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Compilation of Henry's law constants (version 5.0.0) for water as solvent

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Abstract. Many atmospheric chemicals occur in the gas phase as well as in liquid cloud droplets and aerosol particles. Therefore, it is necessary to understand their distribution between the phases. According to Henry's law, the equilibrium ratio between the abundances in the gas phase and in the aqueous phase is constant for a dilute solution. Henry's law constants of trace gases of potential importance in environmental chemistry have been collected and converted into a uniform format. The compilation contains 46 434 values of Henry's law constants for 10 173 species, collected from 995 references. It is also available on the internet at https://www.henrys-law.org (last access: October 2023). This article is a living review that supersedes the now obsolete publication by Sander (2015).

1 Introduction

Henry's law is named after the English chemist William Henry, who studied the topic in the early 19th century. In his publication about the quantity of gases absorbed by water (Henry, 1803), he described the results of his experiments:

> "[. . .] water takes up, of gas condensed by one, two, or more additional atmospheres, a quantity which, ordinarily compressed, would be equal to twice, thrice, &c. the volume absorbed under the common pressure of the atmosphere."

In other words, the amount of dissolved gas is proportional to its partial pressure in the gas phase. The proportionality factor is called a Henry's law constant. In atmospheric chemistry, these constants are needed to describe the exchange of trace species between the air and liquid cloud droplets, aerosol particles, oceans, and other bodies of water. In other areas of environmental research, the constants are needed to calculate the vaporization of contaminants, e.g., from rivers and during waste water treatment (e.g., Shen, 1982; Hawthorne et al., 1985; David et al., 2000).

Section 2 provides theoretical background about Henry's law and commonly used quantities and units. In Sect. 3, the compilation of Henry's law constants is described in detail. Additional information can be found in the Supplement, which is described in Sect. 4.

This article is a living review describing version 5.0.0. Compared to the now obsolete version 4.0 (Sander, 2015), the compilation contains 29 084 additional values of Henry's law constants for 5541 additional species, collected from 306 additional references. In cases where experimental data are available for a large temperature range, the values were refitted to a three-parameter equation in addition to the two-parameter fits that were used previously. The symbols of the Henry's law constants have been adjusted in order to follow the new recommendations of the International Union of Pure and Applied Chemistry (IUPAC) by Sander et al. (2022). In addition to the CAS registry numbers, chemical species are now also identified by their InChIKeys (Heller et al., 2015).

2 Theoretical background

2.1 Fundamental types of Henry's law constants

There are many variants of Henry's law constants which can all be classified into two fundamental types: one possibility is to put the aqueous phase into the numerator and the gas phase into the denominator, i.e., define the constant as the quotient A/G. Here, A and G are quantities describing the equilib-

Table 1. Variants of Henry's law constants H.

Symbol	Definition[a]	SI unit	Other commonly used (non-SI) units[b]	Conversion[c] from H_s^{cp}
		Henry's law solubility constants H_s		
H_s^{cp}	c_a/p	$\mathrm{mol\,m^{-3}\,Pa^{-1}}$	$\mathrm{M\,atm^{-1}}$	
H_s^{xp}	x/p	$\mathrm{Pa^{-1}}$	$\mathrm{atm^{-1}}$	$H_s^{xp} = H_s^{cp} \times M_{H_2O}/\varrho_{H_2O}$
H_s^{bp}	b/p	$\mathrm{mol\,kg^{-1}\,Pa^{-1}}$	$\mathrm{mol\,kg^{-1}\,atm^{-1}}$	$H_s^{bp} = H_s^{cp}/\varrho_{H_2O}$
H_s^{cc}	c_a/c_g	1 (dimensionless)		$H_s^{cc} = H_s^{cp} \times RT$
		Henry's law volatility constants H_v		
H_v^{pc}	p/c_a	$\mathrm{Pa\,m^3\,mol^{-1}}$	$\mathrm{atm\,m^3\,mol^{-1}}$	$H_v^{pc} = 1/H_s^{cp}$
H_v^{px}	p/x	Pa	atm	$H_v^{px} = (\varrho_{H_2O}/M_{H_2O})/H_s^{cp}$
H_v^{pw}	p/w	Pa	atm	$H_v^{pw} = (\varrho_{H_2O}/M_B)/H_s^{cp}$
H_v^{cc}	c_g/c_a	1 (dimensionless)		$H_v^{cc} = 1/(H_s^{cp} \times RT)$

[a] The definitions apply only at equilibrium and in the limit of infinite dilution.
[b] Here, M = $\mathrm{mol\,L^{-1}}$ and atm = 101 325 Pa.
[c] Here, M_{H_2O} and ϱ_{H_2O} are the molar mass and density of water, respectively. M_B is the molar mass of the solute. The simplified conversion formulas are valid only for binary solutions and ideal gases. More conversion formulas can be found in Table 2 of Sander et al. (2022).

rium composition (at infinite dilution) of the aqueous phase and the gas phase, respectively. Alternatively, the Henry's law constant can be defined as the quotient G/A, which results in the inverse value. There is no advantage or disadvantage in using one or the other; the two types exist purely for historical reasons. Unfortunately, the name "Henry's law constant" is used for both types. Therefore, expressions like "a large Henry's law constant" are meaningless unless the type is specified. Especially the dimensionless constants are very error-prone because their type cannot be deduced from the unit. In order to have a consistent terminology, the name "Henry's law solubility constant" (or "Henry solubility" for conciseness) should be used when referring to A/G. When referring to G/A, the name "Henry's law volatility constant" (or "Henry volatility") should be used.

2.2 Variants of Henry's law constants

For both of the fundamental types described in the previous section, there are several variants. This results from the multiplicity of quantities that can be chosen to describe the composition of the two phases. Typical choices for the aqueous phase are molar concentration (c_a), molality (b), and amount fraction (x). For the gas phase, molar concentration (c_g) and partial pressure (p) are often used. Note, however, that it is not possible to use the gas-phase amount fraction (y). At a given gas-phase amount fraction, the aqueous-phase concentration c_a depends on the total pressure, and thus the ratio y/c_a is not a constant.

There are numerous combinations of these quantities. The eight variants recommended by IUPAC are summarized in Table 1. Numerical values of conversion factors between them are shown in Tables 2, 3, and 4.

2.3 Symbols

In the current literature, a plethora of different symbols is used for Henry's law constants. Several symbols are used for the same variant, and sometimes the same symbol is used for different variants. However, for this work a consistent terminology is indispensable. Here, the IUPAC recommendations by Sander et al. (2022) are used: for Henry's law solubility constants, the symbol H_s is used, and for Henry's law volatility constants, the symbol H_v is used.

To specify the exact variant of the Henry's law constant, two superscripts are used. They refer to the numerator and the denominator of the definition. For example, H_s^{cp} refers to the Henry solubility defined as c/p. If H_s refers to the reference temperature $T^\ominus = 298.15\,\mathrm{K}$, it will be denoted as $H_s^\ominus$. A summary of the symbols is shown in Table 5.

2.4 Temperature dependence of Henry's law constants

In spite of the name Henry's law *constant*, it should be kept in mind that its value still depends on some parameters, e.g., the temperature T. The temperature dependence of equilibrium constants can be described with the van't Hoff equation, which also applies to Henry's law:

$$\frac{\mathrm{d}\ln H_s}{\mathrm{d}(1/T)} = \frac{-\Delta_{sol}H}{R}, \tag{1}$$

where $\Delta_{sol}H$ is the enthalpy of dissolution, and R is the gas constant. Note that the letter H in the symbol $\Delta_{sol}H$ refers to enthalpy and is not related to the letter H for Henry's law constants. Integrating the above equation leads to

$$\ln H_s = \frac{-\Delta_{sol}H}{R}\frac{1}{T} + \mathrm{const.} \tag{2}$$

Table 2. Conversion factors between several Henry's law solubility constants H_s (at $T^\ominus = 298.15\,\mathrm{K}$ and $\varrho^\ominus = 997\,\mathrm{kg\,m^{-3}}$). For example, the second table entry indicates that $H_s^{cp} = 1\,\mathrm{mol\,m^{-3}\,Pa^{-1}} \Leftrightarrow H_s^{cp} = 101.325\,\mathrm{M\,atm^{-1}}$.

	$H_s^{cp} = \ldots \frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}$	$H_s^{cp} = \ldots \frac{\mathrm{M}}{\mathrm{atm}}$	$H_s^{cc} = \ldots$	$H_s^{bp} = \ldots \frac{\mathrm{mol}}{\mathrm{kg\,Pa}}$	$H_s^{bp} = \ldots \frac{\mathrm{mol}}{\mathrm{kg\,atm}}$	$H_s^{xp} = \ldots \frac{1}{\mathrm{atm}}$	$\alpha = \ldots$
$H_s^{cp} = 1 \frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}$	1.00000	101.325	2478.96	1.00301×10^{-3}	101.630	1.83089	2271.10
$H_s^{cp} = 1 \frac{\mathrm{M}}{\mathrm{atm}}$	9.86923×10^{-3}	1.00000	24.4654	9.89893×10^{-6}	1.00301	0.0180695	22.4140
$H_s^{cc} = 1$	4.03395×10^{-4}	0.0408740	1.00000	4.04609×10^{-7}	0.0409970	7.38573×10^{-4}	0.916150
$H_s^{bp} = 1 \frac{\mathrm{mol}}{\mathrm{kg\,Pa}}$	997.000	1.01021×10^{5}	2.47152×10^{6}	1.00000	1.01325×10^{5}	1825.40	2.26428×10^{6}
$H_s^{bp} = 1 \frac{\mathrm{mol}}{\mathrm{kg\,atm}}$	9.83962×10^{-3}	0.997000	24.3920	9.86923×10^{-6}	1.00000	0.0180153	22.3467
$H_s^{xp} = 1 \frac{1}{\mathrm{atm}}$	0.546182	55.3419	1353.96	5.47826×10^{-4}	55.5084	1.00000	1240.43
$\alpha = 1$	4.40316×10^{-4}	0.0446150	1.09152	4.41641×10^{-7}	0.0447493	8.06171×10^{-4}	1.00000

Table 3. Conversion factors between several Henry's law volatility constants H_v (at $T^\ominus = 298.15\,\mathrm{K}$ and $\varrho^\ominus = 997\,\mathrm{kg\,m^{-3}}$). For example, the second table entry indicates that $H_v^{px} = 1\,\mathrm{atm} \Leftrightarrow H_v^{pc} = 1.83089\,\mathrm{m^3\,Pa\,mol^{-1}}$.

	$H_v^{px} = \ldots\,\mathrm{atm}$	$H_v^{pc} = \ldots \frac{\mathrm{m^3\,Pa}}{\mathrm{mol}}$	$H_v^{pc} = \ldots \frac{\mathrm{m^3\,atm}}{\mathrm{mol}}$	$H_v^{cc} = \ldots$
$H_v^{px} = 1\,\mathrm{atm}$	1.00000	1.83089	1.80695×10^{-5}	7.38573×10^{-4}
$H_v^{pc} = 1 \frac{\mathrm{m^3\,Pa}}{\mathrm{mol}}$	0.546182	1.00000	9.86923×10^{-6}	4.03395×10^{-4}
$H_v^{pc} = 1 \frac{\mathrm{m^3\,atm}}{\mathrm{mol}}$	55341.9	1.01325×10^{5}	1.00000	40.8740
$H_v^{cc} = 1$	1353.96	2478.96	0.0244654	1.00000

Table 4. Products of Henry's law solubility constants H_s and Henry's law volatility constants H_v (at $T^\ominus = 298.15\,\mathrm{K}$ and $\varrho^\ominus = 997\,\mathrm{kg\,m^{-3}}$). For example, if $H_v^{px} = 5\,\mathrm{atm}$, then $H_s^{bp} \approx 11\,\mathrm{mol\,kg^{-1}\,atm^{-1}}$ because $5 \times 11 \approx 55.5084$.

	$\frac{H_s^{cp}}{\mathrm{mol\,m^{-3}\,Pa^{-1}}}$	$\frac{H_s^{cp}}{\mathrm{M\,atm^{-1}}}$	$\frac{H_s^{cc}}{1}$	$\frac{H_s^{bp}}{\mathrm{mol\,kg^{-1}\,Pa^{-1}}}$	$\frac{H_s^{bp}}{\mathrm{mol\,kg^{-1}\,atm^{-1}}}$	$\frac{H_s^{xp}}{\mathrm{atm^{-1}}}$	$\frac{\alpha}{1}$
$\frac{H_v^{px}}{\mathrm{atm}}$	0.546182	55.3419	1353.96	5.47826×10^{-4}	55.5084	1.00000	1240.43
$\frac{H_v^{pc}}{\mathrm{m^3\,Pa\,mol^{-1}}}$	1.00000	101.325	2478.96	1.00301×10^{-3}	101.630	1.83089	2271.10
$\frac{H_v^{pc}}{\mathrm{m^3\,atm\,mol^{-1}}}$	9.86923×10^{-6}	1.00000×10^{-3}	0.0244654	9.89893×10^{-9}	1.00301×10^{-3}	1.80695×10^{-5}	0.0224140
$\frac{H_v^{cc}}{1}$	4.03395×10^{-4}	0.0408740	1.00000	4.04609×10^{-7}	0.0409970	7.38573×10^{-4}	0.916150

Table 5. List of symbols.

Symbol	Quantity	SI unit*
ϱ	density	$\mathrm{kg\,m^{-3}}$
A	parameter for the temperature dependence of H_s	1
b	molality	$\mathrm{mol\,kg^{-1}}$
B	parameter for the temperature dependence of H_s	K
C	parameter for the temperature dependence of H_s	1
c_a	aqueous-phase concentration	$\mathrm{mol\,m^{-3}}$
c_g	gas-phase concentration	$\mathrm{mol\,m^{-3}}$
D	parameter for the temperature dependence of H_s	$\mathrm{K^{-1}}$
$\Delta_{sol}G$	free energy of dissolution	$\mathrm{J\,mol^{-1}}$
$\Delta_{sol}H$	molar enthalpy of dissolution	$\mathrm{J\,mol^{-1}}$
H_s	Henry solubility (all variants)	miscellaneous
$H_s^{\ominus}$	Henry solubility at the reference temperature $T^{\ominus}$	miscellaneous
H_s^{bp}	Henry solubility (defined as b/p)	$\mathrm{mol\,kg^{-1}\,Pa^{-1}}$
H_s^{cc}	Henry solubility (defined as c/c)	1
H_s^{cp}	Henry solubility (defined as c/p)	$\mathrm{mol\,m^{-3}\,Pa^{-1}}$
$H_{s,eff}$	effective Henry solubility	miscellaneous
H_s'	$H_s \times K_A$ (for strong acids)	miscellaneous
H_v	Henry volatility (all variants)	miscellaneous
$H_v^{\ominus}$	Henry volatility at the reference temperature $T^{\ominus}$	miscellaneous
H_v^{cc}	Henry volatility (defined as c/c)	1
H_v^{pc}	Henry volatility (defined as p/c)	$\mathrm{Pa\,m^3\,mol^{-1}}$
H_v^{px}	Henry volatility (defined as p/x)	Pa
K_A	acid constant	$\mathrm{mol\,m^{-3}}$
K_s	Sechenov parameter	miscellaneous
M	molar mass	$\mathrm{kg\,mol^{-1}}$
p	partial pressure $= c_g RT$	Pa
p_{sat}	saturation vapor pressure of water	Pa
p_{tot}	total pressure (solute + water)	Pa
R	gas constant	$8.314\,\mathrm{J\,mol^{-1}\,K^{-1}}$
T	temperature	K
$T^{\ominus}$	reference temperature	298.15 K
w	mass fraction in the aqueous phase	$\mathrm{kg\,kg^{-1}}$ (dimensionless)
x	amount fraction (molar mixing ratio) in the aqueous phase	$\mathrm{mol\,mol^{-1}}$ (dimensionless)
y	amount fraction (molar mixing ratio) in the gas phase	$\mathrm{mol\,mol^{-1}}$ (dimensionless)

* A unit of "1" denotes a quantity of dimension 1, commonly called "dimensionless quantity".

Calling the constant of integration A, and defining the parameter $B = -\Delta_{sol}H/R$, we get

$$\ln H_s = A + \frac{B}{T} \tag{3}$$

or

$$H_s = \exp(A) \times \exp\left(\frac{B}{T}\right). \tag{4}$$

To determine the parameters A and B experimentally, Henry's law constants are measured at several temperatures, and the method of least squares is used to fit the points to a function. Note that functions (3) and (4) produce slightly different fit parameters because the logarithmic function (3) puts less weight on errors of large Henry's law constants than the linear function (4) does. In this work, linear regression is performed using Eq. (3).

Thermodynamic data are often available at the temperature $T^{\ominus} = 298.15$ K. To present Henry's law constants at $T^{\ominus}$ and also show their temperature dependence, an alternative form of Eq. (4) can be used:

$$H_s = H_s^{\ominus} \times \exp\left(B\left(\frac{1}{T} - \frac{1}{T^{\ominus}}\right)\right). \tag{5}$$

where $H_s^{\ominus} = \exp(A) \times \exp(B/T^{\ominus})$. The enthalpy of dissolution $\Delta_{sol}H$ is independent of temperature here:

$$\frac{-\Delta_{sol}H}{R} = \frac{\mathrm{d}\ln H_s}{\mathrm{d}(1/T)} = B. \tag{6}$$

In this work, the values $H_s^{\ominus}$ and $\mathrm{d}\ln H_s/\mathrm{d}(1/T)$ are tabulated.

Table 6. Temperature-dependent terms and their analytical derivatives. Here, C, C_1, and C_2 are the empirical fit parameters defining $\ln H_s$. See Sect. 2.4 for details.

$\ln H_s$	$\frac{d \ln H_s}{d(1/T)}$
C	0
C/T	C
CT	$-CT^2$
CT^2	$-2CT^3$
C/T^2	$2C/T$
C/T^3	$3C/T^2$
$C \ln(T)$	$-CT$
$C_1 \ln(C_2 T)$	$-C_1 T$ (independent of C_2)
$C \log_{10}(T)$	$-CT/\ln(10)$

A simple equation based on the two parameters A and B is valid only for a limited temperature range, in which the enthalpy of dissolution $\Delta_{sol}H$ can be considered constant. To accommodate a larger temperature range, a third parameter C is often added:

$$\ln H_s = A + \frac{B}{T} + C \times \ln T. \tag{7}$$

Here, the fit parameters A and B are different from those calculated for function (3). The enthalpy of dissolution $\Delta_{sol}H$ changes linearly with temperature in the three-parameter fit:

$$\frac{-\Delta_{sol}H}{R} = \frac{d \ln H_s}{d(1/T)} = B - CT. \tag{8}$$

To cover an even larger temperature range with an empirical formula, the dependence of $\ln H_s$ on T can be expressed as the sum of several terms. For example, Wilhelm et al. (1977) used the following formula:

$$\ln H_s = A + B \times T^{-1} + C \times \ln T + D \times T. \tag{9}$$

The analytical derivative is simply the sum of the derivatives of the individual terms. Using the derivatives from Table 6, the temperature dependence of this expression can be calculated as

$$\frac{d \ln H_s}{d(1/T)} = 0 + B - C \times T - D \times T^2. \tag{10}$$

When reporting Henry's law constants as such a function, it is important to present sufficient significant digits because H_s depends exponentially on the parameters.

Note that the temperature dependences for H_s^{cp} and H_s^{cc} are different since the conversion factor between them includes the temperature:

$$\begin{aligned} H_s^{cp} &= H_s^{cc}/(RT) \\ \Leftrightarrow \ln H_s^{cp} &= \ln H_s^{cc} + \ln(1/R) + \ln(1/T) \\ \Rightarrow \frac{d \ln H_s^{cp}}{d(1/T)} &= \frac{d \ln H_s^{cc}}{d(1/T)} + \frac{d \ln(1/T)}{d(1/T)} \\ &= \frac{d \ln H_s^{cc}}{d(1/T)} + T. \end{aligned} \tag{11}$$

2.5 Effective Henry's law solubility constants $H_{s,eff}$

The Henry's law constants mentioned so far describe the equilibrium between a chemical species in the gas phase and exactly the same species in the aqueous phase. This type is called the "intrinsic" Henry's law constant.

Once transferred, some species react in the aqueous phase. If these chemical reactions are fast and result in irreversible destruction, Henry's law cannot be applied. If, however, the species enters a fast equilibrium in the aqueous phase, it is possible to define an "effective" Henry's law constant $H_{s,eff}$, using a "total concentration" c_{tot}. Depending on the chemical class, there are different ways to define such a total concentration.

2.5.1 $H_{s,eff}$ for aldehydes

Aldehydes can be hydrated, forming geminal diols. For example, methanal (HCHO) is almost completely hydrated in aqueous solution:

$$HCHO + H_2O \rightleftharpoons H_2C(OH)_2. \tag{12}$$

The total concentration of dissolved methanal is

$$c_{tot} = c(HCHO) + c(H_2C(OH)_2). \tag{13}$$

The intrinsic Henry's law solubility constant of HCHO is

$$H_s = \frac{c(HCHO)}{p(HCHO)}. \tag{14}$$

In contrast, the effective Henry's law constant $H_{s,eff}$ is defined as

$$H_{s,eff} = \frac{c_{tot}}{p(HCHO)} = \frac{c(HCHO) + c(H_2C(OH)_2)}{p(HCHO)}. \tag{15}$$

2.5.2 $H_{s,eff}$ for acids and bases

Acids and bases undergo ionic dissociation upon dissolution, e.g.,

$$HCl \rightleftharpoons H^+ + Cl^-. \tag{16}$$

Defining the total concentration c_{tot} as

$$c_{tot} = c(HCl) + c(Cl^-), \tag{17}$$

the effective Henry's law constant is

$$H_{s,eff} = \frac{c_{tot}}{p(HCl)} = \frac{c(HCl) + c(Cl^-)}{p(HCl)}. \quad (18)$$

Considering the acidity constant

$$K_a = \frac{c(H^+)\,c(Cl^-)}{c(HCl)}, \quad (19)$$

the relation between the intrinsic and the effective Henry's law constant for HCl can be written as

$$H_{s,eff} = H_s \times \left(1 + \frac{K_a}{c(H^+)}\right). \quad (20)$$

Since the factor on the right-hand side contains $c(H^+)$, the conversion between the intrinsic and the effective Henry's law constant is pH-dependent. Thus, effective Henry's law constants of acids and bases are not material constants but depend on solution pH. Proportionality between $p(HCl)$ and c_{tot} is restricted to conditions under which the uptake of gaseous HCl does not affect the acidity of the solution.

In order to obtain a pH-independent constant, the product of the intrinsic Henry's law constant H_s^{cp} and the acidity constant K_a is often used for HCl and other strong acids:

$$H_s' = H_s^{cp} \times K_a = \frac{c(H^+) \times c(Cl^-)}{p(HCl)}. \quad (21)$$

Although H_s' is usually also called a Henry's law constant, it should be noted that it is a different quantity, and it has different units than H_s^{cp}.

2.5.3 $H_{s,eff}$ for halogens

In the aqueous phase, halogens are in equilibrium with their hypohalous acids, e.g.,

$$Cl_2 + H_2O \rightleftharpoons HOCl + H^+ + Cl^-. \quad (22)$$

The equilibrium constant is

$$K = \frac{c(HOCl)\,c(H^+)\,c(Cl^-)}{c(Cl_2)}. \quad (23)$$

Since the sum of Cl_2 and HOCl is not affected by this equilibrium, a "total chlorine concentration" c_{tot} can be defined as

$$c_{tot} = c(Cl_2) + c(HOCl). \quad (24)$$

Using c_{tot}, it is formally possible to define an effective Henry's law constant as

$$H_{s,eff} = \frac{c_{tot}}{p(Cl_2)} = \frac{c(Cl_2) + c(HOCl)}{p(Cl_2)}. \quad (25)$$

However, this definition is problematic because it does not work at infinite dilution. With decreasing Cl_2 concentration, the equilibrium in Eq. (22) will shift to the right (Le Chatelier's principle), i.e., $c(HOCl) \gg c(Cl_2)$, and the effective Henry's law solubility constant goes to infinity (see, e.g., Fig. 2 in Jones, 1911 or Fig. A1 in Lin and Pehkonen, 1998). Therefore, the intrinsic Henry's law constant should be used for halogens, and the term "effective Henry's law constant" should be avoided here.

Instead of extrapolating to infinite dilution, the total chlorine solubility is sometimes reported at the fixed partial pressure of $p(Cl_2) = 101\,325$ Pa. However, even in the vicinity of 101 325 Pa, the total chlorine concentration c_{tot} is not proportional to $p(Cl_2)$.

In order to convert experimentally determined chlorine solubilities to the intrinsic constant $H_s(Cl_2)$, additional processes may have to be considered, e.g., aqueous-phase diffusion (Brian et al., 1962; Leaist, 1986) and the formation of chlorine hydrates (Adams and Edmonds, 1937; Young, 1983).

2.6 Dependence of Henry's law constants on the composition of the solution

Values of Henry's law constants for aqueous solutions depend on the composition of the solution, i.e., on its ionic strength and on dissolved organics. In general, the solubility of a gas decreases with increasing salinity ("salting out"). However, a "salting in" effect has also been observed, e.g., for the effective Henry's law constant of glyoxal (Kampf et al., 2013; Kurtén et al., 2015). The effect can be described with the Sechenov equation (Setschenow, 1889). Note that the scientific transliteration from Cyrillic is "Sechenov", but the original article was written in German and used the German transliteration "Setschenow". There are many alternative ways to define the Sechenov equation, depending on how the aqueous-phase composition is described (based on concentration, molality, or amount fraction) and which variant of the Henry's law constant is used. Describing the solution in terms of molality is preferred because molality is invariant to temperature and to the addition of dry salt to the solution (see Sander, 1999 for details). Thus, the Sechenov equation can be written as

$$\log_{10}\left(\frac{H_{s0}^{bp}}{H_s^{bp}}\right) = K_s \times b(\text{salt}), \quad (26)$$

where H_{s0}^{bp} is Henry's law constant in pure water, H_s^{bp} is Henry's law constant in the salt solution, K_s is the molality-based Sechenov parameter for a given salt, and b(salt) is the molality of the salt. For mixed electrolyte solutions with more than one salt, an extension of the Sechenov equation developed by Schumpe (1993) and Weisenberger and Schumpe (1996) can be used. Sechenov parameters are not suitable for systems in which a species reacts irreversibly with the salt (e.g., $N_2O_5 + Cl^-$).

Since the atmosphere contains very dilute cloud droplets as well as highly concentrated aerosols, adequate values of Henry's law constants should be used. Unfortunately, Sechenov parameters are unknown for many species.

3 Values of Henry's law constants

3.1 The data compilation

The compilation of Henry's law constants is presented in the Appendix, and it is also available online at https://www.henrys-law.org (last access: October 2023). It contains Henry's law constants for inorganic and organic species of potential importance in environmental chemistry. Most data were measured at ambient conditions (around 298 K and 1 atm). Data at high temperatures are excluded or (if possible) extrapolated to $T^{\ominus} = 298.15$ K. The data refer to aqueous solutions; octanol and other solvents are not considered. The constants refer to pure water as solvent unless noted otherwise (e.g., sea water).

All Henry's law constants have been converted to a uniform format: H_s^{cp} with the unit $\mathrm{mol\,m^{-3}\,Pa^{-1}}$. In cases where the conversion involves the temperature-dependent density of water, the parameterization by Bettin and Spieweck (1990) was used to calculate ϱ_{H_2O} at the temperature T. The temperature-dependent vapor pressure of water p_{sat} was calculated using the parameterization by Buck (1981).

Inorganic substances are sorted according to the elements they contain. The order chosen is O, H, N, F, Cl, Br, I, S, rare gases, and others. Compounds with several of these elements are put into the last of the applicable sections. For example, nitryl chloride, which contains O, N, and Cl, is listed in the Cl section. Carbon-containing compounds (including CO and CO_2) are sorted somewhat arbitrarily by increasing chain length and complexity. Heteroatoms (O, N, F, Cl, Br, I, S, P, etc.) are sorted in the same order as for inorganic compounds. The table contains the following groups of species:

The first column of the table shows the systematic name, the chemical formula, trivial names (if any), the CAS registry number (in square brackets), and the InChIKey.

The column labeled "H_s^{cp}" contains Henry's law solubility constants at the reference temperature $T^{\ominus} = 298.15\,\mathrm{K}$. Values are rounded to two significant digits and given in the unit $\mathrm{mol\,m^{-3}\,Pa^{-1}}$.

The column labeled "$\mathrm{d}\ln H_s/\mathrm{d}(1/T)$" contains the temperature dependence of the Henry solubility as defined in Eq. (5), rounded to two significant digits and given in the unit K. If the term $\Delta_{sol}H$ is temperature-dependent, the value of $\mathrm{d}\ln H_s/\mathrm{d}(1/T)$ is calculated at $T^{\ominus} = 298.15\,\mathrm{K}$. If a three-parameter fit according to Eq. (7) allows the parameterization over a larger temperature range, it is presented in the notes.

For each table entry, the column labeled "type" denotes how the Henry's law constant was obtained in the given reference. Literature reviews are usually most reliable, followed by original publications of experimental determinations of H_s. Other data have to be treated more carefully. The types listed here are roughly ordered by decreasing reliability. Note, however, that recent measurements which are newer than the latest review article should always be considered.

"L" The cited paper is a *literature* review.

"M" The cited paper presents the original *measurements*.

"V" The *vapor* pressure of the pure substance was divided by its aqueous solubility (sometimes called the "VP/AS" method).

"R" The cited paper presents a *recalculation* of previously published material (e.g. extrapolation to a different temperature or concentration range).

"T" The value was obtained from a *thermodynamical* calculation ($\Delta_{sol}G = -RT\ln H$; see Sander, 1999 for details).

"X" The original paper was not available for this study. The data listed here were found in a secondary source.

"C" The paper is a *citation* of a reference which I could not obtain (personal communication, PhD theses, grey literature).

"Q" The value was calculated using a "*quantitative* structure–property relationship" (QSPR) or a similar theoretical method.

"E" The value is an *estimate*. Estimates are listed only if no reliable data are available.

"?" The cited paper does not clearly state how the value was obtained.

"W" The value is probably *wrong*. It is not listed in the table, in order to avoid spreading of erroneous data. More information can be found in the notes.

In some cases there might be good agreement between different authors. However, if the original work they refer to is not known, one has to be careful when evaluating the reliability. It is possible that they were recalculating data from the same source. The similarity in that case would not be due to independent investigations.

The table entries in the pdf of this document are hyperlinked to endnotes with additional information. Symbols and acronyms used here refer to those in the original publications.

The CAS numbers in the tables are hyperlinked to the NIST Chemistry WebBook.

3.2 Further sources of information

3.2.1 Review articles

Several reviews about Henry's law have been published, starting with Markham and Kobe (1941) up to more recent publications such as Wilhelm et al. (1977), Mackay and Shiu (1981), Staudinger and Roberts (1996), Staudinger and Roberts (2001), Fogg and Sangster (2003), and Burkholder et al. (2019). Practical guidance on the use of Henry's law has been published by Smith and Harvey (2007).

Experimental methods to obtain Henry's law constants as well as indirect (theoretical) methods have been described and compared by several authors. Only a brief summary of some articles is given here. For details, the reader is referred to the original publications:

- Battino and Clever (1966) – miscellaneous methods, partially of historical interest;
- Betterton (1992) – head-space method, bubble column method, thermodynamic cycles, calculation from vapor pressure and solubility, linear correlations;
- Turner et al. (1996) – static methods, mechanical recirculation methods, separate measurement of solubility and pure species vapor pressure, ebulliometry, perturbation chromatography;

- Staudinger and Roberts (1996) – batch air stripping, concurrent flow technique, Equilibrium Partitioning in Closed Systems (EPICS), calculation via quantitative property–property relationships (QPPRs), quantitative structure–property relationships (QSPRs), UNIversal quasichemical Functional group Activity Coefficients (UNIFAC);
- Brennan et al. (1998) – comparison of predictive methods;
- Sander (1999) – QPPR, QSPR, thermodynamic calculations;
- Fogg and Sangster (2003) – miscellaneous methods;
- Dupeux et al. (2022) – QSPR.

3.2.2 Internet

On the internet, several pages provide Henry's law constants, e.g., the following:

- the PubChem database at https://pubchem.ncbi.nlm.nih.gov (last access: 16 September 2023)
- the NIST Chemistry WebBook at https://webbook.nist.gov/chemistry (last access: 16 September 2023)
- the ChemSpider database at https://www.chemspider.com (last access: 16 September 2023)
- the Generator for Explicit Chemistry and Kinetics of Organics in the Atmosphere (GECKO-A), which provides Henry's law constants on the basis of experimental data and structure–activity relationships, at https://geckoa.lisa.u-pec.fr/generateur_form.php (last access: 16 September 2023)
- the Pesticide Properties Database (PPD) at https://www.ars.usda.gov/Services/docs.htm?docid=14199 (last access: 16 September 2023)
- HENRYWIN, a program to calculate Henry's law constants, at https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface (last access: 16 September 2023)
- vapor–liquid equilibrium data (mostly at elevated temperatures) from the Dortmund Data Bank at http://www.ddbst.com/en/EED/VLE/VLEindex.php (last access: 16 September 2023)
- EPI Suite estimates from the Arctic Monitoring and Assessment Programme (AMAP) database at https://chemicals.amap.no/about (last access: 16 September 2023).

3.2.3 Vapor–liquid equilibrium data

Henry's law constants can be obtained from vapor–liquid equilibrium (VLE) data. For example, consider a binary mixture that consists of a solute dissolved in water. The total pressure p_{tot} over the solution is the sum of the partial pressures of the components. The partial pressure of the solute can be defined via Henry's law, and the partial pressure of the water can be defined via Raoult's law:

$$\begin{aligned} p_{tot} &= p_{solute} + p_{water} \\ &= x H_v^{px} + (1-x) p_{sat} \\ &= x(H_v^{px} - p_{sat}) + p_{sat} \end{aligned} \tag{27}$$

where p_{sat} is the saturation vapor pressure of water. If VLE data with the total pressure at several small solute fractions x are available, the derivative $\mathrm{d}p_{tot}/\mathrm{d}x$ (i.e., the slope of a plot p_{tot} vs x) can be used to obtain the Henry's law constant:

$$\frac{\mathrm{d}p_{tot}}{\mathrm{d}x} = H_v^{px} - p_{sat} \Rightarrow H_v^{px} = \frac{\mathrm{d}p_{tot}}{\mathrm{d}x} + p_{sat}. \tag{28}$$

4 The electronic supplement

The Supplement contains several files with additional information about the compiled Henry's law constants. It includes a `README` file with a detailed description. Here, only a short summary is given:

- The files `henry_*.f90` contain the Fortran 90 code that was used to convert the values from the original publications to the uniform format H_s^{cp} with the unit mol m^{-3} Pa^{-1}. The code and the comments in the code can be used to double-check that the conversion was done correctly.
- If the original publications contain measurements at different temperatures, the code often contains all individual data points, not just the regression line that was used to calculate the temperature dependence. In addition, the Supplement contains data files with the temperature-dependent values of H_s^{cp} in `output/Tdep_data/*.dat` and plots of the data points as well as the regression lines according to Eqs. (5) and (7) in `output/gnuplot/Tdep.pdf`.
- If the Henry's law constants are needed in electronic form, it is cumbersome to extract them from the pdf of this article. Therefore, the Supplement contains the files `output/*.f90` with declarations of the Henry's law constants (H_s^{cp}, H_s^{xp}, H_s^{bp}, H_s^{cc}, H_v^{pc}, H_v^{px}, and H_v^{cc}) in Fortran 90 syntax.
- For some references, the `util/` directory contains Python scripts that preprocess input and perform other calculations related to the original data.

5 Summary and outlook

An updated and extended version of a compilation of Henry's law constants has been presented. The collection, which is also available at https://www.henrys-law.org, will be continuously maintained, updated, and extended in the future. If necessary, errata will be posted on the web page. In addition to providing a source of information, I hope that this work will help to identify gaps in our current knowledge and stimulate research projects. In particular, it seems that even for some well-known chemicals like isoprene, HCl, Br_2, or BrCl, there is a large uncertainty in the value of the Henry's law constants. I always welcome emails informing me about new measurements of Henry's law constants to be included in the table.

Appendix A: Appendix with data tables

A1 Inorganic species

A1.1 Oxygen (O)

Table A1.1: Oxygen (O)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
oxygen	1.3×10^{-5}	1500	Burkholder et al. (2019)	L	1
O_2	1.3×10^{-5}	1500	Burkholder et al. (2015)	L	1
[7782-44-7]			Clever et al. (2014)	L	2
MYMOFIZGZYHOMD-UHFFFAOYSA-N	1.2×10^{-5}	1700	Warneck and Williams (2012)	L	
	1.3×10^{-5}	1500	Sander et al. (2011)	L	1
	1.3×10^{-5}	1500	Sander et al. (2006)	L	1
	1.3×10^{-5}	1400	Fernández-Prini et al. (2003)	L	3
	1.3×10^{-5}	1500	Battino et al. (1983)	L	
	1.3×10^{-5}	1500	Battino (1981)	L	1
	1.3×10^{-5}	1500	Wilhelm et al. (1977)	L	
	1.2×10^{-5}	1400	Himmelblau (1960)	L	1
	1.2×10^{-5}	1600	Millero et al. (2002a)	M	4, 5
	1.2×10^{-5}	1600	Millero et al. (2002b)	M	6, 7
	1.3×10^{-5}	1500	Rettich et al. (2000)	M	8
	1.3×10^{-5}	1400	Sherwood et al. (1991)	M	9
	1.3×10^{-5}	1500	Rettich et al. (1981)	M	10
	1.3×10^{-5}	1500	Cosgrove and Walkley (1981)	M	11
	1.2×10^{-5}		da Silva et al. (1980)	M	12
	1.3×10^{-5}	1400	Cramer (1980)	M	
	1.3×10^{-5}	1400	Benson et al. (1979)	M	
	1.4×10^{-4}		Razumovskii and Zaikov (1971)	M	13
	1.1×10^{-5}		Power and Stegall (1970)	M	14
	1.3×10^{-5}	1500	Murray and Riley (1969)	M	15
	1.2×10^{-5}	1200	Shoor et al. (1969)	M	16
	1.2×10^{-5}	1600	Carpenter (1966)	M	17
	1.3×10^{-5}	1500	Morrison and Billett (1952)	M	18
	1.2×10^{-5}		Orcutt and Seevers (1937a)	M	
	1.3×10^{-5}	1500	Fox (1909)	M	
	1.2×10^{-5}	1700	Geffcken (1904)	M	
	1.3×10^{-5}	1400	Winkler (1891b)	M	19
	1.3×10^{-5}	1400	Bohr and Bock (1891)	M	
	1.2×10^{-5}	1800	Timofejew (1890)	M	
	1.2×10^{-5}	1200	Bunsen (1855a)	M	
	1.2×10^{-5}	1600	Wauchope and Haque (1972)	V	
	1.2×10^{-5}	1600	Wauchope and Haque (1972)	V	
	1.3×10^{-5}	1500	Wauchope and Haque (1972)	V	
	1.3×10^{-5}		Pierotti (1965)	T	
	1.4×10^{-5}		Nunn (1958)	C	12
	7.9×10^{-6}		Hayer et al. (2022)	Q	20
	1.3×10^{-5}	1500	Yaws et al. (1999)	?	21

Table A1.1: Oxygen (O) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^{-5}		Abraham and Weathersby (1994)	?	21
	1.2×10^{-5}	1500	Dean and Lange (1999)	?	22, 23
	1.3×10^{-5}		Seinfeld (1986)	?	21
	1.3×10^{-4}		Smith and Bomberger (1980)	?	24
ozone	1.0×10^{-4}	2800	Burkholder et al. (2019)	L	
O_3	1.0×10^{-4}	2800	Burkholder et al. (2015)	L	
[10028-15-6]			Clever et al. (2014)	L	25
CBENFWSGALASAD-UHFFFAOYSA-N	1.0×10^{-4}	2800	Sander et al. (2011)	L	
	1.0×10^{-4}	2800	Sander et al. (2006)	L	
	7.6×10^{-5}	3700	Biń (2005)	L	
	1.1×10^{-4}	2400	Warneck (2003)	L	
			Battino (1981)	L	26
	1.3×10^{-4}	2000	Wilhelm et al. (1977)	L	
	1.1×10^{-4}		Levanov et al. (2008)	M	12
	1.1×10^{-4}	2300	Gershenzon et al. (2001)	M	
	9.9×10^{-5}	2600	Rischbieter et al. (2000)	M	
	9.2×10^{-5}	2600	Andreozzi et al. (1996)	M	
	1.2×10^{-4}	1400	Sotelo et al. (1989)	M	
	1.1×10^{-4}	2300	Kosak-Channing and Helz (1983)	M	
	1.7×10^{-4}		Gurol and Singer (1982)	M	12
			Roth and Sullivan (1981)	M	27
	1.2×10^{-4}	1900	Stumm (1958)	M	
	9.9×10^{-5}	2600	Kilpatrick et al. (1956)	M	
	1.3×10^{-4}	2000	Briner and Perrottet (1939)	M	
	2.0×10^{-4}		Fischer and Tropsch (1917)	M	
	8.0×10^{-5}	2900	Luther (1905)	M	
	1.2×10^{-4}	4100	Mailfert (1894)	M	
	1.2×10^{-4}		Schöne (1873)	M	28
	1.1×10^{-4}	2600	Chameides (1984)	T	
	1.2×10^{-4}		Perry and Chilton (1973)	X	29
	1.2×10^{-4}		Hayer et al. (2022)	Q	20
			Lide and Frederikse (1995)	?	30
	9.3×10^{-5}	2500	Seinfeld (1986)	?	21
	9.3×10^{-5}	2500	Hoffmann and Jacob (1984)	?	21

A1.2 Hydrogen (H)

Table A1.2: Hydrogen (H)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hydrogen atom	2.6×10^{-6}		Burkholder et al. (2019)	L	
H	2.6×10^{-6}		Burkholder et al. (2015)	L	
[12385-13-6]	2.6×10^{-6}		Sander et al. (2011)	L	
YZCKVEUIGOORGS-UHFFFAOYSA-N	2.6×10^{-6}		Sander et al. (2006)	L	
	3.1×10^{-6}		Armstrong et al. (2015)	T	
	3.4×10^{-6}		Parker (1992)	E	31
			Roduner and Bartels (1992)	?	32
hydrogen	7.8×10^{-6}	530	Fernández-Prini et al. (2003)	L	3
H_2	7.7×10^{-6}	490	Young (1981a)	L	1
[1333-74-0]	7.7×10^{-6}	490	Wilhelm et al. (1977)	L	
UFHFLCQGNIYNRP-UHFFFAOYSA-N	7.8×10^{-6}	600	Himmelblau (1960)	L	1
	7.8×10^{-6}	620	Schmidt (1979)	M	33, 34
	7.7×10^{-6}	480	Gordon et al. (1977)	M	35
	7.7×10^{-6}	520	Crozier and Yamamoto (1974)	M	36
	7.2×10^{-6}		Longo et al. (1970)	M	14
	7.2×10^{-6}		Power and Stegall (1970)	M	14
			Shoor et al. (1969)	M	37
	7.5×10^{-6}		Ruetschi and Amlie (1966)	M	38
	7.8×10^{-6}	510	Morrison and Billett (1952)	M	39
	7.8×10^{-6}	540	Geffcken (1904)	M	
	7.7×10^{-6}	1500	Braun (1900)	M	40
	7.7×10^{-6}	500	Winkler (1891a)	M	41
	7.5×10^{-6}	550	Bohr and Bock (1891)	M	
	7.8×10^{-6}	610	Timofejew (1890)	M	
	8.5×10^{-6}	20	Bunsen (1855a)	M	42, 43
	7.8×10^{-6}	500	Wauchope and Haque (1972)	V	
	7.7×10^{-6}		Hine and Weimar (1965)	R	
	8.3×10^{-6}		Pierotti (1965)	T	
	6.4×10^{-6}		Hayer et al. (2022)	Q	20
	7.7×10^{-6}	490	Yaws et al. (1999)	?	21
	7.7×10^{-6}		Abraham and Weathersby (1994)	?	21
	7.7×10^{-6}	500	Dean and Lange (1999)	?	44, 23
deuterium			Young (1981a)	L	45
D_2	7.9×10^{-6}	720	Muccitelli and Wen (1978)	M	46
[7782-39-0]	7.9×10^{-6}	720	Muccitelli and Wen (1978)	M	
UFHFLCQGNIYNRP-VVKOMZTBSA-N	8.2×10^{-6}		Hayer et al. (2022)	Q	20

Table A1.2: Hydrogen (H) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hydroxyl radical	3.8×10^{-1}		Burkholder et al. (2019)	T	47
OH	3.8×10^{-1}		Burkholder et al. (2015)	T	47
[3352-57-6]	3.8×10^{-1}		Sander et al. (2011)	T	47
TUJKJAMUKRIRHC-UHFFFAOYSA-N	3.8×10^{-1}		Sander et al. (2006)	T	47
	2.9×10^{-1}	4300	Hanson et al. (1992)	T	
	3.2×10^{-1}		Mozurkewich (1986)	T	
	2.9×10^{-1}	3100	Berdnikov and Bazhin (1970)	T	48
	2.5×10^{-1}		Lelieveld and Crutzen (1991)	C	
	2.0		Lelieveld and Crutzen (1991)	C	
	8.9×10^{1}		Lelieveld and Crutzen (1991)	C	
	2.5×10^{-1}	5300	Jacob (1986)	C	49
hydroperoxy radical	5.7×10^{1}		Régimbal and Mozurkewich (1997)	R	
HO_2	6.8		Burkholder et al. (2019)	T	47
[3170-83-0]	6.8		Burkholder et al. (2015)	T	47
MHAJPDPJQMAIIY-UHFFFAOYSA-M	6.8		Sander et al. (2011)	T	47
	6.8		Sander et al. (2006)	T	47
	3.8×10^{1}	5900	Hanson et al. (1992)	T	
	8.9×10^{1}		Weinstein-Lloyd and Schwartz (1991)	T	
	8.9×10^{1}		Chameides (1984)	T	
	1.2×10^{1}		Schwartz (1984)	T	50
	4.6×10^{1}	4800	Berdnikov and Bazhin (1970)	T	48
		6600	Jacob (1986)	E	51
hydrogen peroxide	8.6×10^{2}	7300	Burkholder et al. (2019)	L	
H_2O_2	8.6×10^{2}	7300	Burkholder et al. (2015)	L	
[7722-84-1]	9.5×10^{2}	7200	Brockbank (2013)	L	
MHAJPDPJQMAIIY-UHFFFAOYSA-N	9.1×10^{2}	6600	Warneck and Williams (2012)	L	
	8.3×10^{2}	7600	Sander et al. (2011)	L	
	7.6×10^{2}	7300	Sander et al. (2006)	L	
	9.8×10^{2}	6100	Fogg and Sangster (2003)	L	52
	1.2×10^{3}	5900	Rivera-Rios (2018)	M	
	1.1×10^{3}	7000	Huang and Chen (2010)	M	
	8.2×10^{2}	7400	O'Sullivan et al. (1996)	M	
	9.9×10^{2}	6300	Lind and Kok (1994)	M	53
			Staffelbach and Kok (1993)	M	54
	8.5×10^{2}	6500	Zhou and Lee (1992)	M	
	6.7×10^{2}	7900	Hwang and Dasgupta (1985)	M	
	1.4×10^{3}		Yoshizumi et al. (1984)	M	12
	9.6×10^{2}	6600	Chameides (1984)	T	
	7.0×10^{2}	7000	Martin and Damschen (1981)	T	
	6.4×10^{1}		Hilal et al. (2008)	Q	
	7.0×10^{2}	7300	Seinfeld (1986)	?	21
	7.0×10^{2}	7300	Hoffmann and Jacob (1984)	?	21
			Pandis and Seinfeld (1989)	W	55

A1.3 Nitrogen (N)

Table A1.3: Nitrogen (N)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
nitrogen	6.4×10^{-6}	1300	Burkholder et al. (2019)	L	1
N_2	6.4×10^{-6}	1300	Burkholder et al. (2015)	L	1
[7727-37-9]	6.4×10^{-6}	1600	Warneck and Williams (2012)	L	
IJGRMHOSHXDMSA-UHFFFAOYSA-N	6.4×10^{-6}	1300	Sander et al. (2011)	L	1
	6.4×10^{-6}	1300	Sander et al. (2006)	L	1
	6.5×10^{-6}	1200	Fernández-Prini et al. (2003)	L	3
	6.5×10^{-6}	1200	Battino et al. (1984)	L	
	6.5×10^{-6}	1200	Battino (1982)	L	1
	6.4×10^{-6}	1300	Wilhelm et al. (1977)	L	
	5.4×10^{-6}		Steward et al. (1973)	L	14
	6.5×10^{-6}	1400	Allott et al. (1973)	L	
	6.3×10^{-6}	1300	Himmelblau (1960)	L	1
	6.4×10^{-6}	1300	Rettich et al. (1984)	M	56
	6.6×10^{-6}	1300	Cosgrove and Walkley (1981)	M	11
	5.5×10^{-6}		Power and Stegall (1970)	M	14
	6.4×10^{-6}	1300	Murray et al. (1969)	M	57
	6.5×10^{-6}	1400	Morrison and Billett (1952)	M	58
	6.6×10^{-6}		Orcutt and Seevers (1937a)	M	
	6.5×10^{-6}	1100	Van Slyke et al. (1934)	M	
	5.6×10^{-6}		Grollman (1929)	M	59
	6.4×10^{-6}	1200	Fox (1909)	M	
	6.3×10^{-6}	2200	Braun (1900)	M	60
	6.3×10^{-6}	1300	Winkler (1891b)	M	61
	6.7×10^{-6}	1400	Bohr and Bock (1891)	M	
	5.8×10^{-6}	1200	Bunsen (1855a)	M	43
	6.4×10^{-6}	1300	Wauchope and Haque (1972)	V	
	6.5×10^{-6}	1300	Wauchope and Haque (1972)	V	
	6.5×10^{-6}		Pierotti (1965)	T	
	7.2×10^{-6}		Nunn (1958)	C	12
	5.6×10^{-6}		Hayer et al. (2022)	Q	20
	6.4×10^{-6}	1600	Battino et al. (2018)	?	
	6.3×10^{-6}	1200	Yaws et al. (1999)	?	21
	5.7×10^{-6}		Abraham and Weathersby (1994)	?	21
	6.3×10^{-6}	1300	Dean and Lange (1999)	?	62, 23
ammonia	5.9×10^{-1}	4200	Burkholder et al. (2019)	L	
NH_3	5.9×10^{-1}	4200	Burkholder et al. (2015)	L	
[7664-41-7]	5.9×10^{-1}	4200	Sander et al. (2011)	L	
QGZKDVFQNNGYKY-UHFFFAOYSA-N	5.9×10^{-1}	4200	Sander et al. (2006)	L	
	5.8×10^{-1}	4400	Yoo et al. (1986)	L	1
	6.0×10^{-1}	4200	Edwards et al. (1978)	L	1
	1.0×10^{-1}	1500	Wilhelm et al. (1977)	L	
	2.8×10^{-1}	3200	Shi et al. (1999)	M	
	9.9	6600	Tsuji et al. (1990)	M	63

Table A1.3: Nitrogen (N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.0×10^{-1}	4200	Clegg and Brimblecombe (1989)	M	
	5.5×10^{-1}	4100	Dasgupta and Dong (1986)	M	
	7.7×10^{-1}		Holzwarth et al. (1984)	M	
	7.4×10^{-1}	3700	Hales and Drewes (1979)	M	
	5.6×10^{-1}	4200	Dasgupta and Dong (1986)	T	
	5.7×10^{-1}	4100	Chameides (1984)	T	
	5.9×10^{-1}	4100	Edwards et al. (1975)	T	1
	6.1×10^{-1}		Van Krevelen et al. (1949)	X	64
	2.9×10^{-1}		Hayer et al. (2022)	Q	20
	2.7×10^{-1}	2400	Dean and Lange (1999)	?	65, 23
	5.7×10^{-1}		Abraham et al. (1990)	?	
	6.1×10^{-1}	4100	Seinfeld (1986)	?	21
	5.8×10^{-1}	4100	Hoffmann and Jacob (1984)	?	21
	5.2×10^{-1}		Bone et al. (1983)	?	66
hydrazoic acid HN_3 [7782-79-8] JUINSXZKUKVTMD-UHFFFAOYSA-N	1.2×10^{-1}	3800	Sander et al. (2011)	L	67
	9.8×10^{-2}	3100	Wilhelm et al. (1977)	L	
	1.2×10^{-1}	3700	Betterton and Robinson (1997)	M	
	9.9×10^{-2}		Templeton and King (1971)	M	38
	1.2×10^{-1}	4200	D'Orazio and Wood (1963)	M	
	7.6×10^{-1}		Modarresi et al. (2007)	Q	68
			Burkholder et al. (2019)	W	69
			Burkholder et al. (2015)	W	70
hydrazine H_4N_2 [302-01-2] OAKJQQAXSVQMHS-UHFFFAOYSA-N	1.6×10^{1}		HSDB (2015)	V	
dinitrogen monoxide N_2O (nitrous oxide; laughing gas) [10024-97-2] GQPLMRYTRLFLPF-UHFFFAOYSA-N	2.4×10^{-4}	2600	Burkholder et al. (2019)	L	1
	2.1×10^{-4}	2600	Burkholder et al. (2019)	L	71
	2.4×10^{-4}	2600	Burkholder et al. (2015)	L	1
	2.1×10^{-4}	2600	Burkholder et al. (2015)	L	71
	2.4×10^{-4}	2700	Warneck and Williams (2012)	L	
	2.4×10^{-4}	2600	Sander et al. (2011)	L	1
	2.4×10^{-4}	2600	Sander et al. (2006)	L	1
	2.4×10^{-4}	2500	Young (1981b)	L	1
	2.4×10^{-4}	2600	Wilhelm et al. (1977)	L	
	1.8×10^{-4}		Steward et al. (1973)	L	14
	2.5×10^{-4}	2500	Allott et al. (1973)	L	
	2.4×10^{-4}	2500	Weiss and Price (1980)	M	72
	2.5×10^{-4}	2300	Gabel and Schultz (1973)	M	
	2.4×10^{-4}		Joosten and Danckwerts (1972)	M	
	1.9×10^{-4}		Bachofen and Farhi (1971)	M	14
	2.4×10^{-4}	2400	Saidman et al. (1966)	M	
	1.4×10^{-4}		Sy and Hasbrouck (1964)	M	14
	2.2×10^{-4}		Nunn (1958)	M	73

Table A1.3: Nitrogen (N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.4×10^{-4}		Orcutt and Seevers (1937a)	M	
	2.4×10^{-4}	2500	Kunerth (1922)	M	
	2.4×10^{-4}	2400	Siebeck (1909)	M	
	2.4×10^{-4}	2700	Geffcken (1904)	M	
	2.3×10^{-4}	2900	Roth (1897)	M	74
	2.5×10^{-4}	2600	Carius (1855)	M	
	2.6×10^{-4}	2500	Gordon (1895)	X	75
	1.7×10^{-4}		Harris (1951)	X	14, 76
	3.0×10^{-4}		Macintosh et al. (1958)	X	12, 76
	1.7×10^{-4}		Orcutt and Seevers (1937b)	X	59, 76
	2.8×10^{-4}		Nunn (1958)	C	12
	2.2×10^{-4}		Hayer et al. (2022)	Q	20
		3600	Kühne et al. (2005)	Q	
		2700	Kühne et al. (2005)	?	
	2.4×10^{-4}	2500	Yaws et al. (1999)	?	21
	1.8×10^{-4}		Abraham and Weathersby (1994)	?	21
	2.4×10^{-4}	2800	Dean and Lange (1999)	?	23
	2.5×10^{-4}		Seinfeld (1986)	?	21
	2.5×10^{-4}		Liss and Slater (1974)	?	
nitrogen monoxide	1.9×10^{-5}	1600	Warneck and Williams (2012)	L	
NO	1.9×10^{-5}	1600	Sander et al. (2011)	L	77, 1
(nitric oxide)	1.9×10^{-5}	1600	Sander et al. (2006)	L	78, 1
[10102-43-9]	1.9×10^{-5}	1500	Schwartz and White (1981)	L	
MWUXSHHQAYIFBG-UHFFFAOYSA-N	1.9×10^{-5}	1400	Young (1981b)	L	79, 1
	1.3×10^{-5}		Zafiriou and McFarland (1980)	M	80
	2.3×10^{-5}		Komiyama and Inoue (1980)	M	81
	1.9×10^{-5}	1500	Komiyama and Inoue (1978)	M	
	1.9×10^{-5}	1400	Winkler (1901)	M	82
	3.4×10^{-5}		Pierotti (1965)	T	
	1.9×10^{-5}	1300	Loomis (1928)	C	83
	1.5×10^{-5}		Hayer et al. (2022)	Q	20
		1500	Kühne et al. (2005)	Q	
		1600	Kühne et al. (2005)	?	
	1.9×10^{-5}	1400	Yaws et al. (1999)	?	21
	1.9×10^{-5}	1500	Dean and Lange (1999)	?	84, 23
	1.9×10^{-5}		Seinfeld (1986)	?	21
	1.9×10^{-5}		Andrew and Hanson (1961)	?	
			Burkholder et al. (2019)	W	85
			Burkholder et al. (2015)	W	86
			Wilhelm et al. (1977)	W	87

Table A1.3: Nitrogen (N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
nitrogen dioxide	1.2×10^{-4}	2400	Burkholder et al. (2019)	L	
NO_2	1.2×10^{-4}	2400	Burkholder et al. (2015)	L	
[10102-44-0]	9.9×10^{-5}		Warneck and Williams (2012)	L	
JCXJVPUVTGWSNB-UHFFFAOYSA-N	1.2×10^{-4}	2400	Sander et al. (2011)	L	
	1.4×10^{-4}		Sander et al. (2006)	L	
	1.2×10^{-4}		Schwartz and White (1981)	L	
	1.2×10^{-4}	2400	Cheung et al. (2000)	M	
	6.9×10^{-5}		Lee and Schwartz (1981)	M	88
	2.3×10^{-4}		Komiyama and Inoue (1980)	M	81
	1.2×10^{-4}	2500	Chameides (1984)	T	
	3.4×10^{-4}	1800	Berdnikov and Bazhin (1970)	T	48
	9.9×10^{-5}		Pandis and Seinfeld (1989)	?	89
	9.9×10^{-5}		Seinfeld (1986)	?	21
	4.0×10^{-4}		Andrew and Hanson (1961)	?	
nitrogen trioxide	1.8×10^{-2}		Thomas et al. (1998)	M	
NO_3	5.9×10^{-3}		Rudich et al. (1996)	M	90
(nitrate radical)	3.8×10^{-4}		Burkholder et al. (2019)	T	47
[12033-49-7]	3.8×10^{-4}		Burkholder et al. (2015)	T	47
YPJKMVATUPSWOH-UHFFFAOYSA-N	3.8×10^{-4}		Sander et al. (2011)	T	47
	3.8×10^{-4}		Sander et al. (2006)	T	47
	1.2×10^{-1}	1900	Chameides (1986)	T	
	3.4×10^{-4}	2000	Berdnikov and Bazhin (1970)	T	48
			Jacob (1986)	E	91
			Seinfeld and Pandis (1997)	?	92
dinitrogen trioxide	5.9×10^{-3}		Schwartz and White (1981)	L	
N_2O_3	2.5×10^{-1}		Komiyama and Inoue (1978)	M	
[10544-73-7]					
LZDSILRDTDCIQT-UHFFFAOYSA-N					
dinitrogen tetroxide	1.4×10^{-2}		Schwartz and White (1981)	L	
N_2O_4	2.0×10^{-2}		Komiyama and Inoue (1980)	M	81
[10544-72-6]	1.6×10^{-2}	3500	Komiyama and Inoue (1978)	M	
WFPZPJSADLPSON-UHFFFAOYSA-N	3.1×10^{-2}		Andrew and Hanson (1961)	M	
	1.3×10^{-2}	1100	Kramers et al. (1961)	M	
dinitrogen pentoxide	3.0×10^{-2}		Cruzeiro et al. (2022)	T	93
N_2O_5	3.9×10^{-3}		Galib and Limmer (2021)	T	94
(nitric anhydride)	4.9×10^{-3}		Hirshberg et al. (2018)	T	95
[10102-03-1]	8.7×10^{-4}	3600	Fried et al. (1994)	T	96
ZWWCURLKEXEFQT-UHFFFAOYSA-N	3.9×10^{-2}	4300	Robinson et al. (1997)	Q	97
	4.9×10^{-2}		Mentel et al. (1999)	E	98
	∞		Sander and Crutzen (1996)	E	99
	∞		Jacob (1986)	E	99

Table A1.3: Nitrogen (N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hydroxylamine H_3NO [7803-49-8] AVXURJPOCDRRFD-UHFFFAOYSA-N	1.4×10^{3}		HSDB (2015)	Q	100
nitrous acid	4.8×10^{-1}	4800	Schwartz and White (1981)	L	
HNO_2	4.7×10^{-1}	4900	Becker et al. (1998)	M	
[7782-77-6]	4.7×10^{-1}	4900	Becker et al. (1996)	M	
IOVCWXUNBOPUCH-UHFFFAOYSA-N	4.8×10^{-1}	4900	Park and Lee (1988)	M	
	3.7×10^{-1}	9000	Komiyama and Inoue (1978)	M	
	4.7×10^{-1}	4700	Martin (1984)	T	
	4.8×10^{-1}	4800	Chameides (1984)	T	
	4.8×10^{-1}		Seinfeld (1986)	?	21
nitric acid	8.8×10^{2}		Durham et al. (1981)	V	
HNO_3	2.1×10^{3}	8700	Lelieveld and Crutzen (1991)	R	101
[7697-37-2]			Clegg and Brimblecombe (1990)	T	102, 1
GRYLNZFGIOXLOG-UHFFFAOYSA-N			Brimblecombe and Clegg (1989)	T	103
	2.6×10^{4}	8700	Chameides (1984)	T	
	2.1×10^{3}		Schwartz and White (1981)	T	
	2.1×10^{3}		Pandis and Seinfeld (1989)	?	104
	2.1×10^{3}		Seinfeld (1986)	?	21
	3.4×10^{3}	8800	Hoffmann and Jacob (1984)	?	21
			Brimblecombe and Clegg (1988)	W	105
pernitric acid	3.9×10^{-1}	8400	Leu and Zhang (1999)	L	
HNO_4	3.9×10^{1}		Amels et al. (1996)	M	
[26404-66-0]	1.2×10^{2}	6900	Régimbal and Mozurkewich (1997)	T	
UUZZMWZGAZGXSF-UHFFFAOYSA-N	1.4×10^{2}		Warneck (1999)	C	
	2.0×10^{2}	0	Jacob et al. (1989)	C	
			Möller and Mauersberger (1992)	E	106

A1.4 Fluorine (F)

Table A1.4: Fluorine (F)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
fluorine atom F [14762-94-8] YCKRFDGAMUMZLT-UHFFFAOYSA-N	2.0×10^{-4}	400	Berdnikov and Bazhin (1970)	T	48
hydrogen fluoride HF [7664-39-3] KRHYYFGTRYWZRS-UHFFFAOYSA-N	1.3×10^{2}		Fredenhagen and Wellmann (1932a)	M	
			Brimblecombe and Clegg (1989)	T	107
	6.8×10^{-4}		Hayer et al. (2022)	Q	20
			Brimblecombe and Clegg (1988)	W	105
difluorine monoxide F_2O [7783-41-7] UJMWVICAENGCRF-UHFFFAOYSA-N	2.9×10^{-5}		Schäfer and Lax (1962)	C	
nitrogen trifluoride NF_3 [7783-54-2] GVGCUCJTUSOZKP-UHFFFAOYSA-N	7.9×10^{-6}	1900	Burkholder et al. (2019)	L	1
	7.9×10^{-6}	1900	Burkholder et al. (2015)	L	1
	7.9×10^{-6}	1900	Sander et al. (2011)	L	1
	7.9×10^{-6}	1900	Wilhelm et al. (1977)	L	
	7.7×10^{-6}	1700	Dean et al. (1973)	M	108
	7.8×10^{-6}	1900	Ashton et al. (1968)	M	109
dinitrogen tetrafluoride N_2F_4 (tetrafluorohydrazine) [10036-47-2] GFADZIUESKAXAK-UHFFFAOYSA-N	8.4×10^{-6}	2500	Burkholder et al. (2019)	L	1
	8.4×10^{-6}	2500	Burkholder et al. (2015)	L	1
	8.4×10^{-6}	2500	Sander et al. (2011)	L	1
	8.4×10^{-6}	2500	Wilhelm et al. (1977)	L	
	8.4×10^{-6}	2400	Dean et al. (1973)	M	110

A1.5 Chlorine (Cl)

Table A1.5: Chlorine (Cl)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chlorine (molecular) Cl_2 [7782-50-5] KZBUYRJDOAKODT-UHFFFAOYSA-N			Burkholder et al. (2019)	L	111
			Burkholder et al. (2015)	L	111
			Sander et al. (2011)	L	111
			Sander et al. (2006)	L	111
			Young (1983)	L	112
	6.1×10^{-4}	3200	Aieta and Roberts (1986)	M	
	6.2×10^{-4}	3500	Whitney and Vivian (1941a)	M	113
			Jones (1911)	M	111
			Winkler (1907)	M	111
	6.0×10^{-4}	3000	Yakovkin (1900)	M	114
			Bakhuis Roozeboom (1884)	M	111
			Goodwin (1883)	M	111
			Schoenfeld (1855)	M	111
	7.4×10^{-4}	2600	Lin and Pehkonen (1998)	R	
	5.9×10^{-4}		Leaist (1986)	R	115
		3200	Brian et al. (1962)	R	
			Adams and Edmonds (1937)	R	116
			Arkadiev (1918)	R	117
	6.1×10^{-4}	2800	Wagman et al. (1982)	T	
	8.7×10^{-4}		Hayer et al. (2022)	Q	20
			Bartlett and Margerum (1999)	?	111, 21, 118
			Yaws et al. (1999)	?	111
			Dean and Lange (1999)	?	111
			Wilhelm et al. (1977)	?	119, 111
chlorine atom Cl [22537-15-1] ZAMOUSCENKQFHK-UHFFFAOYSA-N	2.3×10^{-2}		Burkholder et al. (2019)	T	47
	2.3×10^{-2}		Burkholder et al. (2015)	T	47
	2.3×10^{-2}		Sander et al. (2011)	T	47
	2.3×10^{-2}		Sander et al. (2006)	T	47
	2.0×10^{-3}		Mozurkewich (1986)	T	120
	1.5×10^{-4}	1500	Berdnikov and Bazhin (1970)	T	48
hydrogen chloride HCl [7647-01-0] VEXZGXHMUGYJMC-UHFFFAOYSA-N			Clegg and Brimblecombe (1986)	L	121
	1.5×10^{1}		Chen et al. (1979)	R	
			Carslaw et al. (1995)	T	122, 1
			Brimblecombe and Clegg (1989)	T	123
	1.1×10^{-2}	2300	Marsh and McElroy (1985)	T	
			Wagman et al. (1982)	T	124
	2.0×10^{-1}		Graedel and Goldberg (1983)	C	
	2.4×10^{-1}		Hayer et al. (2022)	Q	20
			Seinfeld and Pandis (1997)	?	92
	1.9×10^{-1}	620	Dean and Lange (1999)	?	125, 23
	7.2	2000	Pandis and Seinfeld (1989)	?	126
	2.5×10^{1}		Seinfeld (1986)	?	21

Table A1.5: Chlorine (Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
			Brimblecombe and Clegg (1988)	W	105
hypochlorous acid	6.5	5900	Burkholder et al. (2019)	L	
HOCl	6.5	5900	Burkholder et al. (2015)	L	
[7790-92-3]	6.5	5900	Sander et al. (2011)	L	
QWPPOHNGKGFGJK-UHFFFAOYSA-N	6.5	5900	Sander et al. (2006)	L	
	6.5	5900	Huthwelker et al. (1995)	L	
	9.1		Blatchley et al. (1992)	M	12
	4.7	1600	Hanson and Ravishankara (1991)	M	127
	9.0		McCoy et al. (1990)	M	12
	6.0	4900	Holzwarth et al. (1984)	M	128
	1.2×10^{1}	5200	Imagawa (1950)	M	11
	6.4	8900	Ourisson and Kastner (1939)	M	
	2.6	5100	Wagman et al. (1982)	T	
	5.4		Hilal et al. (2008)	Q	
perchloric acid	9.9×10^{3}		Jaeglé et al. (1996)	E	129
$HClO_4$					
[7601-90-3]					
VLTRZXGMWDSKGL-UHFFFAOYSA-N					
monochlorine monoxide	7.0×10^{-3}		Burkholder et al. (2019)	T	47
ClO	7.0×10^{-3}		Burkholder et al. (2015)	T	47
[14989-30-1]	7.0×10^{-3}		Sander et al. (2011)	T	47
MLWGAEVSWJXOQJ-UHFFFAOYSA-N	7.0×10^{-3}		Sander et al. (2006)	T	47
dichlorine monoxide			Secoy and Cady (1941)	M	130
Cl_2O			Ourisson and Kastner (1939)	M	131
[7791-21-1]	3.4×10^{-2}	5900	this work	R	132, 133, 134
RCJVRSBWZCNNQT-UHFFFAOYSA-N	7.6×10^{-2}	5600	this work	R	133, 135
	7.0×10^{-2}		Roth (1942)	R	136
			Burkholder et al. (2019)	?	137
			Burkholder et al. (2015)	?	137
			Sander et al. (2011)	?	137
			Sander et al. (2006)	?	137
			Young (1983)	?	138
			Wilhelm et al. (1977)	W	139
chlorine dioxide	1.0×10^{-2}	3500	Burkholder et al. (2019)	L	
ClO_2	1.0×10^{-2}	3500	Burkholder et al. (2015)	L	
[10049-04-4]	1.0×10^{-2}	3500	Sander et al. (2011)	L	
OSVXSBDYLRYLIG-UHFFFAOYSA-N	1.0×10^{-2}	3500	Sander et al. (2006)	L	
	1.0×10^{-2}	3300	Young (1983)	L	1
	1.0×10^{-2}	3300	Wilhelm et al. (1977)	L	
	1.0×10^{-2}	3200	Kepinski and Trzeszczynski (1964)	M	
	1.1×10^{-2}	3100	Ishi (1958)	M	
	1.0×10^{-2}		Taube and Dodgen (1949)	M	
	6.6×10^{-3}	1200	Bigorgne (1947)	M	

Table A1.5: Chlorine (Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.7×10^{-3}	3600	Holst (1944)	M	
			Haller and Northgraves (1955)	C	140
	1.1×10^{-2}	3100	Mavu (2011)	?	
	9.7×10^{-3}		Morrow et al. (2006)	?	
	1.0×10^{-2}	3300	Yaws et al. (1999)	?	21
perchloryl fluoride ClO_3F [7616-94-6] XHFXMNZYIKFCPN-UHFFFAOYSA-N	4.4×10^{-5}		Hayer et al. (2022)	Q	20
nitrosyl chloride NOCl [2696-92-6] VPCDQGACGWYTMC-UHFFFAOYSA-N	$>4.9\times10^{-4}$		Burkholder et al. (2019)	L	
	$>4.9\times10^{-4}$		Burkholder et al. (2015)	L	
	$>4.9\times10^{-4}$		Scheer et al. (1997)	M	
nitryl chloride $ClNO_2$ [13444-90-1] HSSFHZJIMRUXDM-UHFFFAOYSA-M	4.5×10^{-4}		Frenzel et al. (1998)	E	
	2.4×10^{-4}		Behnke et al. (1997)	E	141
	3.9×10^{-4}		Roberts et al. (2008)	?	
chlorine nitrate $ClNO_3$ [14545-72-3] XYLGPCWDPLOBGP-UHFFFAOYSA-N	7.0×10^{-2}	4500	Robinson et al. (1997)	Q	142
	∞		Sander and Crutzen (1996)	E	99
chloramine NH_2Cl (chloramide) [10599-90-3] QDHHCQZDFGDHMP-UHFFFAOYSA-N	8.6×10^{-1}	6000	Burkholder et al. (2019)	L	
	8.6×10^{-1}	6000	Burkholder et al. (2015)	L	
	8.6×10^{-1}	6000	Sander et al. (2011)	L	
	8.6×10^{-1}	6000	Sander et al. (2006)	L	
	9.2×10^{-1}	4800	Holzwarth et al. (1984)	M	
	4.6×10^{-5}		Hayer et al. (2022)	Q	20
dichloramine $NHCl_2$ (chlorimide) [3400-09-7] JSYGRUBHOCKMGQ-UHFFFAOYSA-N	2.9×10^{-1}	4200	Burkholder et al. (2019)	L	
	2.9×10^{-1}	4200	Burkholder et al. (2015)	L	
	2.9×10^{-1}	4200	Sander et al. (2011)	L	
	2.9×10^{-1}	4200	Sander et al. (2006)	L	
	2.8×10^{-1}	4200	Holzwarth et al. (1984)	M	
nitrogen trichloride NCl_3 [10025-85-1] QEHKBHWEUPXBCW-UHFFFAOYSA-N	9.9×10^{-4}	4100	Burkholder et al. (2019)	L	
	9.9×10^{-4}	4100	Burkholder et al. (2015)	L	
	9.9×10^{-4}	4100	Sander et al. (2011)	L	
	9.9×10^{-4}	4100	Sander et al. (2006)	L	
	9.9×10^{-4}	4100	Holzwarth et al. (1984)	M	

A1.6 Bromine (Br)

Table A1.6: Bromine (Br)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bromine (molecular)	7.2×10^{-3}	4400	Burkholder et al. (2019)	L	
Br_2	7.2×10^{-3}	4400	Burkholder et al. (2015)	L	
[7726-95-6]	7.2×10^{-3}	4400	Sander et al. (2011)	L	
GDTBXPJZTBHREO-UHFFFAOYSA-N	7.2×10^{-3}	4400	Sander et al. (2006)	L	
	1.8×10^{-2}	3600	Dubik et al. (1987)	M	143
	6.8×10^{-3}		Hill et al. (1968)	M	
	9.6×10^{-3}		Jenkins and King (1965)	M	12
	7.0×10^{-3}	4100	Kelley and Tartar (1956)	M	
	1.4×10^{-2}		Jones (1911)	M	81
	7.8×10^{-3}	3800	Winkler (1906)	M	
	7.9×10^{-3}	3600	Winkler (1899)	M	
	8.3×10^{-3}	4100	Fogg and Sangster (2003)	V	
	7.9×10^{-3}	3900	Jenkins and King (1965)	R	
	7.2×10^{-3}	4000	Wagman et al. (1982)	T	
	9.2×10^{-3}		Giona et al. (1969)	X	144, 12
	7.6×10^{-3}		Bartlett and Margerum (1999)	?	21, 118
	7.5×10^{-3}	3900	Dean and Lange (1999)	?	145, 23
bromine atom	1.2×10^{-2}		Mozurkewich (1986)	T	120
Br	3.4×10^{-4}	1800	Berdnikov and Bazhin (1970)	T	48
[10097-32-2]					
WKBOTKDWSSQWDR-UHFFFAOYSA-N					
hydrogen bromide			Carslaw et al. (1995)	T	146, 1
HBr			Brimblecombe and Clegg (1989)	T	147
[10035-10-6]			Wagman et al. (1982)	T	148
CPELXLSAUQHCOX-UHFFFAOYSA-N	6.8×10^{-2}		Hayer et al. (2022)	Q	20
			Chameides and Stelson (1992)	?	149
	2.4×10^{-1}	250	Dean and Lange (1999)	?	150, 23
			Brimblecombe and Clegg (1988)	W	105
hypobromous acid	$>1.3\times10^{1}$		Burkholder et al. (2019)	L	
HOBr	$>1.3\times10^{1}$		Burkholder et al. (2015)	L	
[13517-11-8]	$>1.9\times10^{1}$		Blatchley et al. (1992)	M	12
CUILPNURFADTPE-UHFFFAOYSA-N	1.9×10^{1}		McCoy et al. (1990)	M	12
	1.8×10^{-2}	4000	Mozurkewich (1995)	T	151
	6.0×10^{1}		Frenzel et al. (1998)	E	
	9.1×10^{-1}		Vogt et al. (1996)	E	
			Sander et al. (2011)	W	152
			Sander et al. (2006)	W	152
			Fickert (1998)	W	153

Table A1.6: Bromine (Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
nitryl bromide $BrNO_2$ [13536-70-4] SEYAFCXQVVHRPY-UHFFFAOYSA-M	3.0×10^{-3}		Frenzel et al. (1998)	E	
bromine nitrate $BrNO_3$ [40423-14-1] RRTWEEAEXPZMPY-UHFFFAOYSA-N	∞		Sander and Crutzen (1996)	E	99
bromine chloride	9.7×10^{-3}	5600	Burkholder et al. (2019)	L	
BrCl	9.7×10^{-3}	5600	Burkholder et al. (2015)	L	
[13863-41-7]	9.7×10^{-3}	5600	Sander et al. (2011)	L	
CODNYICXDISAEA-UHFFFAOYSA-N	9.7×10^{-3}	5600	Sander et al. (2006)	L	
	$<6.2\times10^{-2}$		Katrib et al. (2001)	M	154
	1.5×10^{-2}		Disselkamp et al. (1999)	M	155
	9.3×10^{-3}	5600	Bartlett and Margerum (1999)	M	
	4.2×10^{-2}	4000	Dubik et al. (1987)	M	143
	1.1×10^{-2}		this work	T	156
	6.9×10^{-4}	4000	Ordóñez et al. (2012)	E	
	5.8×10^{-3}		Frenzel et al. (1998)	E	

A1.7 Iodine (I)

Table A1.7: Iodine (I)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
iodine (molecular) I_2 [7553-56-2] PNDPGZBMCMUPRI-UHFFFAOYSA-N	2.8×10^{-2} 2.8×10^{-2} 3.0×10^{-2} 3.1×10^{-2} 3.2×10^{-2} 1.1×10^{-2}	4300 3900 4400 4600 4800	Eguchi et al. (1973) Fogg and Sangster (2003) Palmer et al. (1985) Berdnikov and Bazhin (1970) Wagman et al. (1982) Thompson and Zafiriou (1983)	M V R R T C	 1 157
iodine atom I [14362-44-8] ZCYVEMRRCGMTRW-UHFFFAOYSA-N	7.9×10^{-4} 6.2×10^{-5}	 2300	Mozurkewich (1986) Berdnikov and Bazhin (1970)	T T	158 48
hydrogen iodide HI [10034-85-2] XMBWDFGMSWQBCA-UHFFFAOYSA-N	 2.5×10^{-1} ∞	 9800	Brimblecombe and Clegg (1989) Wagman et al. (1982) Ordóñez et al. (2012) Vogt et al. (1999) Brimblecombe and Clegg (1988)	T T E E W	159 160 99 105
iodine monoxide IO [14696-98-1] AFSVSXMRDKPOEW-UHFFFAOYSA-N	4.4		Saiz-Lopez et al. (2014)	?	161
iodine dioxide OIO [13494-92-3] WXDJHDMIIZKXSK-UHFFFAOYSA-N	9.9×10^{1}		Saiz-Lopez et al. (2014)	?	161
diiodine dioxide I_2O_2 [215239-62-6] IELAHHPSAVYAOC-UHFFFAOYSA-N	∞ ∞ 9.9×10^{1}		Badia et al. (2019) Vogt et al. (1999) Saiz-Lopez et al. (2014)	E E ?	162, 163 162, 99 162, 161
diiodine trioxide I_2O_3 [11085-17-9] NMNCVPKLBXOKQA-UHFFFAOYSA-N	∞ 9.9×10^{1}		Badia et al. (2019) Saiz-Lopez et al. (2014)	E ?	162, 163 162, 161
diiodine tetroxide I_2O_4 [1024652-24-1] XHTWXUOEQMOFEJ-UHFFFAOYSA-N	∞ 9.9×10^{1}		Badia et al. (2019) Saiz-Lopez et al. (2014)	E ?	162, 163 162, 161
hypoiodous acid HOI [14332-21-9] GEOVEUCEIQCBKH-UHFFFAOYSA-N	>4.1		Palmer et al. (1985) Thompson and Zafiriou (1983)	C E	 164

Table A1.7: Iodine (I) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
iodine nitrite INO_2 [15465-40-4] PSZTWRLUACEPOW-UHFFFAOYSA-N	3.0×10^{-3} ∞		Badia et al. (2019) Vogt et al. (1999)	E E	165 99
iodine nitrate INO_3 [14696-81-2] CCJHDZZUWZIVJF-UHFFFAOYSA-N	∞		Vogt et al. (1999)	E	99
iodine chloride ICl [7790-99-0] QZRGKCOWNLSUDK-UHFFFAOYSA-N	1.1		Wagman et al. (1982)	T	
iodine bromide IBr [7789-33-5] CBEQRNSPHCCXSH-UHFFFAOYSA-N	2.4×10^{-1}		Wagman et al. (1982)	T	

A1.8 Sulfur (S)

Table A1.8: Sulfur (S)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
sulfur S [7704-34-9] NINIDFKCEFEMDL-UHFFFAOYSA-N	2.0×10^{1}		Maniere et al. (2011)	?	12, 166
hydrogen sulfide H_2S [7783-06-4] RWSOTUBLDIXVET-UHFFFAOYSA-N	1.0×10^{-3}	2100	Burkholder et al. (2019)	L	1
	1.0×10^{-3}	2100	Burkholder et al. (2015)	L	1
	1.0×10^{-3}	2100	Sander et al. (2011)	L	1
	1.0×10^{-3}	2100	Sander et al. (2006)	L	1
	1.0×10^{-3}	2000	Fernández-Prini et al. (2003)	L	3
	1.0×10^{-3}	2200	Carroll and Mather (1989)	L	
	1.0×10^{-3}	2000	Fogg and Young (1988)	L	1, 167
	1.0×10^{-3}	2000	Yoo et al. (1986)	L	1
	1.0×10^{-3}	2100	Edwards et al. (1978)	L	1
	1.0×10^{-3}	2100	Wilhelm et al. (1977)	L	
	9.1×10^{-4}	1700	Rinker and Sandall (2000)	M	
	9.2×10^{-4}	1600	Munder et al. (2000)	M	
	8.6×10^{-4}	2100	De Bruyn et al. (1995b)	M	
	1.1×10^{-3}	2300	Suleimenov and Krupp (1994)	M	1
	1.2×10^{-3}	1700	Tsuji et al. (1990)	M	63
	9.4×10^{-4}	2300	Barrett et al. (1988)	M	
	1.0×10^{-3}	2100	Clarke and Glew (1971)	M	168
	1.0×10^{-3}	2300	Winkler (1907)	M	
	1.0×10^{-3}	2100	Winkler (1906)	M	
	1.1×10^{-3}	2000	Schoenfeld (1855)	M	169
	9.6×10^{-4}	2000	Iliuta and Larachi (2007)	R	1
	1.0×10^{-3}		Hine and Weimar (1965)	R	
	1.0×10^{-3}	2300	Edwards et al. (1975)	T	1
	7.0×10^{-4}		Hayer et al. (2022)	Q	20
	1.0×10^{-3}	2000	Yaws et al. (1999)	?	21
	1.0×10^{-3}	2100	Dean and Lange (1999)	?	170, 23
			Chapoy et al. (2005)	W	171, 1
deuterium sulfide D_2S [13536-94-2] RWSOTUBLDIXVET-ZSJDYOACSA-N	9.9×10^{-4}	2100	Clarke and Glew (1971)	M	172, 173
sulfur dioxide SO_2 [7446-09-5] RAHZWNYVWXNFOC-UHFFFAOYSA-N	1.3×10^{-2}	2900	Burkholder et al. (2019)	L	1
	1.3×10^{-2}	2900	Burkholder et al. (2015)	L	1
	1.3×10^{-2}	2900	Sander et al. (2011)	L	1
	1.3×10^{-2}	2900	Sander et al. (2006)	L	1
	1.2×10^{-2}	3100	Yoo et al. (1986)	L	1
	1.3×10^{-2}	2900	Young (1983)	L	1
	1.2×10^{-2}	3200	Maahs (1982)	L	

Table A1.8: Sulfur (S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-2}	3000	Edwards et al. (1978)	L	1
	1.4×10^{-2}	2800	Wilhelm et al. (1977)	L	
	4.0×10^{-1}		St-Pierre et al. (2014)	M	174
	1.2×10^{-2}	3100	Johnstone and Leppla (1934)	M	
	1.4×10^{-2}	3400	Schoenfeld (1855)	M	175
	1.1×10^{-2}	1200	Terraglio and Manganelli (1967)	V	
	1.2×10^{-2}	3100	Chameides (1984)	T	
	1.2×10^{-2}	3100	Edwards et al. (1975)	T	1
	1.2×10^{-2}		Rodríguez-Sevilla et al. (2001)	X	176
	1.2×10^{-2}	3100	Pandis and Seinfeld (1989)	C	
	1.2×10^{-2}	3300	Beilke and Gravenhorst (1978)	C	
	2.9×10^{-2}		Hayer et al. (2022)	Q	20
	1.3×10^{-2}	2900	Yaws et al. (1999)	?	21
	1.5×10^{-2}	3100	Dean and Lange (1999)	?	177, 23
	1.2×10^{-2}	3100	Seinfeld (1986)	?	21
	1.2×10^{-2}	3100	Hoffmann and Jacob (1984)	?	21
sulfur trioxide SO_3 [7446-11-9] AKEJUJNQAAGONA-UHFFFAOYSA-N	5.1×10^{-8}		Hayer et al. (2022)	Q	20
	∞		Sander and Crutzen (1996)	E	99
sulfuric acid H_2SO_4 [7664-93-9] QAOWNCQODCNURD-UHFFFAOYSA-N			Marti et al. (1997)	M	178
			Ayers et al. (1980)	M	179
			Gmitro and Vermeulen (1964)	M	180
			Clegg et al. (1998)	V	181
	1.3×10^{13}	20000	Hoffmann and Calvert (1985)	T	
	2.9×10^{7}	10000	Ayers (1983)	T	
sulfur hexafluoride SF_6 [2551-62-4] SFZCNBIFKDRMGX-UHFFFAOYSA-N	2.4×10^{-6}	3100	Warneck and Williams (2012)	L	
	2.5×10^{-6}	2100	Fernández-Prini et al. (2003)	L	3
	2.4×10^{-6}	2400	Wilhelm et al. (1977)	L	
	2.3×10^{-6}	2700	Bullister et al. (2002)	M	182
	1.4×10^{-6}		Guitart et al. (1989)	M	14
	2.4×10^{-6}		Park et al. (1982)	M	
	2.5×10^{-6}	260	Cosgrove and Walkley (1981)	M	42, 11
	1.7×10^{-6}		Longo et al. (1970)	M	14
	1.7×10^{-6}		Power and Stegall (1970)	M	14
			Shoor et al. (1969)	M	183
	2.4×10^{-6}	2400	Ashton et al. (1968)	M	184
	2.2×10^{-6}	3500	Friedman (1954)	M	
	2.2×10^{-6}		Giardino et al. (1988)	V	
	2.6×10^{-6}		Hayer et al. (2022)	Q	20
	2.2×10^{-5}		Keshavarz et al. (2022)	Q	
	2.6×10^{-5}		Duchowicz et al. (2020)	Q	185
		3200	Kühne et al. (2005)	Q	
	2.2×10^{-6}		Duchowicz et al. (2020)	?	186, 21
		2800	Kühne et al. (2005)	?	

Table A1.8: Sulfur (S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.4×10^{-6}	2400	Yaws et al. (1999)	?	21
	1.9×10^{-6}		Abraham and Weathersby (1994)	?	21
sulfuryl fluoride	8.9×10^{-5}	3100	Cady and Misra (1974)	M	
SO_2F_2	7.3×10^{-5}		Duchowicz et al. (2020)	V	187
[2699-79-8]	3.2		Duchowicz et al. (2020)	Q	
OBTWBSRJZRCYQV-UHFFFAOYSA-N	6.3×10^{-6}		Maniere et al. (2011)	?	12, 166

A1.9 Rare gases (He, Ne, Ar, Kr, Xe, Rn)

Table A1.9: Rare gases (He, Ne, Ar, Kr, Xe, Rn)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
helium	3.9×10^{-6}	15	Fernández-Prini et al. (2003)	L	3
He	3.8×10^{-6}	83	Abraham and Matteoli (1988)	L	
[7440-59-7]	3.8×10^{-6}	83	Clever (1979a)	L	1
SWQJXJOGLNCZEY-UHFFFAOYSA-N	3.8×10^{-6}	92	Wilhelm et al. (1977)	L	
	3.7×10^{-6}	320	Himmelblau (1960)	L	1
	3.9×10^{-6}	69	Krause and Benson (1989)	M	
			Shoor et al. (1969)	M	188
	3.7×10^{-6}	120	Morrison and Johnstone (1954)	M	189
	3.8×10^{-6}		Friedman (1954)	M	
	3.8×10^{-6}	210	Lannung (1930)	M	190
	3.7×10^{-6}	380	Cady et al. (1922)	M	
	6.3×10^{-6}	-700	von Antropoff (1910)	M	42
	3.7×10^{-6}	220	Wauchope and Haque (1972)	V	
	5.3×10^{-6}		Pierotti (1965)	T	
	4.5×10^{-6}		Hayer et al. (2022)	Q	20
	3.3×10^{-6}	4	Linnemann et al. (2020)	Q	42
	3.3×10^{-6}	71	Linnemann et al. (2020)	Q	42, 191
	3.9×10^{-6}		Warr et al. (2015)	Q	12
	3.8×10^{-6}	83	Yaws et al. (1999)	?	21
	3.9×10^{-6}		Abraham and Weathersby (1994)	?	21
	3.7×10^{-6}	200	Dean and Lange (1999)	?	192, 23
	3.8×10^{-6}		Abraham et al. (1990)	?	
neon	4.5×10^{-6}	430	Fernández-Prini et al. (2003)	L	3
Ne	4.4×10^{-6}	470	Abraham and Matteoli (1988)	L	
[7440-01-9]	4.5×10^{-6}	470	Clever (1979a)	L	1
GKAOGPIIYCISHV-UHFFFAOYSA-N	4.4×10^{-6}	450	Wilhelm et al. (1977)	L	
	4.5×10^{-6}	440	Krause and Benson (1989)	M	
	4.4×10^{-6}	510	Crovetto et al. (1982)	M	
	4.3×10^{-6}		Power and Stegall (1970)	M	14
	4.5×10^{-6}	460	Morrison and Johnstone (1954)	M	193
	4.6×10^{-6}	37	Lannung (1930)	M	194
	6.6×10^{-6}	-990	von Antropoff (1910)	M	
	4.5×10^{-6}	510	Wauchope and Haque (1972)	V	
	8.8×10^{-6}		Pierotti (1965)	T	
	4.5×10^{-6}		Hayer et al. (2022)	Q	20
	3.4×10^{-6}	250	Linnemann et al. (2020)	Q	33
	4.7×10^{-6}	470	Linnemann et al. (2020)	Q	33, 191
	3.6×10^{-6}		Warr et al. (2015)	Q	12
	4.5×10^{-6}	470	Yaws et al. (1999)	?	21
	4.4×10^{-6}		Abraham and Weathersby (1994)	?	21
	4.5×10^{-6}	550	Dean and Lange (1999)	?	195, 23
	4.4×10^{-6}		Abraham et al. (1990)	?	

Table A1.9: Rare gases (He, Ne, Ar, Kr, Xe, Rn) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
argon	1.4×10^{-5}	1700	Warneck and Williams (2012)	L	
Ar	1.4×10^{-5}	1400	Fernández-Prini et al. (2003)	L	3
[7440-37-1]	1.4×10^{-5}	1500	Abraham and Matteoli (1988)	L	
XKRFYHLGVUSROY-UHFFFAOYSA-N	1.4×10^{-5}	1500	Clever (1980)	L	1
	1.4×10^{-5}	1500	Wilhelm et al. (1977)	L	
	1.4×10^{-5}	1400	Rettich et al. (1992)	M	196
	1.4×10^{-5}	1400	Krause and Benson (1989)	M	
	1.4×10^{-5}		Park et al. (1982)	M	
	1.4×10^{-5}	1500	Crovetto et al. (1982)	M	
	1.4×10^{-5}	1200	Cosgrove and Walkley (1981)	M	11
	1.4×10^{-5}	1300	Potter II and Clynne (1978)	M	
	1.4×10^{-5}	1500	Murray and Riley (1970)	M	197
	1.4×10^{-5}	1600	Shoor et al. (1969)	M	198
	1.4×10^{-5}	1500	Ashton et al. (1968)	M	199
	1.3×10^{-5}	1500	Morrison and Johnstone (1954)	M	200
	1.4×10^{-5}	1800	Friedman (1954)	M	
	1.4×10^{-5}	1400	Lannung (1930)	M	201
	1.6×10^{-5}	1300	von Antropoff (1910)	M	
	1.5×10^{-5}	1400	Winkler (1906)	M	
	1.4×10^{-5}	1400	Wauchope and Haque (1972)	V	
	1.4×10^{-5}	1400	Wauchope and Haque (1972)	V	
	1.8×10^{-5}		Pierotti (1965)	T	
	9.5×10^{-6}		Hayer et al. (2022)	Q	20
	7.8×10^{-6}	1200	Linnemann et al. (2020)	Q	191
	1.1×10^{-5}	1100	Linnemann et al. (2020)	Q	202
	1.2×10^{-5}		Warr et al. (2015)	Q	12
	1.4×10^{-5}	1500	Yaws et al. (1999)	?	21
	1.2×10^{-5}		Abraham and Weathersby (1994)	?	21
	1.4×10^{-5}	1500	Dean and Lange (1999)	?	203, 23
	1.4×10^{-5}		Abraham et al. (1990)	?	
krypton	2.5×10^{-5}	1700	Fernández-Prini et al. (2003)	L	3
Kr	2.5×10^{-5}	1900	Abraham and Matteoli (1988)	L	
[7439-90-9]	2.5×10^{-5}	1900	Clever (1979b)	L	1
DNNSSWSSYDEUBZ-UHFFFAOYSA-N	2.5×10^{-5}	1900	Wilhelm et al. (1977)	L	
	2.0×10^{-5}		Steward et al. (1973)	L	14
	2.5×10^{-5}	2000	Allott et al. (1973)	L	
	2.5×10^{-5}	1800	Krause and Benson (1989)	M	
	2.5×10^{-5}	1900	Crovetto et al. (1982)	M	
	2.6×10^{-5}	1800	Cosgrove and Walkley (1981)	M	11
	2.4×10^{-5}	1700	Morrison and Johnstone (1954)	M	204
	3.4×10^{-5}	1400	von Antropoff (1910)	M	205
	2.8×10^{-5}	1900	von Antropoff (1910)	M	205
	2.4×10^{-5}	1800	Wauchope and Haque (1972)	V	
	4.4×10^{-5}		Pierotti (1965)	T	
	2.6×10^{-5}		Hayer et al. (2022)	Q	20

Table A1.9: Rare gases (He, Ne, Ar, Kr, Xe, Rn) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.5×10^{-5}	1600	Linnemann et al. (2020)	Q	191
	1.6×10^{-5}	1400	Linnemann et al. (2020)	Q	202
	2.5×10^{-5}		Warr et al. (2015)	Q	12
	2.5×10^{-5}	1900	Yaws et al. (1999)	?	21
	2.0×10^{-5}		Abraham and Weathersby (1994)	?	21
	2.5×10^{-5}	1800	Dean and Lange (1999)	?	206, 23
	2.5×10^{-5}		Abraham et al. (1990)	?	
xenon Xe [7440-63-3] FHNFHKCVQCLJFQ-UHFFFAOYSA-N	4.4×10^{-5}	2200	Fernández-Prini et al. (2003)	L	3
	4.3×10^{-5}	2300	Abraham and Matteoli (1988)	L	
	4.3×10^{-5}	2300	Clever (1979b)	L	1
	4.2×10^{-5}	2200	Wilhelm et al. (1977)	L	
	3.3×10^{-5}		Steward et al. (1973)	L	14
	4.5×10^{-5}	2400	Allott et al. (1973)	L	
	4.0×10^{-5}	2400	Himmelblau (1960)	L	1, 207
	4.3×10^{-5}	2300	Krause and Benson (1989)	M	
	4.2×10^{-5}	2400	Crovetto et al. (1982)	M	
	4.2×10^{-5}	2200	Morrison and Johnstone (1954)	M	208
	4.4×10^{-5}	2500	von Antropoff (1910)	M	
	4.2×10^{-5}	2200	Wauchope and Haque (1972)	V	
	5.5×10^{-5}		Pierotti (1965)	T	
	2.5×10^{-5}		Hayer et al. (2022)	Q	20
	7.0×10^{-5}	2300	Linnemann et al. (2020)	Q	191
	2.9×10^{-5}	1800	Linnemann et al. (2020)	Q	202
	8.2×10^{-5}		Warr et al. (2015)	Q	12
	4.3×10^{-5}	2300	Yaws et al. (1999)	?	21
	3.4×10^{-5}		Abraham and Weathersby (1994)	?	21
	4.9×10^{-5}	2200	Dean and Lange (1999)	?	209, 23
	4.3×10^{-5}		Abraham et al. (1990)	?	
xenon-133 ^{133}Xe [14932-42-4] FHNFHKCVQCLJFQ-NJFSPNSNSA-N	3.2×10^{-5}		Ercan (1979)	M	14
radon Rn [10043-92-2] SYUHGPGVQRZVTB-UHFFFAOYSA-N	9.1×10^{-5}	2900	Abraham and Matteoli (1988)	L	
	9.1×10^{-5}	2600	Clever (1979b)	L	1
	9.2×10^{-5}	2600	Wilhelm et al. (1977)	L	
	9.4×10^{-5}	2600	Lewis et al. (1987)	M	210
	1.0×10^{-4}	2700	Ramstedt (1911)	M	
	1.2×10^{-4}		Pierotti (1965)	T	
	1.0×10^{-4}		Hayer et al. (2022)	Q	20
	7.4×10^{-5}	2400	Linnemann et al. (2020)	Q	211
	9.1×10^{-5}	2600	Yaws et al. (1999)	?	21
	8.3×10^{-5}	2800	Dean and Lange (1999)	?	212, 23
	9.1×10^{-5}		Abraham et al. (1990)	?	

A1.10 Other elements (B, Se, P, As, Hg)

Table A1.10: Other elements (B, Se, P, As, Hg)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
boric acid H_3BO_3 [10043-35-3] KGBXLFKZBHKPEV-UHFFFAOYSA-N	3.8×10^{6}		HSDB (2015)	V	
selenium hydride	8.1×10^{-4}	1700	Fogg and Young (1988)	L	1
H_2Se	8.3×10^{-4}	1900	Wilhelm et al. (1977)	L	
[7783-07-5]	8.3×10^{-4}	1900	Sisi et al. (1971)	M	213
BUGBHKTXTAQXES-UHFFFAOYSA-N					
phosphorus trihydride	8.1×10^{-5}	2000	Wilhelm et al. (1977)	L	
PH_3	5.9×10^{-5}	3000	Fu et al. (2013)	M	214
(phosphine)	8.1×10^{-5}	2000	Yaws et al. (1999)	?	21
[7803-51-2]					
XYFCBTPGUUZFHI-UHFFFAOYSA-N					
arsenic hydride AsH_3 (arsine) [7784-42-1] RQNWIZPPADIBDY-UHFFFAOYSA-N	8.8×10^{-5}	2100	Wilhelm et al. (1977)	L	
mercury	1.3×10^{-3}	2600	Burkholder et al. (2019)	L	
Hg	1.3×10^{-3}	2600	Burkholder et al. (2015)	L	
[7439-97-6]	1.2×10^{-3}	5400	Clever (1987)	L	1
QSHDDOUJBYECFT-UHFFFAOYSA-N	1.1×10^{-3}	4800	Clever et al. (1985)	L	1
	1.3×10^{-3}	2600	Andersson et al. (2008)	M	
	1.3×10^{-3}	2500	Sanemasa (1975)	M	
	8.7×10^{-4}		Mackay and Leinonen (1975)	V	
	1.1×10^{-3}	5700	Glew and Hames (1971)	V	1
	1.2×10^{-3}		Shon et al. (2005)	C	
	1.4×10^{-3}		WHO (1990)	C	12
		2300	Abraham et al. (2008)	Q	215
	1.4×10^{-3}		Schroeder and Munthe (1998)	?	12, 21
	1.3×10^{-3}	2700	Schroeder and Munthe (1998)	?	21
	1.3×10^{-3}		Petersen et al. (1998)	?	216
	9.2×10^{-4}		Brimblecombe (1986)	?	81
mercury(II) oxide	3.2×10^{4}		Shon et al. (2005)	?	217
HgO	2.7×10^{10}		Schroeder and Munthe (1998)	?	21
[21908-53-2]	1.4×10^{4}		Petersen et al. (1998)	?	216
UKWHYYKOEPRTIC-UHFFFAOYSA-N					

Table A1.10: Other elements (B, Se, P, As, Hg) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
mercury dihydroxide	1.3×10^{2}	4200	WHO (1990)	C	
$Hg(OH)_2$	1.3×10^{2}	4200	Lindqvist and Rodhe (1985)	C	
[12135-13-6]					
VLKKXDVIWIBHHS-UHFFFAOYSA-L					
mercury dichloride	1.0×10^{3}		Severit (1997)	M	218
$HgCl_2$	1.6×10^{4}		Abraham et al. (2008)	V	
[7487-94-7]	4.2×10^{4}		Abraham et al. (2008)	V	
LWJROJCJINYWOX-UHFFFAOYSA-L	1.3×10^{4}	7400	Kanefke (2008)	R	
	2.4×10^{5}		Shon et al. (2005)	C	
	1.4×10^{4}	5300	WHO (1990)	C	
	1.4×10^{4}	5300	Lindqvist and Rodhe (1985)	C	
	4.2×10^{4}	7400	Abraham et al. (2008)	Q	219
	2.7×10^{4}		Schroeder and Munthe (1998)	?	12, 21
	1.4×10^{4}	9500	Braun and Dransfeld (1989)	?	11
	6.3×10^{2}		Iverfeldt and Persson (1985)	?	220
mercury dibromide	1.2×10^{3}		Abraham et al. (2008)	V	
$HgBr_2$	9.6×10^{2}	7400	Kanefke (2008)	C	
[7789-47-1]	4.4×10^{3}	7100	Abraham et al. (2008)	Q	219
NGYIMTKLQULBOO-UHFFFAOYSA-L	2.7×10^{4}		Hedgecock et al. (2005)	?	221
	5.2×10^{1}		Iverfeldt and Persson (1985)	?	220
mercury diiodide	5.7×10^{1}		Abraham et al. (2008)	V	
HgI_2	2.0×10^{2}	6700	Abraham et al. (2008)	Q	219
[7774-29-0]	1.9		Iverfeldt and Persson (1985)	?	220
YFDLHELOZYVNJE-UHFFFAOYSA-L					

A2 Hydrocarbons (C, H)

A2.1 Alkanes

Table A2.1: Alkanes

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methane	1.4×10^{-5}	1600	Burkholder et al. (2019)	L	1
CH_4	1.2×10^{-5}	1100	Burkholder et al. (2019)	L	71
[74-82-8]	1.4×10^{-5}	1600	Burkholder et al. (2015)	L	1
VNWKTOKETHGBQD-UHFFFAOYSA-N	1.2×10^{-5}	1100	Burkholder et al. (2015)	L	71
	1.4×10^{-5}	1900	Warneck and Williams (2012)	L	
	1.4×10^{-5}	1600	Sander et al. (2011)	L	1
	1.4×10^{-5}	1600	Sander et al. (2006)	L	1
	1.4×10^{-5}	1500	Fernández-Prini et al. (2003)	L	3
	1.4×10^{-5}	1600	Plyasunov and Shock (2000)	L	
	1.4×10^{-5}	1600	Abraham and Matteoli (1988)	L	
			Clever and Young (1987)	L	222
	1.5×10^{-5}		Mackay and Shiu (1981)	L	
	1.4×10^{-5}	1700	Wilhelm et al. (1977)	L	
	1.3×10^{-5}	1500	Himmelblau (1960)	L	1
	1.6×10^{-5}		Liu et al. (2021)	M	
	1.4×10^{-5}	1800	Lutsyk et al. (2005)	M	
	1.2×10^{-5}	2400	Lekvam and Bishnoi (1997)	M	
	1.3×10^{-5}	1400	Reichl (1995)	M	223
	1.4×10^{-5}	1600	Scharlin and Battino (1995)	M	224
	1.2×10^{-5}		Guitart et al. (1989)	M	14
	1.4×10^{-5}	1800	Ben-Naim and Battino (1985)	M	
	1.4×10^{-5}	1600	Crovetto et al. (1982)	M	
	1.4×10^{-5}	1600	Rettich et al. (1981)	M	
	1.4×10^{-5}	1600	Cosgrove and Walkley (1981)	M	11
	1.3×10^{-5}	1700	Shoor et al. (1969)	M	225
	1.5×10^{-5}		McAuliffe (1966)	M	226
	1.4×10^{-5}	1600	Wetlaufer et al. (1964)	M	
	1.5×10^{-5}		McAuliffe (1963)	M	227
	1.3×10^{-5}	1600	Morrison and Billett (1952)	M	228
	1.3×10^{-5}	1700	Winkler (1901)	M	229
	1.5×10^{-5}		Duchowicz et al. (2020)	V	187
	1.5×10^{-5}		HSDB (2015)	V	
	1.5×10^{-5}		Meylan and Howard (1991)	V	
	1.5×10^{-5}		Hine and Mookerjee (1975)	V	
	1.3×10^{-5}	1600	Wauchope and Haque (1972)	V	
	9.2×10^{-5}		Butler and Ramchandani (1935)	V	
	1.4×10^{-5}		Hine and Weimar (1965)	R	
	1.4×10^{-5}		Pierotti (1965)	T	
	9.6×10^{-6}		Liss and Slater (1974)	C	
	1.3×10^{-5}		Deno and Berkheimer (1960)	C	
	1.1×10^{-5}		Hayer et al. (2022)	Q	20
	3.4×10^{-3}		Duchowicz et al. (2020)	Q	

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.0×10^{-7}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-5}		Hilal et al. (2008)	Q	
		2300	Kühne et al. (2005)	Q	
	3.0×10^{-5}		Yao et al. (2002)	Q	230
	3.0×10^{-5}		English and Carroll (2001)	Q	231, 232
	8.6×10^{-6}		Katritzky et al. (1998)	Q	
	1.6×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	2.1×10^{-5}		Suzuki et al. (1992)	Q	233
	2.4×10^{-5}		Meylan and Howard (1991)	Q	
		1700	Kühne et al. (2005)	?	
	1.6×10^{-5}		Yaws (1999)	?	21
	1.4×10^{-5}	1600	Yaws et al. (1999)	?	21
	1.2×10^{-5}		Abraham and Weathersby (1994)	?	21
	1.3×10^{-5}	1700	Dean and Lange (1999)	?	234, 23
	1.5×10^{-5}		Yaws and Yang (1992)	?	21
	1.4×10^{-5}		Abraham et al. (1990)	?	
ethane	1.9×10^{-5}	2400	Burkholder et al. (2019)	L	1
C_2H_6	1.9×10^{-5}	2400	Burkholder et al. (2015)	L	1
[74-84-0]	1.9×10^{-5}	2400	Sander et al. (2011)	L	1
OTMSDBZUPAUEDD-UHFFFAOYSA-N	1.9×10^{-5}	2400	Sander et al. (2006)	L	1
	1.9×10^{-5}	2400	Fernández-Prini et al. (2003)	L	3
	1.9×10^{-5}	2300	Plyasunov and Shock (2000)	L	
	1.9×10^{-5}	2300	Abraham and Matteoli (1988)	L	
	1.9×10^{-5}	2300	Hayduk (1982)	L	1
	2.0×10^{-5}		Mackay and Shiu (1981)	L	
	1.8×10^{-5}	2400	Wilhelm et al. (1977)	L	
	2.0×10^{-5}	2300	Reichl (1995)	M	235
	1.3×10^{-5}		Guitart et al. (1989)	M	14
	1.8×10^{-5}	2700	Ben-Naim and Battino (1985)	M	
	1.9×10^{-5}	2300	Rettich et al. (1981)	M	
	1.8×10^{-5}	2700	Cosgrove and Walkley (1981)	M	11
	2.0×10^{-5}		McAuliffe (1966)	M	226
	2.0×10^{-5}	2400	Wetlaufer et al. (1964)	M	
	2.0×10^{-5}		McAuliffe (1963)	M	227
	1.7×10^{-5}	2100	Morrison and Billett (1952)	M	236
	1.8×10^{-5}	2400	Winkler (1901)	M	237
	2.0×10^{-5}		Duchowicz et al. (2020)	V	187
	2.0×10^{-5}		HSDB (2015)	V	
	2.0×10^{-5}		Hine and Mookerjee (1975)	V	
	1.7×10^{-5}	2000	Wauchope and Haque (1972)	V	
	1.0×10^{-4}		Butler and Ramchandani (1935)	V	
	4.0×10^{-5}		Pierotti (1965)	T	
	2.0×10^{-5}		Yaws (2003)	X	238
	1.8×10^{-5}		Deno and Berkheimer (1960)	C	
	1.8×10^{-5}		Hayer et al. (2022)	Q	20

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.3×10^{-3}		Duchowicz et al. (2020)	Q	
	1.1×10^{-4}		Wang et al. (2017)	Q	81, 239
	1.1×10^{-5}		Wang et al. (2017)	Q	81, 240
	2.0×10^{-5}		Wang et al. (2017)	Q	81, 241
	2.0×10^{-5}		Li et al. (2014)	Q	242
	3.3×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	4.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
	2.0×10^{-5}		Hilal et al. (2008)	Q	
	7.8×10^{-6}		Modarresi et al. (2007)	Q	68
		2600	Kühne et al. (2005)	Q	
	4.6×10^{-6}		Modarresi et al. (2005)	Q	248
	2.1×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	2.1×10^{-5}		Yao et al. (2002)	Q	230
	1.8×10^{-5}		English and Carroll (2001)	Q	231, 232
	1.5×10^{-5}		Katritzky et al. (1998)	Q	
	2.4×10^{-5}		Suzuki et al. (1992)	Q	233
	2.2×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	1.1×10^{-5}		Irmann (1965)	Q	
		2500	Kühne et al. (2005)	?	
	2.0×10^{-5}		Yaws (1999)	?	21
	1.9×10^{-5}	2300	Yaws et al. (1999)	?	21
	1.5×10^{-5}		Abraham and Weathersby (1994)	?	21
	1.8×10^{-5}	2400	Dean and Lange (1999)	?	251, 23
	2.0×10^{-5}		Yaws and Yang (1992)	?	21
	1.9×10^{-5}		Abraham et al. (1990)	?	
propane	1.5×10^{-5}	2700	Burkholder et al. (2019)	L	1
C_3H_8	1.5×10^{-5}	2700	Burkholder et al. (2015)	L	1
[74-98-6]	1.5×10^{-5}	2700	Sander et al. (2011)	L	1
ATUOYWHBWRKTHZ-UHFFFAOYSA-N	1.5×10^{-5}	2700	Sander et al. (2006)	L	1
	1.5×10^{-5}	2800	Plyasunov and Shock (2000)	L	
	1.5×10^{-5}	2800	Abraham and Matteoli (1988)	L	
	1.5×10^{-5}	2700	Hayduk (1986)	L	1
	1.4×10^{-5}		Mackay and Shiu (1981)	L	
	1.5×10^{-5}	2700	Wilhelm et al. (1977)	L	
	1.6×10^{-5}	2700	Chapoy et al. (2004)	M	1
	1.5×10^{-5}	2700	Reichl (1995)	M	252
	9.7×10^{-6}		Guitart et al. (1989)	M	14
	1.4×10^{-5}	3000	Ben-Naim and Battino (1985)	M	
	1.4×10^{-5}		McAuliffe (1966)	M	226
	1.6×10^{-5}	2700	Wetlaufer et al. (1964)	M	
	1.4×10^{-5}		McAuliffe (1963)	M	227
	1.5×10^{-5}	2600	Morrison and Billett (1952)	M	253

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.4×10^{-5}		Duchowicz et al. (2020)	V	187
	1.4×10^{-5}		HSDB (2015)	V	
	1.4×10^{-5}		Hine and Mookerjee (1975)	V	
	1.5×10^{-5}	2600	Wauchope and Haque (1972)	V	
	1.5×10^{-5}	2700	Wauchope and Haque (1972)	V	
	1.3×10^{-5}		Irmann (1965)	V	
	1.4×10^{-5}		Yaws (2003)	X	238
	1.4×10^{-5}		Deno and Berkheimer (1960)	C	
	1.7×10^{-5}		Hayer et al. (2022)	Q	20
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	8.7×10^{-5}		Wang et al. (2017)	Q	81, 239
	9.3×10^{-6}		Wang et al. (2017)	Q	81, 240
	1.9×10^{-5}		Wang et al. (2017)	Q	81, 241
	4.1×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	2.4×10^{-5}		Gharagheizi et al. (2010)	Q	247
	1.4×10^{-5}		Hilal et al. (2008)	Q	
	7.2×10^{-6}		Modarresi et al. (2007)	Q	68
		2900	Kühne et al. (2005)	Q	
	3.7×10^{-6}		Modarresi et al. (2005)	Q	248
	1.4×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	2.0×10^{-5}		Yao et al. (2002)	Q	230
	1.4×10^{-5}		English and Carroll (2001)	Q	231, 232
	1.5×10^{-5}		Katritzky et al. (1998)	Q	
	1.7×10^{-5}		Suzuki et al. (1992)	Q	233
	1.6×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	1.3×10^{-5}		Irmann (1965)	Q	
		2800	Kühne et al. (2005)	?	
	1.4×10^{-5}		Yaws (1999)	?	21
	1.5×10^{-5}	4500	Yaws et al. (1999)	?	21
	1.4×10^{-5}		Yaws and Yang (1992)	?	21
	1.5×10^{-5}		Abraham et al. (1990)	?	
butane	1.2×10^{-5}	3100	Burkholder et al. (2019)	L	254, 1
C_4H_{10}	1.2×10^{-5}	3100	Burkholder et al. (2015)	L	255, 1
[106-97-8]	1.2×10^{-5}	3100	Sander et al. (2011)	L	256, 1
IJDNQMDRQITEOD-UHFFFAOYSA-N	1.2×10^{-5}	3100	Sander et al. (2006)	L	257, 1
	1.2×10^{-5}	3100	Plyasunov and Shock (2000)	L	
	1.3×10^{-5}	3100	Abraham and Matteoli (1988)	L	
	1.2×10^{-5}	3000	Hayduk (1986)	L	1
	1.0×10^{-5}		Mackay and Shiu (1981)	L	
	1.2×10^{-5}	3100	Wilhelm et al. (1977)	L	
	1.3×10^{-5}	2300	Carroll et al. (1997)	M	1
	8.0×10^{-6}		Guitart et al. (1989)	M	14

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-5}	3200	Ben-Naim and Battino (1985)	M	
	1.1×10^{-5}		McAuliffe (1966)	M	226
	1.3×10^{-5}	3200	Wetlaufer et al. (1964)	M	
	1.1×10^{-5}		McAuliffe (1963)	M	227
	1.1×10^{-5}	2900	Morrison and Billett (1952)	M	258
	1.0×10^{-5}		Duchowicz et al. (2020)	V	187
	1.0×10^{-5}		HSDB (2015)	V	
	1.0×10^{-5}		Mackay et al. (2006a)	V	
	1.0×10^{-5}		Mackay et al. (1993)	V	
	9.6×10^{-6}		Hwang et al. (1992)	V	
	1.1×10^{-5}		Hine and Mookerjee (1975)	V	
	1.1×10^{-5}	2900	Wauchope and Haque (1972)	V	
	1.2×10^{-5}	3100	Wauchope and Haque (1972)	V	
	1.2×10^{-5}		Irmann (1965)	V	
	4.8×10^{-5}		Butler and Ramchandani (1935)	V	
	1.1×10^{-5}		Yaws (2003)	X	259
	1.1×10^{-5}		Yaws (2003)	X	238
	1.1×10^{-5}		Deno and Berkheimer (1960)	C	
	1.6×10^{-5}		Dupeux et al. (2022)	Q	260
	1.6×10^{-5}		Hayer et al. (2022)	Q	20
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	7.8×10^{-5}		Wang et al. (2017)	Q	81, 239
	1.1×10^{-5}		Wang et al. (2017)	Q	81, 240
	1.8×10^{-5}		Wang et al. (2017)	Q	81, 241
	1.1×10^{-5}		Li et al. (2014)	Q	242
	4.6×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	247
	1.2×10^{-5}		Hilal et al. (2008)	Q	
		3300	Kühne et al. (2005)	Q	
	3.5×10^{-6}		Modarresi et al. (2005)	Q	248
	1.1×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	1.6×10^{-5}		Yao et al. (2002)	Q	230
	1.0×10^{-5}		English and Carroll (2001)	Q	231, 261
	1.5×10^{-5}		Katritzky et al. (1998)	Q	
	1.3×10^{-5}		Suzuki et al. (1992)	Q	233
	1.2×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	1.2×10^{-5}		Irmann (1965)	Q	
		3300	Kühne et al. (2005)	?	
	1.1×10^{-5}		Yaws (1999)	?	21
	1.2×10^{-5}	3000	Yaws et al. (1999)	?	21
	1.1×10^{-5}		Yaws and Yang (1992)	?	21
	1.2×10^{-5}		Abraham et al. (1990)	?	

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methylpropane	9.1×10^{-6}	2700	Burkholder et al. (2019)	L	262, 1
$HC(CH_3)_3$	9.1×10^{-6}	2700	Burkholder et al. (2015)	L	263, 1
(isobutane)	9.1×10^{-6}	2700	Sander et al. (2011)	L	264, 1
[75-28-5]	9.1×10^{-6}	2700	Sander et al. (2006)	L	265, 1
NNPPMTNAJDCUHE-UHFFFAOYSA-N			Fogg and Sangster (2003)	L	266
	9.2×10^{-6}	2900	Plyasunov and Shock (2000)	L	
	9.1×10^{-6}	2700	Hayduk (1986)	L	267, 1
	8.3×10^{-6}		Mackay and Shiu (1981)	L	
	8.0×10^{-6}	2700	Wilhelm et al. (1977)	L	
	1.1×10^{-4}	5100	Mohebbi et al. (2012)	M	
	8.5×10^{-6}		McAuliffe (1966)	M	226
	9.9×10^{-6}	2700	Wetlaufer et al. (1964)	M	
	8.5×10^{-6}		McAuliffe (1963)	M	227
	8.3×10^{-6}		Duchowicz et al. (2020)	V	187
	8.3×10^{-6}		HSDB (2015)	V	
	8.3×10^{-6}		Mackay et al. (2006a)	V	
	8.3×10^{-6}		Mackay et al. (1993)	V	
	8.4×10^{-6}		Hine and Mookerjee (1975)	V	
	9.7×10^{-6}		Irmann (1965)	V	
	8.5×10^{-6}		Yaws (2003)	X	238
	1.3×10^{-5}		Hayer et al. (2022)	Q	20
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	8.3×10^{-5}		Wang et al. (2017)	Q	81, 239
	5.3×10^{-6}		Wang et al. (2017)	Q	81, 240
	2.0×10^{-5}		Wang et al. (2017)	Q	81, 241
	3.1×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
	5.6×10^{-6}		Hilal et al. (2008)	Q	
	5.8×10^{-6}		Modarresi et al. (2007)	Q	68
		3300	Kühne et al. (2005)	Q	
	3.7×10^{-6}		Modarresi et al. (2005)	Q	248
	8.4×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	8.4×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	9.8×10^{-6}		Yao et al. (2002)	Q	230, 268
	1.0×10^{-5}		English and Carroll (2001)	Q	231, 232
	1.5×10^{-5}		Katritzky et al. (1998)	Q	
	1.1×10^{-5}		Suzuki et al. (1992)	Q	233
	1.0×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	1.1×10^{-5}		Irmann (1965)	Q	
		2900	Kühne et al. (2005)	?	
	8.6×10^{-6}		Yaws (1999)	?	21
	9.1×10^{-6}	2700	Yaws et al. (1999)	?	21
	8.5×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.0×10^{-6}		Abraham et al. (1990)	?	
	7.9×10^{-6}		Abraham (1979)	?	
pentane	7.2×10^{-6}	3900	Brockbank (2013)	L	1, 269
C_5H_{12}	8.7×10^{-6}	3500	Plyasunov and Shock (2000)	L	
[109-66-0]	8.0×10^{-6}	3400	Abraham and Matteoli (1988)	L	
OFBQJSOFQDEBGM-UHFFFAOYSA-N	8.0×10^{-6}		Mackay and Shiu (1981)	L	
	8.7×10^{-6}	3400	Jou and Mather (2000)	M	270, 271
	8.2×10^{-6}	3600	Jönsson et al. (1982)	M	
	7.8×10^{-6}		Rytting et al. (1978)	M	
	7.8×10^{-6}		Mackay et al. (2006a)	V	
	7.8×10^{-6}		Mackay et al. (1993)	V	
	8.3×10^{-6}		Eastcott et al. (1988)	V	
	7.8×10^{-6}		Amoore and Buttery (1978)	V	
	7.9×10^{-6}		Hine and Mookerjee (1975)	V	
	8.3×10^{-6}		McAuliffe (1966)	V	226
	8.3×10^{-6}		McAuliffe (1963)	V	227
		3000	Gill et al. (1976)	T	
	7.8×10^{-6}		Yaws (2003)	X	259
	7.8×10^{-6}		Yaws (2003)	X	238
	1.3×10^{-5}		Dupeux et al. (2022)	Q	260
	4.9×10^{-5}		Keshavarz et al. (2022)	Q	
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	185
	6.5×10^{-5}		Wang et al. (2017)	Q	81, 239
	9.3×10^{-6}		Wang et al. (2017)	Q	81, 240
	1.7×10^{-5}		Wang et al. (2017)	Q	81, 241
	4.7×10^{-6}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	8.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
	9.9×10^{-6}		Hilal et al. (2008)	Q	
	6.6×10^{-6}		Modarresi et al. (2007)	Q	68
		3600	Kühne et al. (2005)	Q	
	3.1×10^{-6}		Modarresi et al. (2005)	Q	248
	8.4×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	1.5×10^{-5}		Yao et al. (2002)	Q	230
	8.0×10^{-6}		English and Carroll (2001)	Q	231, 232
	1.5×10^{-5}		Katritzky et al. (1998)	Q	
	1.0×10^{-5}		Suzuki et al. (1992)	Q	233
	9.9×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
	7.9×10^{-6}		Duchowicz et al. (2020)	?	186, 21
		4200	Kühne et al. (2005)	?	
	7.8×10^{-6}		Yaws (1999)	?	21
	5.1×10^{-6}		Abraham and Weathersby (1994)	?	21
	7.8×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.0×10^{-6}		Abraham et al. (1990)	?	
2-methylbutane	7.7×10^{-6}	3000	Plyasunov and Shock (2000)	L	
C_5H_{12}	7.2×10^{-6}		Mackay and Shiu (1981)	L	
(isopentane)	7.0×10^{-6}		Duchowicz et al. (2020)	V	187
[78-78-4]	7.0×10^{-6}		HSDB (2015)	V	
QWTDNUCVQCZILF-UHFFFAOYSA-N	7.2×10^{-6}		Mackay et al. (2006a)	V	
	2.1×10^{-6}		Mackay et al. (1993)	V	
	7.2×10^{-6}		Eastcott et al. (1988)	V	
	7.2×10^{-6}		Cabani et al. (1981)	V	
	7.6×10^{-6}		McAuliffe (1966)	V	226
	7.6×10^{-6}		McAuliffe (1963)	V	227
	7.2×10^{-6}		Yaws (2003)	X	238
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	7.3×10^{-5}		Wang et al. (2017)	Q	81, 239
	6.0×10^{-6}		Wang et al. (2017)	Q	81, 240
	2.0×10^{-5}		Wang et al. (2017)	Q	81, 241
	3.8×10^{-6}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	272, 244
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	8.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
	6.4×10^{-6}		Hilal et al. (2008)	Q	
	7.2×10^{-6}		Modarresi et al. (2007)	Q	68
	3.8×10^{-6}		Modarresi et al. (2005)	Q	248
	5.8×10^{-6}		Yaffe et al. (2003)	Q	249, 273
	8.4×10^{-6}		Yao et al. (2002)	Q	230
	7.9×10^{-6}		English and Carroll (2001)	Q	231, 232
	1.5×10^{-5}		Katritzky et al. (1998)	Q	
	8.4×10^{-6}		Nirmalakhandan et al. (1997)	Q	
	7.2×10^{-6}		Yaws (1999)	?	21
	7.2×10^{-6}		Yaws and Yang (1992)	?	21
dimethylpropane	6.0×10^{-6}	3000	Plyasunov and Shock (2000)	L	
$C(CH_3)_4$	2.7×10^{-6}		Mackay and Shiu (1981)	L	
(neopentane)	5.9×10^{-6}	3300	Wilhelm et al. (1977)	L	
[463-82-1]	5.5×10^{-6}	2800	Shoor et al. (1969)	M	274
CRSOQBOWXPBRES-UHFFFAOYSA-N	4.7×10^{-6}		McAuliffe (1966)	M	
	6.3×10^{-6}	3200	Wetlaufer et al. (1964)	M	
	2.7×10^{-6}		Duchowicz et al. (2020)	V	187
	2.7×10^{-6}		HSDB (2015)	V	
	4.5×10^{-6}		Mackay et al. (2006a)	V	
	4.5×10^{-6}		Mackay et al. (1993)	V	
	4.5×10^{-6}		Hine and Mookerjee (1975)	V	
	4.7×10^{-6}		Yaws (2003)	X	238
	7.5×10^{-5}		Duchowicz et al. (2020)	Q	
	4.5×10^{-5}		Wang et al. (2017)	Q	81, 239

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.1×10^{-6}		Wang et al. (2017)	Q	81, 240
	2.5×10^{-5}		Wang et al. (2017)	Q	81, 241
	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	8.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
	2.5×10^{-6}		Hilal et al. (2008)	Q	
	5.3×10^{-6}		Modarresi et al. (2007)	Q	68
		3600	Kühne et al. (2005)	Q	
	3.6×10^{-6}		Modarresi et al. (2005)	Q	248
	4.6×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	3.8×10^{-6}		Yao et al. (2002)	Q	230, 268
	8.0×10^{-6}		English and Carroll (2001)	Q	231, 275
	1.4×10^{-5}		Katritzky et al. (1998)	Q	
	7.3×10^{-6}		Suzuki et al. (1992)	Q	233
	6.2×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
		3100	Kühne et al. (2005)	?	
	4.7×10^{-6}		Yaws (1999)	?	21
	4.7×10^{-6}		Yaws and Yang (1992)	?	21
	5.8×10^{-6}		Abraham et al. (1990)	?	
	5.9×10^{-6}		Abraham (1979)	?	
hexane	5.7×10^{-6}	4400	Brockbank (2013)	L	1, 276
C_6H_{14}	6.9×10^{-6}	3800	Plyasunov and Shock (2000)	L	
[110-54-3]	6.1×10^{-6}	3800	Abraham and Matteoli (1988)	L	
VLKZOEOYAKHREP-UHFFFAOYSA-N	5.9×10^{-6}		Mackay and Shiu (1981)	L	
	6.1×10^{-6}		Ryu and Park (1999)	M	
	7.4×10^{-6}		Park et al. (1997)	M	277
	2.4×10^{-4}	8700	Kolb et al. (1992)	M	278
	6.7×10^{-6}		Guitart et al. (1989)	M	14
	9.9×10^{-6}	7500	Ashworth et al. (1988)	M	279
	6.7×10^{-6}	4200	Tsonopoulos and Wilson (1983)	M	1
	5.9×10^{-6}	4000	Jönsson et al. (1982)	M	
	5.4×10^{-6}		Rytting et al. (1978)	M	
	5.5×10^{-6}		Duchowicz et al. (2020)	V	187
	5.5×10^{-6}		HSDB (2015)	V	
	5.5×10^{-6}		Mackay et al. (2006a)	V	
	5.5×10^{-6}		Mackay et al. (1993)	V	
	5.5×10^{-6}		Hwang et al. (1992)	V	
	7.1×10^{-6}		Eastcott et al. (1988)	V	
	6.1×10^{-6}		Cabani et al. (1981)	V	
	5.4×10^{-6}		Hine and Mookerjee (1975)	V	
	5.9×10^{-6}		McAuliffe (1966)	V	226
	5.9×10^{-6}		McAuliffe (1963)	V	227
	6.7×10^{-6}	3800	Plyasunov et al. (2001)	T	

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		3800	Gill et al. (1976)	T	
	7.6×10^{-6}		Yaws (2003)	X	259
	7.6×10^{-6}		Yaws (2003)	X	238
	1.0×10^{-5}		Dupeux et al. (2022)	Q	260
	5.7×10^{-6}		Hayer et al. (2022)	Q	20
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	5.0×10^{-5}		Wang et al. (2017)	Q	81, 239
	6.9×10^{-6}		Wang et al. (2017)	Q	81, 240
	1.6×10^{-5}		Wang et al. (2017)	Q	81, 241
	2.3×10^{-5}		Li et al. (2014)	Q	242
	4.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	5.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
	7.7×10^{-6}		Hilal et al. (2008)	Q	
	5.2×10^{-6}		Modarresi et al. (2007)	Q	68
		4000	Kühne et al. (2005)	Q	
	2.9×10^{-6}		Modarresi et al. (2005)	Q	248
	5.8×10^{-6}		Yaffe et al. (2003)	Q	249, 273
	6.0×10^{-6}		Yao et al. (2002)	Q	230
	6.2×10^{-6}		English and Carroll (2001)	Q	231, 232
	1.4×10^{-5}		Katritzky et al. (1998)	Q	
	1.4×10^{-5}		Russell et al. (1992)	Q	280
	7.9×10^{-6}		Suzuki et al. (1992)	Q	233
	7.9×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
		4100	Kühne et al. (2005)	?	
	7.6×10^{-6}		Yaws (1999)	?	21
	3.4×10^{-6}		Abraham and Weathersby (1994)	?	21
	7.6×10^{-6}		Yaws and Yang (1992)	?	21
	6.1×10^{-6}		Abraham et al. (1990)	?	
2-methylpentane	6.4×10^{-6}	4500	Brockbank (2013)	L	1
C_6H_{14}	5.7×10^{-6}	3900	Plyasunov and Shock (2000)	L	
(isohexane)	5.9×10^{-6}		Mackay and Shiu (1981)	L	
[107-83-5]	1.3×10^{-5}	960	Ashworth et al. (1988)	M	42, 279
AFABGHUZZDYHJO-UHFFFAOYSA-N	5.8×10^{-6}		Duchowicz et al. (2020)	V	187
	5.8×10^{-6}		HSDB (2015)	V	
	5.7×10^{-6}		Mackay et al. (2006a)	V	
	5.7×10^{-6}		Mackay et al. (1993)	V	
	5.7×10^{-6}		Eastcott et al. (1988)	V	
	5.7×10^{-6}		Hine and Mookerjee (1975)	V	
	6.0×10^{-6}		McAuliffe (1966)	V	226
	6.0×10^{-6}		McAuliffe (1963)	V	227
			Staudinger and Roberts (1996)	R	281
	5.7×10^{-6}		Yaws (2003)	X	238

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.2×10^{-6}		Hilal et al. (2008)	C	
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	6.0×10^{-5}		Wang et al. (2017)	Q	81, 239
	4.5×10^{-6}		Wang et al. (2017)	Q	81, 240
	1.9×10^{-5}		Wang et al. (2017)	Q	81, 241
	3.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	5.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
	4.8×10^{-6}		Hilal et al. (2008)	Q	
	5.9×10^{-6}		Modarresi et al. (2007)	Q	68
		4000	Kühne et al. (2005)	Q	
	3.9×10^{-6}		Modarresi et al. (2005)	Q	248
	5.8×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	8.0×10^{-6}		Yao et al. (2002)	Q	230
	6.1×10^{-6}		English and Carroll (2001)	Q	231, 232
	1.4×10^{-5}		Katritzky et al. (1998)	Q	
	7.0×10^{-6}		Suzuki et al. (1992)	Q	233
	6.7×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
		4000	Kühne et al. (2005)	?	
	5.7×10^{-6}		Yaws (1999)	?	21
	3.6×10^{-6}		Abraham and Weathersby (1994)	?	21
	5.7×10^{-6}		Yaws and Yang (1992)	?	21
3-methylpentane C_6H_{14} [96-14-0] PFEOZHBOMNWTJB-UHFFFAOYSA-N	5.9×10^{-6}		Brockbank (2013)	L	
	5.9×10^{-6}		Plyasunov and Shock (2000)	L	
	5.8×10^{-6}		Mackay and Shiu (1981)	L	
	5.9×10^{-6}		Duchowicz et al. (2020)	V	187
	5.8×10^{-6}		HSDB (2015)	V	
	5.9×10^{-6}		Mackay et al. (2006a)	V	
	5.9×10^{-6}		Mackay et al. (1993)	V	
	5.9×10^{-6}		Eastcott et al. (1988)	V	
	5.8×10^{-6}		Hine and Mookerjee (1975)	V	
	6.0×10^{-6}		McAuliffe (1966)	V	
	8.2×10^{-6}		Yaws (2003)	X	238
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	6.0×10^{-5}		Wang et al. (2017)	Q	81, 239
	5.8×10^{-6}		Wang et al. (2017)	Q	81, 240
	1.9×10^{-5}		Wang et al. (2017)	Q	81, 241
	4.1×10^{-6}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	272, 244
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	5.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
	6.2×10^{-6}		Hilal et al. (2008)	Q	

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.0×10^{-6}		Modarresi et al. (2007)	Q	68
		4000	Kühne et al. (2005)	Q	
	3.1×10^{-6}		Modarresi et al. (2005)	Q	248
	5.8×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	6.7×10^{-6}		Yao et al. (2002)	Q	230
	6.1×10^{-6}		English and Carroll (2001)	Q	231, 261
	1.4×10^{-5}		Katritzky et al. (1998)	Q	
	7.2×10^{-6}		Suzuki et al. (1992)	Q	233
	7.0×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
		4700	Kühne et al. (2005)	?	
	8.2×10^{-6}		Yaws (1999)	?	21
	3.7×10^{-6}		Abraham and Weathersby (1994)	?	21
	8.8×10^{-6}		Yaws and Yang (1992)	?	21
2,2-dimethylbutane	5.7×10^{-6}		Brockbank (2013)	L	
C_6H_{14}	5.6×10^{-6}	3500	Plyasunov and Shock (2000)	L	
[75-83-2]	5.8×10^{-6}		Mackay and Shiu (1981)	L	
HNRMPXKDFBEGFZ-UHFFFAOYSA-N	6.5×10^{-6}		Duchowicz et al. (2020)	V	187
	5.8×10^{-6}		HSDB (2015)	V	
	5.0×10^{-6}		Mackay et al. (2006a)	V	
	5.0×10^{-6}		Mackay et al. (1993)	V	
	5.8×10^{-6}		Eastcott et al. (1988)	V	
	5.1×10^{-6}		Hine and Mookerjee (1975)	V	
	5.5×10^{-6}		McAuliffe (1966)	V	226
	5.5×10^{-6}		McAuliffe (1963)	V	227
	6.5×10^{-6}		Yaws (2003)	X	238
	7.5×10^{-5}		Duchowicz et al. (2020)	Q	
	4.0×10^{-5}		Wang et al. (2017)	Q	81, 239
	2.8×10^{-6}		Wang et al. (2017)	Q	81, 240
	2.5×10^{-5}		Wang et al. (2017)	Q	81, 241
	2.7×10^{-6}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	272, 244
	3.1×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	4.9×10^{-6}		Gharagheizi et al. (2010)	Q	247
	3.4×10^{-6}		Hilal et al. (2008)	Q	
	7.2×10^{-6}		Modarresi et al. (2007)	Q	68
	3.9×10^{-6}		Modarresi et al. (2005)	Q	248
	5.3×10^{-6}		Yaffe et al. (2003)	Q	249, 273
	3.4×10^{-6}		Yao et al. (2002)	Q	230
	6.2×10^{-6}		English and Carroll (2001)	Q	231, 232
	1.3×10^{-5}		Katritzky et al. (1998)	Q	
	6.0×10^{-6}		Suzuki et al. (1992)	Q	233
	5.3×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
	6.5×10^{-6}		Yaws (1999)	?	21
	3.4×10^{-6}		Abraham and Weathersby (1994)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.5×10^{-6}		Yaws and Yang (1992)	?	21
2,3-dimethylbutane	8.0×10^{-6}	4400	Brockbank (2013)	L	1
C_6H_{14}	7.6×10^{-6}		Plyasunov and Shock (2000)	L	
[79-29-8]	7.7×10^{-6}		Mackay and Shiu (1981)	L	
ZFFMLCVRJBZUDZ-UHFFFAOYSA-N	8.4×10^{-6}		Duchowicz et al. (2020)	V	187
	8.2×10^{-6}		HSDB (2015)	V	
	6.9×10^{-6}		Mackay et al. (2006a)	V	
	6.9×10^{-6}		Mackay et al. (1993)	V	
	7.1×10^{-6}		Eastcott et al. (1988)	V	
	7.6×10^{-6}		Yaws (2003)	X	238
	6.7×10^{-5}		Duchowicz et al. (2020)	Q	
	6.8×10^{-5}		Wang et al. (2017)	Q	81, 239
	4.9×10^{-6}		Wang et al. (2017)	Q	81, 240
	2.2×10^{-5}		Wang et al. (2017)	Q	81, 241
	3.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	5.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
	5.3×10^{-6}		Hilal et al. (2008)	Q	
	7.6×10^{-6}		Modarresi et al. (2007)	Q	68
		4000	Kühne et al. (2005)	Q	
	5.2×10^{-6}		Modarresi et al. (2005)	Q	248
	7.7×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	4.2×10^{-6}		Yao et al. (2002)	Q	230
	6.1×10^{-6}		English and Carroll (2001)	Q	231, 275
	1.3×10^{-5}		Katritzky et al. (1998)	Q	
	5.8×10^{-6}		Nirmalakhandan et al. (1997)	Q	
		4200	Kühne et al. (2005)	?	
	7.6×10^{-6}		Yaws (1999)	?	21
	7.6×10^{-6}		Yaws and Yang (1992)	?	21
heptane	4.4×10^{-6}	4500	Brockbank (2013)	L	1
C_7H_{16}	4.9×10^{-6}	4200	Plyasunov and Shock (2000)	L	
[142-82-5]	4.4×10^{-6}	4100	Abraham and Matteoli (1988)	L	
IMNFDUFMRHMDMM-UHFFFAOYSA-N	4.3×10^{-6}		Mackay and Shiu (1981)	L	
	4.5×10^{-6}		Ryu and Park (1999)	M	
	5.5×10^{-6}		Park et al. (1997)	M	277
	1.2×10^{-5}	3700	Hansen et al. (1993)	M	282
	6.0×10^{-6}		Guitart et al. (1989)	M	14
	4.2×10^{-6}	4700	Jönsson et al. (1982)	M	
	4.8×10^{-6}		Rytting et al. (1978)	M	
	4.9×10^{-6}		Duchowicz et al. (2020)	V	187
	5.5×10^{-6}		HSDB (2015)	V	
	4.8×10^{-6}		Mackay et al. (2006a)	V	
	4.8×10^{-6}		Mackay et al. (1993)	V	

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.0×10^{-6}		Eastcott et al. (1988)	V	
	4.8×10^{-6}		Hine and Mookerjee (1975)	V	
	5.2×10^{-6}		McAuliffe (1966)	V	226
	5.2×10^{-6}		McAuliffe (1963)	V	227
	3.7×10^{-6}		Yaws (2003)	X	259
	3.7×10^{-6}		Yaws (2003)	X	238
	8.2×10^{-6}		Dupeux et al. (2022)	Q	260
	1.1×10^{-5}		Hayer et al. (2022)	Q	20
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	4.7×10^{-5}		Wang et al. (2017)	Q	81, 239
	4.9×10^{-6}		Wang et al. (2017)	Q	81, 240
	8.0×10^{-6}		Wang et al. (2017)	Q	81, 241
	4.1×10^{-6}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-6}		Raventos-Duran et al. (2010)	Q	272, 244
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	3.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
	5.4×10^{-6}		Hilal et al. (2008)	Q	
	5.3×10^{-6}		Modarresi et al. (2007)	Q	68
		4300	Kühne et al. (2005)	Q	
	2.4×10^{-6}		Modarresi et al. (2005)	Q	248
	4.1×10^{-6}		Yaffe et al. (2003)	Q	249, 273
	5.1×10^{-6}		Yao et al. (2002)	Q	230
	1.3×10^{-5}		Katritzky et al. (1998)	Q	
	6.5×10^{-6}		Russell et al. (1992)	Q	280
	6.0×10^{-6}		Suzuki et al. (1992)	Q	233
	6.2×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
		4900	Kühne et al. (2005)	?	
	3.7×10^{-6}		Yaws (1999)	?	21
	2.8×10^{-6}		Abraham and Weathersby (1994)	?	21
	3.6×10^{-6}		Yaws and Yang (1992)	?	21
	4.4×10^{-6}		Abraham et al. (1990)	?	
2-methylhexane	2.9×10^{-6}		Brockbank (2013)	L	
C_7H_{16}	2.9×10^{-6}		Plyasunov and Shock (2000)	L	
(isoheptane)	2.9×10^{-6}		Mackay and Shiu (1981)	L	
[591-76-4]	1.9×10^{-5}	-3600	Hansen et al. (1993)	M	282, 283
GXDHCNNESPLIKD-UHFFFAOYSA-N	2.9×10^{-6}		Duchowicz et al. (2020)	V	187
	2.9×10^{-6}		Mackay et al. (2006a)	V	
	2.9×10^{-6}		Mackay et al. (1993)	V	
	2.9×10^{-6}		Eastcott et al. (1988)	V	
	2.9×10^{-6}		Yaws (2003)	X	238
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	4.7×10^{-5}		Wang et al. (2017)	Q	81, 239
	3.2×10^{-6}		Wang et al. (2017)	Q	81, 240
	1.7×10^{-5}		Wang et al. (2017)	Q	81, 241

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.2×10^{-6}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-6}		Raventos-Duran et al. (2010)	Q	272, 244
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	3.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
	3.7×10^{-6}		Hilal et al. (2008)	Q	
	5.2×10^{-6}		Modarresi et al. (2007)	Q	68
	2.8×10^{-6}		Modarresi et al. (2005)	Q	248
	2.9×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	3.4×10^{-6}		Yao et al. (2002)	Q	230
	1.3×10^{-5}		Katritzky et al. (1998)	Q	
	5.2×10^{-6}		Nirmalakhandan et al. (1997)	Q	
	2.9×10^{-6}		Yaws (1999)	?	21
	2.9×10^{-6}		Yaws and Yang (1992)	?	21
3-methylhexane C_7H_{16} [589-34-4] VLJXXKKOSFGPHI-UHFFFAOYSA-N	3.2×10^{-6}		Brockbank (2013)	L	
	4.5×10^{-6}		Plyasunov and Shock (2000)	L	
	4.2×10^{-6}		Mackay and Shiu (1981)	L	
	6.0×10^{-6}		Duchowicz et al. (2020)	V	187
	4.0×10^{-6}		Mackay et al. (2006a)	V	
	4.0×10^{-6}		Mackay et al. (1993)	V	
	3.2×10^{-6}		Eastcott et al. (1988)	V	
	3.2×10^{-6}		Yaws (2003)	X	238
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	4.7×10^{-5}		Wang et al. (2017)	Q	81, 239
	3.8×10^{-6}		Wang et al. (2017)	Q	81, 240
	1.8×10^{-5}		Wang et al. (2017)	Q	81, 241
	3.6×10^{-6}		Gharagheizi et al. (2012)	Q	
	3.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
	4.5×10^{-6}		Hilal et al. (2008)	Q	
	6.1×10^{-6}		Modarresi et al. (2007)	Q	68
	2.7×10^{-6}		Modarresi et al. (2005)	Q	248
	4.1×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	3.4×10^{-6}		Yao et al. (2002)	Q	230
	4.6×10^{-6}		English and Carroll (2001)	Q	231, 232
	1.3×10^{-5}		Katritzky et al. (1998)	Q	
	5.3×10^{-6}		Nirmalakhandan et al. (1997)	Q	
	3.2×10^{-6}		Yaws (1999)	?	21
	2.5×10^{-6}		Abraham and Weathersby (1994)	?	21
	3.2×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2-dimethylpentane	3.1×10^{-6}		Plyasunov and Shock (2000)	L	
C_7H_{16}	3.1×10^{-6}		Mackay and Shiu (1981)	L	
[590-35-2]	3.1×10^{-6}		Duchowicz et al. (2020)	V	187
CXOWYJMDMMMMJO-UHFFFAOYSA-N	3.1×10^{-6}		Mackay et al. (2006a)	V	
	3.1×10^{-6}		Mackay et al. (1993)	V	
	3.1×10^{-6}		Eastcott et al. (1988)	V	
	3.1×10^{-6}		Yaws (2003)	X	238
	7.5×10^{-5}		Duchowicz et al. (2020)	Q	
	2.4×10^{-6}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-6}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	3.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
	2.5×10^{-6}		Hilal et al. (2008)	Q	
	5.2×10^{-6}		Modarresi et al. (2007)	Q	68
	3.1×10^{-6}		Modarresi et al. (2005)	Q	248
	3.1×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	3.7×10^{-6}		Yao et al. (2002)	Q	230
	3.6×10^{-6}		English and Carroll (2001)	Q	231, 232
	1.2×10^{-5}		Katritzky et al. (1998)	Q	
	4.1×10^{-6}		Nirmalakhandan et al. (1997)	Q	
	3.1×10^{-6}		Yaws (1999)	?	21
	3.1×10^{-6}		Yaws and Yang (1992)	?	21
2,3-dimethylpentane	5.7×10^{-6}		Plyasunov and Shock (2000)	L	
C_7H_{16}	5.7×10^{-6}		Mackay and Shiu (1981)	L	
[565-59-3]	5.7×10^{-6}		Duchowicz et al. (2020)	V	187
WGECXQBGLLYSFP-UHFFFAOYSA-N	5.7×10^{-6}		Mackay et al. (1993)	V	
	5.7×10^{-6}		Eastcott et al. (1988)	V	
	5.7×10^{-6}		Yaws (2003)	X	238
	6.7×10^{-5}		Duchowicz et al. (2020)	Q	
	3.6×10^{-6}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-6}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	3.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
	4.8×10^{-6}		Hilal et al. (2008)	Q	
	7.1×10^{-6}		Modarresi et al. (2007)	Q	68
	5.8×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	4.7×10^{-6}		English and Carroll (2001)	Q	231, 232
	1.2×10^{-5}		Katritzky et al. (1998)	Q	
	4.7×10^{-6}		Nirmalakhandan et al. (1997)	Q	
	5.7×10^{-6}		Yaws (1999)	?	21
	5.7×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4-dimethylpentane	2.9×10^{-6}		Brockbank (2013)	L	
C_7H_{16}	3.3×10^{-6}		Plyasunov and Shock (2000)	L	
[108-08-7]	3.3×10^{-6}		Mackay and Shiu (1981)	L	
BZHMBWZPUJHVEE-UHFFFAOYSA-N	5.2×10^{-6}		Duchowicz et al. (2020)	V	187
	3.1×10^{-6}		Mackay et al. (2006a)	V	
	3.1×10^{-6}		Mackay et al. (1993)	V	
	3.4×10^{-6}		Eastcott et al. (1988)	V	
	3.1×10^{-6}		Hine and Mookerjee (1975)	V	
	3.1×10^{-6}		McAuliffe (1966)	V	
	3.3×10^{-6}		Yaws (2003)	X	238
	6.7×10^{-5}		Duchowicz et al. (2020)	Q	
	2.4×10^{-6}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-6}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	3.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
	2.2×10^{-6}		Hilal et al. (2008)	Q	
	5.2×10^{-6}		Modarresi et al. (2007)	Q	68
	3.0×10^{-6}		Modarresi et al. (2005)	Q	248
	5.3×10^{-6}		Yaffe et al. (2003)	Q	249, 273
	4.0×10^{-6}		Yao et al. (2002)	Q	230
	4.7×10^{-6}		English and Carroll (2001)	Q	231, 275
	1.2×10^{-5}		Katritzky et al. (1998)	Q	
	4.7×10^{-6}		Suzuki et al. (1992)	Q	233
	4.5×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
	3.4×10^{-6}		Yaws (1999)	?	21
	3.3×10^{-6}		Yaws and Yang (1992)	?	21
3,3-dimethylpentane	5.6×10^{-6}	3000	Brockbank (2013)	L	1, 284
C_7H_{16}	5.3×10^{-6}		Plyasunov and Shock (2000)	L	
[562-49-2]	5.4×10^{-6}		Mackay and Shiu (1981)	L	
AEXMKKGTQYQZCS-UHFFFAOYSA-N	5.4×10^{-6}		Duchowicz et al. (2020)	V	187
	5.4×10^{-6}		Mackay et al. (2006a)	V	
	5.4×10^{-6}		Mackay et al. (1993)	V	
	5.4×10^{-6}		Eastcott et al. (1988)	V	
	5.4×10^{-6}		Yaws (2003)	X	238
	7.5×10^{-5}		Duchowicz et al. (2020)	Q	
	3.3×10^{-6}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
	4.0×10^{-6}		Hilal et al. (2008)	Q	
	7.5×10^{-6}		Modarresi et al. (2007)	Q	68
		4300	Kühne et al. (2005)	Q	
	3.5×10^{-6}		Modarresi et al. (2005)	Q	248
	5.3×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	2.8×10^{-6}		Yao et al. (2002)	Q	230
	3.6×10^{-6}		English and Carroll (2001)	Q	231, 232

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-5}		Katritzky et al. (1998)	Q	
	4.4×10^{-6}		Nirmalakhandan et al. (1997)	Q	
		3000	Kühne et al. (2005)	?	
	5.4×10^{-6}		Yaws (1999)	?	21
	5.3×10^{-6}		Yaws and Yang (1992)	?	21
3-ethylpentane	3.8×10^{-6}		Yaws (2003)	X	238
C_7H_{16}	3.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[617-78-7]	3.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
AORMDLNPRGXHHL-UHFFFAOYSA-N	5.3×10^{-6}		Hilal et al. (2008)	Q	
	2.5×10^{-6}		Modarresi et al. (2005)	Q	248
	4.8×10^{-6}		Yao et al. (2002)	Q	230, 268
	3.8×10^{-6}		Yaws (1999)	?	21
	3.9×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3-trimethylbutane	3.2×10^{-6}		Mackay et al. (2006a)	V	
C_7H_{16}	3.2×10^{-6}		Mackay et al. (1993)	V	
[464-06-2]	4.2×10^{-6}		Yaws (2003)	X	238
ZISSAWUMDACLOM-UHFFFAOYSA-N	2.8×10^{-6}		Gharagheizi et al. (2012)	Q	
	3.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
	3.3×10^{-6}		Hilal et al. (2008)	Q	
	7.2×10^{-6}		Modarresi et al. (2007)	Q	68
	3.1×10^{-6}		Modarresi et al. (2005)	Q	248
	3.1×10^{-6}		Yaffe et al. (2003)	Q	249, 273
	1.8×10^{-6}		Yao et al. (2002)	Q	230
	4.2×10^{-6}		Yaws (1999)	?	21
	4.1×10^{-6}		Yaws and Yang (1992)	?	21
octane	3.4×10^{-6}	5300	Brockbank (2013)	L	1
C_8H_{18}	4.0×10^{-6}	4600	Plyasunov and Shock (2000)	L	
[111-65-9]	3.1×10^{-6}	4300	Abraham and Matteoli (1988)	L	
TVMXDCGIABBOFY-UHFFFAOYSA-N	3.3×10^{-6}		Mackay and Shiu (1981)	L	
	3.4×10^{-6}		Ryu and Park (1999)	M	
	3.3×10^{-6}		Park et al. (1997)	M	277
	3.0×10^{-5}	8000	Hansen et al. (1993)	M	282
	3.1×10^{-6}	4100	Heidman et al. (1985)	M	1
	2.9×10^{-6}	5400	Jönsson et al. (1982)	M	
	3.1×10^{-6}		Rytting et al. (1978)	M	
	3.1×10^{-6}		Duchowicz et al. (2020)	V	187
	3.1×10^{-6}		HSDB (2015)	V	
	8.6×10^{-7}		Abraham and Acree (2007)	V	
	3.2×10^{-6}		Mackay et al. (2006a)	V	
	3.8×10^{-6}	4800	Sarraute et al. (2004)	V	
	3.2×10^{-6}		Mackay et al. (1993)	V	
	3.0×10^{-6}		Hwang et al. (1992)	V	
	3.1×10^{-6}		Meylan and Howard (1991)	V	
	3.2×10^{-6}		Eastcott et al. (1988)	V	

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.1×10^{-6}		Hine and Mookerjee (1975)	V	
	3.1×10^{-6}		Mackay and Leinonen (1975)	V	
	3.9×10^{-6}		McAuliffe (1966)	V	226
	3.9×10^{-6}		McAuliffe (1963)	V	227
	2.0×10^{-6}		Yaws (2003)	X	259
	2.0×10^{-6}		Yaws (2003)	X	238
	6.8×10^{-6}		Dupeux et al. (2022)	Q	260
	2.8×10^{-5}		Hayer et al. (2022)	Q	20
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	3.6×10^{-5}		Wang et al. (2017)	Q	81, 239
	3.4×10^{-6}		Wang et al. (2017)	Q	81, 240
	4.2×10^{-6}		Wang et al. (2017)	Q	81, 241
	3.1×10^{-6}		Li et al. (2014)	Q	242
	3.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	2.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
	3.9×10^{-6}		Hilal et al. (2008)	Q	
	4.6×10^{-6}		Modarresi et al. (2007)	Q	68
		4700	Kühne et al. (2005)	Q	
	2.9×10^{-6}		Yaffe et al. (2003)	Q	249, 273
	3.7×10^{-6}		English and Carroll (2001)	Q	231, 232
	1.2×10^{-5}		Katritzky et al. (1998)	Q	
	2.6×10^{-6}		Russell et al. (1992)	Q	280
	4.6×10^{-6}		Suzuki et al. (1992)	Q	233
	3.3×10^{-6}		Meylan and Howard (1991)	Q	
	5.0×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
		5400	Kühne et al. (2005)	?	
	2.0×10^{-6}		Yaws (1999)	?	21
	2.0×10^{-6}		Abraham and Weathersby (1994)	?	21
	2.0×10^{-6}		Yaws and Yang (1992)	?	21
	3.1×10^{-6}		Abraham et al. (1990)	?	
2-methylheptane C_8H_{18} [592-27-8] JVSWJIKNEAIKJW-UHFFFAOYSA-N	2.9×10^{-6}		Mackay et al. (2006a)	V	
	2.9×10^{-6}		Mackay et al. (1993)	V	
	2.4×10^{-6}		Yaws (2003)	X	238
	2.8×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
	2.7×10^{-6}		Hilal et al. (2008)	Q	
	2.1×10^{-6}		Modarresi et al. (2005)	Q	248
	3.1×10^{-6}		Yao et al. (2002)	Q	230, 268
	2.4×10^{-6}		Yaws (1999)	?	21
	2.7×10^{-6}		Hoff et al. (1993)	?	21
	2.7×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methylheptane	2.6×10^{-6}		Brockbank (2013)	L	
C_8H_{18}	2.7×10^{-6}		Plyasunov and Shock (2000)	L	
[589-81-1]	2.7×10^{-6}		Mackay and Shiu (1981)	L	
LAIUFBWHERIJIH-UHFFFAOYSA-N	2.7×10^{-6}		Duchowicz et al. (2020)	V	187
	2.7×10^{-6}		Eastcott et al. (1988)	V	
	2.6×10^{-6}		Yaws (2003)	X	238
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	3.0×10^{-6}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
	3.3×10^{-6}		Hilal et al. (2008)	Q	
	5.5×10^{-6}		Modarresi et al. (2007)	Q	68
	2.0×10^{-6}		Modarresi et al. (2005)	Q	248
	2.9×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	3.0×10^{-6}		Yao et al. (2002)	Q	230
	3.6×10^{-6}		English and Carroll (2001)	Q	231, 261
	4.2×10^{-6}		Nirmalakhandan et al. (1997)	Q	
	2.7×10^{-6}		Yaws (1999)	?	21
	2.7×10^{-6}		Yaws and Yang (1992)	?	21
4-methylheptane	2.7×10^{-6}		Brockbank (2013)	L	
C_8H_{18}	2.4×10^{-6}		Yaws (2003)	X	238
[589-53-7]	2.9×10^{-6}		Gharagheizi et al. (2012)	Q	
CHBAWFGIXDBEBT-UHFFFAOYSA-N	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
	3.0×10^{-6}		Hilal et al. (2008)	Q	
	2.2×10^{-6}		Modarresi et al. (2005)	Q	248
	2.7×10^{-6}		Yao et al. (2002)	Q	230
	2.4×10^{-6}		Yaws (1999)	?	21
	2.7×10^{-6}		Yaws and Yang (1992)	?	21
2,2-dimethylhexane	2.4×10^{-6}	4600	Brockbank (2013)	L	1
C_8H_{18}	2.4×10^{-6}	4600	Dohányosová et al. (2004)	M	285
[590-73-8]	2.7×10^{-7}		Duchowicz et al. (2020)	V	187
FLTJDUOFAQWHDF-UHFFFAOYSA-N	2.7×10^{-6}		Yaws (2003)	X	238
	7.5×10^{-5}		Duchowicz et al. (2020)	Q	
	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
	1.9×10^{-6}		Hilal et al. (2008)	Q	
		4700	Kühne et al. (2005)	Q	
	4.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.8×10^{-6}		Yao et al. (2002)	Q	230
		5100	Kühne et al. (2005)	?	
	2.7×10^{-6}		Yaws (1999)	?	21
	2.9×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-dimethylhexane	2.4×10^{-6}		Yaws (2003)	X	238
C_8H_{18}	2.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[584-94-1]	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
JXPOLSKBTUYKJB-UHFFFAOYSA-N	3.4×10^{-6}		Hilal et al. (2008)	Q	
	2.4×10^{-6}		Yaws (1999)	?	21
	2.6×10^{-6}		Yaws and Yang (1992)	?	21
2,4-dimethylhexane	2.6×10^{-6}		Yaws (2003)	X	238
C_8H_{18}	2.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[589-43-5]	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
HDGQICNBXPAKLR-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	2.6×10^{-6}		Yaws (1999)	?	21
	2.8×10^{-6}		Yaws and Yang (1992)	?	21
2,5-dimethylhexane	3.1×10^{-6}	4000	Brockbank (2013)	L	1, 286
C_8H_{18}	2.4×10^{-6}	4000	Dohányosová et al. (2004)	M	287
[592-13-2]	2.6×10^{-6}		Yaws (2003)	X	238
UWNADWZGEHDQAB-UHFFFAOYSA-N	2.2×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
	1.7×10^{-6}		Hilal et al. (2008)	Q	
		4700	Kühne et al. (2005)	Q	
	2.4×10^{-6}		Modarresi et al. (2005)	Q	248
	2.3×10^{-6}		Yao et al. (2002)	Q	230
		4700	Kühne et al. (2005)	?	
	2.7×10^{-6}		Yaws (1999)	?	21
	2.9×10^{-6}		Yaws and Yang (1992)	?	21
3,3-dimethylhexane	2.4×10^{-6}		Yaws (2003)	X	238
C_8H_{18}	2.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[563-16-6]	2.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
KUMXLFIBWFCMOJ-UHFFFAOYSA-N	2.9×10^{-6}		Hilal et al. (2008)	Q	
	1.9×10^{-6}		Modarresi et al. (2005)	Q	248
	1.5×10^{-6}		Yao et al. (2002)	Q	230
	2.4×10^{-6}		Yaws (1999)	?	21
	2.6×10^{-6}		Yaws and Yang (1992)	?	21
3,4-dimethylhexane	2.2×10^{-6}		Yaws (2003)	X	238
C_8H_{18}	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
[583-48-2]	3.8×10^{-6}		Hilal et al. (2008)	Q	
RNTWWGNZUXGTAX-UHFFFAOYSA-N	2.3×10^{-6}		Yaws (1999)	?	21
	2.4×10^{-6}		Yaws and Yang (1992)	?	21
3-ethylhexane	2.3×10^{-6}		Yaws (2003)	X	238
C_8H_{18}	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
[619-99-8]	3.7×10^{-6}		Hilal et al. (2008)	Q	
SFRKSDZMZHIISH-UHFFFAOYSA-N	2.3×10^{-6}		Yaws (1999)	?	21
	2.6×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,3-trimethylpentane	2.4×10^{-6}		Yaws (2003)	X	238
C_8H_{18}	2.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[564-02-3]	2.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
XTDQDBVBDLYELW-UHFFFAOYSA-N	2.7×10^{-6}		Hilal et al. (2008)	Q	
	7.3×10^{-6}		Modarresi et al. (2007)	Q	68
	2.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.7×10^{-6}		Yao et al. (2002)	Q	230
	2.4×10^{-6}		Yaws (1999)	?	21
	2.6×10^{-6}		Yaws and Yang (1992)	?	21
2,2,4-trimethylpentane	3.0×10^{-6}		Plyasunov and Shock (2000)	L	
C_8H_{18}	3.0×10^{-6}		Mackay and Shiu (1981)	L	
(isooctane)	4.6×10^{-6}		Guitart et al. (1989)	M	14
[540-84-1]	3.3×10^{-6}		Mackay et al. (2006a)	V	
NHTMVDHEPJAVLT-UHFFFAOYSA-N	3.3×10^{-6}		Mackay et al. (1993)	V	
	3.1×10^{-6}		Eastcott et al. (1988)	V	
	3.3×10^{-6}		Hine and Mookerjee (1975)	V	
	3.2×10^{-6}		Mackay and Leinonen (1975)	V	
	3.6×10^{-6}		McAuliffe (1966)	V	226
	3.6×10^{-6}		McAuliffe (1963)	V	227
	2.8×10^{-6}		Yaws (2003)	X	238
	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	3.3×10^{-6}		Zhang et al. (2010)	Q	288, 289
	1.7×10^{-6}		Zhang et al. (2010)	Q	288, 290
	2.2×10^{-5}		Zhang et al. (2010)	Q	288, 291
	1.6×10^{-5}		Zhang et al. (2010)	Q	288, 292
	2.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
	1.2×10^{-6}		Hilal et al. (2008)	Q	
	4.8×10^{-6}		Modarresi et al. (2007)	Q	68
		4700	Kühne et al. (2005)	Q	
	3.4×10^{-6}		Modarresi et al. (2005)	Q	248
	6.2×10^{-6}		Yaffe et al. (2003)	Q	249, 273
	2.0×10^{-6}		Yao et al. (2002)	Q	230
	3.7×10^{-6}		English and Carroll (2001)	Q	231, 275
	3.1×10^{-6}		Suzuki et al. (1992)	Q	233
	2.9×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
		4000	Kühne et al. (2005)	?	
	2.9×10^{-6}		Yaws (1999)	?	21
	2.9×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3-trimethylpentane	2.1×10^{-6}		Yaws (2003)	X	238
C_8H_{18}	3.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[560-21-4]	2.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
OKVWYBALHQFVFP-UHFFFAOYSA-N	3.6×10^{-6}		Hilal et al. (2008)	Q	
	2.0×10^{-6}		Modarresi et al. (2005)	Q	248
	1.6×10^{-6}		Yao et al. (2002)	Q	230
	2.2×10^{-6}		Yaws (1999)	?	21
	2.4×10^{-6}		Yaws and Yang (1992)	?	21
2,3,4-trimethylpentane	3.3×10^{-6}		Brockbank (2013)	L	
C_8H_{18}	4.3×10^{-6}		Plyasunov and Shock (2000)	L	
[565-75-3]	5.3×10^{-6}		Mackay and Shiu (1981)	L	
RLPGDEORIPLBNF-UHFFFAOYSA-N			Mackay et al. (2006a)	V	293
	4.9×10^{-6}		Mackay et al. (1993)	V	
	5.6×10^{-6}		Eastcott et al. (1988)	V	
	5.6×10^{-6}		Yaws (2003)	X	238
	2.9×10^{-6}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
	3.1×10^{-6}		Hilal et al. (2008)	Q	
	7.0×10^{-6}		Modarresi et al. (2007)	Q	68
		4700	Kühne et al. (2005)	Q	
	2.0×10^{-6}		Modarresi et al. (2005)	Q	248
	5.3×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	2.1×10^{-6}		Yao et al. (2002)	Q	230
	3.7×10^{-6}		English and Carroll (2001)	Q	231, 232
	1.1×10^{-5}		Katritzky et al. (1998)	Q	
	3.2×10^{-6}		Nirmalakhandan et al. (1997)	Q	
		4900	Kühne et al. (2005)	?	
	5.6×10^{-6}		Yaws (1999)	?	21
	5.6×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2-methylpentane	2.3×10^{-6}		Yaws (2003)	X	238
C_8H_{18}	3.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[609-26-7]	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
DUPUVYJQZSLSJB-UHFFFAOYSA-N	3.6×10^{-6}		Hilal et al. (2008)	Q	
	2.2×10^{-6}		Modarresi et al. (2005)	Q	248
	2.5×10^{-6}		Yao et al. (2002)	Q	230
	2.3×10^{-6}		Yaws (1999)	?	21
	2.6×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-3-methylpentane	2.1×10^{-6}		Yaws (2003)	X	238
C_8H_{18}	3.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[1067-08-9]	2.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
GIEZWIDCIFCQPS-UHFFFAOYSA-N	4.5×10^{-6}		Hilal et al. (2008)	Q	
	2.0×10^{-6}		Modarresi et al. (2005)	Q	248
	2.2×10^{-6}		Yao et al. (2002)	Q	230
	2.1×10^{-6}		Yaws (1999)	?	21
	2.3×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3,3-tetramethylbutane	3.3×10^{-6}		Yaws (2003)	X	238
C_8H_{18}	2.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[594-82-1]	2.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
OMMLUKLXGSRPHK-UHFFFAOYSA-N	3.4×10^{-6}		Hilal et al. (2008)	Q	
	2.6×10^{-6}		Yaws and Yang (1992)	?	21
nonane	2.3×10^{-6}	6600	Brockbank (2013)	L	1, 294
C_9H_{20}	2.1×10^{-6}		Plyasunov and Shock (2000)	L	
[111-84-2]	2.0×10^{-6}		Mackay and Shiu (1981)	L	
BKIMMITUMNQMOS-UHFFFAOYSA-N	2.2×10^{-6}		Ryu and Park (1999)	M	
	1.9×10^{-6}		Park et al. (1997)	M	277
	2.3×10^{-5}	190	Ashworth et al. (1988)	M	42, 279
	1.8×10^{-6}	7300	Jönsson et al. (1982)	M	
	2.9×10^{-6}		Duchowicz et al. (2020)	V	187
	2.9×10^{-6}		HSDB (2015)	V	
	3.0×10^{-6}		Mackay et al. (2006a)	V	
	3.0×10^{-6}		Mackay et al. (1993)	V	
	1.7×10^{-6}		Eastcott et al. (1988)	V	
	2.0×10^{-6}		Abraham (1984)	V	
	1.6×10^{-6}		Yaws (2003)	X	238
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	2.9×10^{-5}		Wang et al. (2017)	Q	81, 239
	2.5×10^{-6}		Wang et al. (2017)	Q	81, 240
	2.3×10^{-5}		Wang et al. (2017)	Q	81, 241
	3.0×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-6}		Raventos-Duran et al. (2010)	Q	272, 244
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	1.8×10^{-6}		Gharagheizi et al. (2010)	Q	247
	3.0×10^{-6}		Hilal et al. (2008)	Q	
	4.3×10^{-6}		Modarresi et al. (2007)	Q	68
		5000	Kühne et al. (2005)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	248
	2.0×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	4.6×10^{-6}		Yao et al. (2002)	Q	230
	1.1×10^{-5}		Katritzky et al. (1998)	Q	
	3.8×10^{-6}		Nirmalakhandan et al. (1997)	Q	
		4100	Kühne et al. (2005)	?	

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
2-methyloctane	1.6×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[3221-61-2]	1.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
ZUBZATZOEPUUQF-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	2.1×10^{-6}		Modarresi et al. (2005)	Q	248
	3.3×10^{-6}		Yao et al. (2002)	Q	230
	1.6×10^{-6}		Yaws (1999)	?	21
	2.1×10^{-6}		Yaws and Yang (1992)	?	21
3-methyloctane	1.5×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[2216-33-3]	1.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
SEEOMASXHIJCDV-UHFFFAOYSA-N	2.4×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	248
	2.8×10^{-6}		Yao et al. (2002)	Q	230
	1.5×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21
4-methyloctane	9.7×10^{-7}		Plyasunov and Shock (2000)	L	
C_9H_{20}	1.0×10^{-6}		Mackay and Shiu (1981)	L	
[2216-34-4]	9.9×10^{-7}		Duchowicz et al. (2020)	V	187
DOGIHOCMZJUJNR-UHFFFAOYSA-N	9.9×10^{-7}		Eastcott et al. (1988)	V	
	9.8×10^{-7}		Yaws (2003)	X	238
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	2.4×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-6}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	1.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
	2.3×10^{-6}		Hilal et al. (2008)	Q	
	4.9×10^{-6}		Modarresi et al. (2007)	Q	68
	1.6×10^{-6}		Modarresi et al. (2005)	Q	248
	2.9×10^{-6}		Yao et al. (2002)	Q	230
	9.8×10^{-7}		Yaws (1999)	?	21
	9.9×10^{-7}		Yaws and Yang (1992)	?	21
2,3-dimethylheptane	1.4×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[3074-71-3]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
WBRFDUJXCLCKPX-UHFFFAOYSA-N	2.4×10^{-6}		Hilal et al. (2008)	Q	
	2.4×10^{-6}		Modarresi et al. (2005)	Q	248
	2.0×10^{-6}		Yao et al. (2002)	Q	230, 268
	1.5×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2-dimethylheptane	1.7×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[1071-26-7]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
PSABUFWDVWCFDP-UHFFFAOYSA-N	1.4×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	248
	2.0×10^{-6}		Yao et al. (2002)	Q	230
	1.7×10^{-6}		Yaws (1999)	?	21
	2.1×10^{-6}		Yaws and Yang (1992)	?	21
2,4-dimethylheptane	1.7×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[2213-23-2]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
AUKVIBNBLXQNIZ-UHFFFAOYSA-N	1.4×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	248
	1.8×10^{-6}		Yao et al. (2002)	Q	230
	1.7×10^{-6}		Yaws (1999)	?	21
	2.1×10^{-6}		Yaws and Yang (1992)	?	21
2,5-dimethylheptane	1.6×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[2216-30-0]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
HQZHQNKZOYIKQC-UHFFFAOYSA-N	1.5×10^{-6}		Hilal et al. (2008)	Q	
	2.0×10^{-6}		Yao et al. (2002)	Q	230
	1.6×10^{-6}		Yaws (1999)	?	21
	2.0×10^{-6}		Yaws and Yang (1992)	?	21
2,6-dimethylheptane	1.7×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[1072-05-5]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
KBPCCVWUMVGXGF-UHFFFAOYSA-N	1.2×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	248
	2.2×10^{-6}		Yao et al. (2002)	Q	230
	1.7×10^{-6}		Yaws (1999)	?	21
	2.1×10^{-6}		Yaws and Yang (1992)	?	21
3,3-dimethylheptane	2.3×10^{-6}		Hilal et al. (2008)	Q	
C_9H_{20}	1.9×10^{-6}		Yaws and Yang (1992)	?	21
[4032-86-4]					
BVAKDOXCVSMKHE-UHFFFAOYSA-N					
3,4-dimethylheptane	1.4×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[922-28-1]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
MAKRYGRRIKSDES-UHFFFAOYSA-N	2.6×10^{-6}		Hilal et al. (2008)	Q	
	1.7×10^{-6}		Modarresi et al. (2005)	Q	248
	1.6×10^{-6}		Yao et al. (2002)	Q	230
	1.4×10^{-6}		Yaws (1999)	?	21
	1.8×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,5-dimethylheptane	1.6×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[926-82-9]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
DZJTZGHZAWTWGA-UHFFFAOYSA-N	1.5×10^{-6}		Hilal et al. (2008)	Q	
	1.7×10^{-6}		Modarresi et al. (2005)	Q	248
	1.6×10^{-6}		Yao et al. (2002)	Q	230
	1.6×10^{-6}		Yaws (1999)	?	21
	2.0×10^{-6}		Yaws and Yang (1992)	?	21
4,4-dimethylheptane	1.5×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[1068-19-5]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
WSOKFYJGNBQDPW-UHFFFAOYSA-N	2.1×10^{-6}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	248
	1.5×10^{-6}		Yao et al. (2002)	Q	230
	1.5×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21
3-ethylheptane	1.4×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-80-4]	1.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
PSVQKOKKLWHNRP-UHFFFAOYSA-N	2.6×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	248
	2.4×10^{-6}		Yao et al. (2002)	Q	230
	1.4×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21
4-ethylheptane	1.5×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[2216-32-2]	1.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
XMROPFQWHHUFFS-UHFFFAOYSA-N	2.5×10^{-6}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	248
	2.8×10^{-6}		Yao et al. (2002)	Q	230
	1.5×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3-trimethylhexane	1.5×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-25-4]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
CBVFSZDQEHBJEQ-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	248
	9.0×10^{-7}		Yao et al. (2002)	Q	230
	1.5×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,4-trimethylhexane	1.7×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-26-5]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
AFTPEBDOGXRMNQ-UHFFFAOYSA-N	1.1×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	248
	1.0×10^{-6}		Yao et al. (2002)	Q	230
	1.7×10^{-6}		Yaws (1999)	?	21
	2.1×10^{-6}		Yaws and Yang (1992)	?	21
2,2,5-trimethylhexane	1.9×10^{-6}	6200	Brockbank (2013)	L	
C_9H_{20}	2.8×10^{-6}		Plyasunov and Shock (2000)	L	
[3522-94-9]	2.9×10^{-6}		Mackay and Shiu (1981)	L	
HHOSMYBYIHNXNO-UHFFFAOYSA-N	4.1×10^{-6}		Mackay et al. (2006a)	V	
	4.1×10^{-6}		Mackay et al. (1993)	V	
	4.1×10^{-6}		Cabani et al. (1981)	V	
	3.9×10^{-6}		McAuliffe (1966)	V	
	1.8×10^{-6}		Yaws (2003)	X	238
	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
	9.0×10^{-7}		Hilal et al. (2008)	Q	
	1.7×10^{-6}		Modarresi et al. (2005)	Q	248
	2.9×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	1.5×10^{-6}		Yao et al. (2002)	Q	230
	2.2×10^{-6}		Nirmalakhandan et al. (1997)	Q	
	1.8×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21
2,3,3-trimethylhexane	1.4×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-28-7]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
DJYSEQMMCZAKGT-UHFFFAOYSA-N	2.4×10^{-6}		Hilal et al. (2008)	Q	
	2.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.0×10^{-6}		Yao et al. (2002)	Q	230
	1.4×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
2,3,4-trimethylhexane	1.4×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[921-47-1]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
RUTNOQHQISEBGT-UHFFFAOYSA-N	2.6×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	248
	1.1×10^{-6}		Yao et al. (2002)	Q	230
	1.4×10^{-6}		Yaws (1999)	?	21
	1.8×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,5-trimethylhexane	1.7×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[1069-53-0]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
ODGLTLJZCVNPBU-UHFFFAOYSA-N	1.4×10^{-6}		Hilal et al. (2008)	Q	
	2.1×10^{-6}		Modarresi et al. (2005)	Q	248
	1.1×10^{-6}		Yao et al. (2002)	Q	230, 268
	2.8×10^{-6}		English and Carroll (2001)	Q	231, 232
	1.7×10^{-6}		Yaws (1999)	?	21
	2.0×10^{-6}		Yaws and Yang (1992)	?	21
2,4,4-trimethylhexane	1.5×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-30-1]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
SVEMKBCPZYWEPH-UHFFFAOYSA-N	1.4×10^{-6}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	248
	1.1×10^{-6}		Yao et al. (2002)	Q	230
	1.5×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21
3,3,4-trimethylhexane	1.3×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-31-2]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
ARWOOWBJJKVYOV-UHFFFAOYSA-N	2.9×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	248
	1.1×10^{-6}		Yao et al. (2002)	Q	230
	1.3×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2-methylhexane	1.5×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[16789-46-1]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
MVLOWDRGPHBNNF-UHFFFAOYSA-N	2.3×10^{-6}		Hilal et al. (2008)	Q	
	2.2×10^{-6}		Modarresi et al. (2005)	Q	248
	1.2×10^{-6}		Yao et al. (2002)	Q	230
	1.5×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21
4-ethyl-2-methylhexane	1.6×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[3074-75-7]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
KYCZJIBOPKRSOV-UHFFFAOYSA-N	1.5×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	248
	1.5×10^{-6}		Yao et al. (2002)	Q	230, 268
	1.7×10^{-6}		Yaws (1999)	?	21
	2.0×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-3-methylhexane	1.3×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[3074-76-8]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
CYWROHZCELEGSE-UHFFFAOYSA-N	3.2×10^{-6}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	248
	1.2×10^{-6}		Yao et al. (2002)	Q	230
	1.3×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-4-methylhexane	1.4×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[3074-77-9]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
OKCRKWVABWILDR-UHFFFAOYSA-N	3.1×10^{-6}		Hilal et al. (2008)	Q	
	1.9×10^{-6}		Modarresi et al. (2005)	Q	248
	1.2×10^{-6}		Yao et al. (2002)	Q	230
	1.4×10^{-6}		Yaws (1999)	?	21
	1.8×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3,3-tetramethylpentane	1.2×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[7154-79-2]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
QUKOJKFJIHSBKV-UHFFFAOYSA-N	3.6×10^{-6}		Hilal et al. (2008)	Q	
	2.1×10^{-6}		Modarresi et al. (2005)	Q	248
	1.0×10^{-6}		Yao et al. (2002)	Q	230, 268
	1.2×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3,4-tetramethylpentane	1.4×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[1186-53-4]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
VZFMYOCAEQDWDY-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	248
	2.8×10^{-6}		Yao et al. (2002)	Q	230
	1.4×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
2,2,4,4-tetramethylpentane	1.7×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[1070-87-7]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
GUMULFRCHLJNDY-UHFFFAOYSA-N	9.0×10^{-7}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	248
	1.4×10^{-6}		Yao et al. (2002)	Q	230
	1.7×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3,4-tetramethylpentane	1.2×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	3.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-38-9]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
JLCYYQOQSAMWTA-UHFFFAOYSA-N	2.7×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	248
	1.2×10^{-6}		Yao et al. (2002)	Q	230
	1.2×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,2-dimethylpentane	1.5×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-32-3]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
CLZCPQKGOAXOJT-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	248
	1.6×10^{-6}		Yao et al. (2002)	Q	230, 268
	1.5×10^{-6}		Yaws (1999)	?	21
	1.8×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,3-dimethylpentane	1.2×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	3.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-33-4]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
MMASVVOQIKCFJZ-UHFFFAOYSA-N	3.5×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	248
	1.6×10^{-6}		Yao et al. (2002)	Q	230
	1.2×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,4-dimethylpentane	1.4×10^{-6}		Yaws (2003)	X	238
C_9H_{20}	2.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[1068-87-7]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
VLHAGZNBWKUMRW-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	2.0×10^{-6}		Modarresi et al. (2005)	Q	248
	1.8×10^{-6}		Yao et al. (2002)	Q	230
	1.4×10^{-6}		Yaws (1999)	?	21
	1.8×10^{-6}		Yaws and Yang (1992)	?	21
3,3-diethylpentane		4900	Abraham and Nasehzadeh (1981)	R	
C_9H_{20}	1.1×10^{-6}		Yaws (2003)	X	238
[1067-20-5]	3.4×10^{-6}		Gharagheizi et al. (2012)	Q	
BGXXXYLRPIRDHJ-UHFFFAOYSA-N	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
	4.1×10^{-6}		Hilal et al. (2008)	Q	
	2.0×10^{-6}		Modarresi et al. (2005)	Q	248
	1.7×10^{-6}		Yao et al. (2002)	Q	230
	1.1×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
	9.5×10^{-6}		Abraham et al. (1990)	?	
	9.4×10^{-6}		Abraham (1979)	?	

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
decane	1.3×10^{-6}		Brockbank (2013)	L	
$C_{10}H_{22}$	1.1×10^{-6}		Plyasunov and Shock (2000)	L	
[124-18-5]	1.4×10^{-6}		Mackay and Shiu (1981)	L	
DIOQZVSQGTUSAI-UHFFFAOYSA-N	1.9×10^{-6}		Duchowicz et al. (2020)	V	187
	1.9×10^{-6}		HSDB (2015)	V	
	2.1×10^{-6}		Mackay et al. (2006a)	V	
	2.1×10^{-6}		Mackay et al. (1993)	V	
	2.0×10^{-6}		Hwang et al. (1992)	V	
	2.3×10^{-6}		Eastcott et al. (1988)	V	
	1.9×10^{-6}		Abraham (1984)	V	
	1.9×10^{-6}		Yaws (2003)	X	259
	1.9×10^{-6}		Yaws (2003)	X	238
	4.4×10^{-6}		Dupeux et al. (2022)	Q	260
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	2.3×10^{-5}		Wang et al. (2017)	Q	81, 239
	1.7×10^{-6}		Wang et al. (2017)	Q	81, 240
	6.5×10^{-6}		Wang et al. (2017)	Q	81, 241
	3.7×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-6}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
	2.2×10^{-6}		Hilal et al. (2008)	Q	
	3.8×10^{-6}		Modarresi et al. (2007)	Q	68
	2.0×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	2.2×10^{-6}		English and Carroll (2001)	Q	231, 232
	1.0×10^{-5}		Katritzky et al. (1998)	Q	
	2.9×10^{-6}		Nirmalakhandan et al. (1997)	Q	
	1.9×10^{-6}		Yaws (1999)	?	21
	2.1×10^{-6}		Yaws and Yang (1992)	?	21
2-methylnonane	1.2×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[871-83-0]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
SGVYKUFIHHTIFL-UHFFFAOYSA-N	1.5×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	3.1×10^{-6}		Yao et al. (2002)	Q	230, 268
	1.2×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
3-methylnonane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[5911-04-6]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
PLZDDPSCZHRBOY-UHFFFAOYSA-N	1.7×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	2.8×10^{-6}		Yao et al. (2002)	Q	230
	1.1×10^{-6}		Yaws (1999)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
4-methylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[17301-94-9]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
IALRSQMWHFKJJA-UHFFFAOYSA-N	1.6×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	2.7×10^{-6}		Yao et al. (2002)	Q	230
	1.0×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
5-methylnonane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-85-9]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
TYSIILFJZXHVPU-UHFFFAOYSA-N	1.7×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	4.2×10^{-6}		Yao et al. (2002)	Q	230
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
2,2-dimethyloctane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-87-1]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
GPBUTTSWJNPYJL-UHFFFAOYSA-N	1.3×10^{-6}		Hilal et al. (2008)	Q	
	1.1×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
2,3-dimethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[7146-60-3]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
YPMNDMUOGQJCLW-UHFFFAOYSA-N	1.7×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	1.6×10^{-6}		Yao et al. (2002)	Q	230
	1.0×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
2,4-dimethyloctane	1.2×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[4032-94-4]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
IXAVTTRPEXFVSX-UHFFFAOYSA-N	1.2×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.7×10^{-6}		Yao et al. (2002)	Q	230
	1.2×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,5-dimethyloctane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-89-3]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
HOAAQUNESXYFDT-UHFFFAOYSA-N	1.3×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	2.0×10^{-6}		Yao et al. (2002)	Q	230, 268
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
2,6-dimethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[2051-30-1]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
ZALHPSXXQIPKTQ-UHFFFAOYSA-N	1.2×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.8×10^{-6}		Yao et al. (2002)	Q	230
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
2,7-dimethyloctane	1.2×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[1072-16-8]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
KEVMYFLMMDUPJE-UHFFFAOYSA-N	1.0×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	1.9×10^{-6}		Yao et al. (2002)	Q	230
	1.2×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
3,3-dimethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[4110-44-5]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
DBULLUBYDONGLT-UHFFFAOYSA-N	1.7×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.4×10^{-6}		Yao et al. (2002)	Q	230
	1.0×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
3,4-dimethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-92-8]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
QQCWGAMGBCGAQJ-UHFFFAOYSA-N	2.0×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	1.6×10^{-6}		Yao et al. (2002)	Q	230
	1.0×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,5-dimethyloctane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-93-9]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
VRHRGVJOUHJULC-UHFFFAOYSA-N	1.4×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	1.6×10^{-6}		Yao et al. (2002)	Q	230
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
3,6-dimethyloctane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-94-0]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
JEEQUUSFXYRPRK-UHFFFAOYSA-N	1.3×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	1.6×10^{-6}		Yao et al. (2002)	Q	230
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
4,4-dimethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-95-1]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
ZMEDGZAGMLTROM-UHFFFAOYSA-N	1.5×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.4×10^{-6}		Yao et al. (2002)	Q	230, 268
	1.1×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
4,5-dimethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-96-2]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
DOYJTLUPPPUSMD-UHFFFAOYSA-N	2.1×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.4×10^{-6}		Yao et al. (2002)	Q	230
	1.0×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyloctane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[5881-17-4]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
OEYGTUAKNZFCDJ-UHFFFAOYSA-N	2.2×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-ethyloctane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-86-0]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
NRJUFUBKIFIKFI-UHFFFAOYSA-N	2.4×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	2.8×10^{-6}		Yao et al. (2002)	Q	230
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3-trimethylheptane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[52896-92-1]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
ACYHSTUWOQNWCX-UHFFFAOYSA-N	1.6×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	9.4×10^{-7}		Yao et al. (2002)	Q	230
	1.0×10^{-6}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
2,2,4-trimethylheptane	1.2×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[14720-74-2]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
IIYGOARYARWJBO-UHFFFAOYSA-N	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.0×10^{-6}		Yao et al. (2002)	Q	230
	1.2×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
2,2,5-trimethylheptane	1.2×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[20291-95-6]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
GZJFAWOTMWATOS-UHFFFAOYSA-N	1.5×10^{-6}		Modarresi et al. (2005)	Q	248
	1.1×10^{-6}		Yao et al. (2002)	Q	230, 268
	1.2×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
2,2,6-trimethylheptane	1.2×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[1190-83-6]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
FHJCGIUZJXWNET-UHFFFAOYSA-N	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	1.3×10^{-6}		Yao et al. (2002)	Q	230
	1.3×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3-trimethylheptane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[52896-93-2]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
QACXEXNKLFWKLK-UHFFFAOYSA-N	1.6×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	9.7×10^{-7}		Yao et al. (2002)	Q	230
	9.5×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
2,3,4-trimethylheptane	9.9×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[52896-95-4]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
UVVYAKOLFKEZEE-UHFFFAOYSA-N	1.6×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	9.0×10^{-7}		Yao et al. (2002)	Q	230
	9.9×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
2,3,5-trimethylheptane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[20278-85-7]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
YKPNYFKOKKKGNM-UHFFFAOYSA-N	1.1×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	1.1×10^{-6}		Yao et al. (2002)	Q	230
	9.5×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
2,3,6-trimethylheptane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[4032-93-3]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
IHPXJGBVRWFEJB-UHFFFAOYSA-N	1.1×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	1.2×10^{-6}		Yao et al. (2002)	Q	230
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
2,4,4-trimethylheptane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[4032-92-2]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
QALGVLROELGEEM-UHFFFAOYSA-N	1.1×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	8.6×10^{-7}		Yao et al. (2002)	Q	230
	1.1×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4,5-trimethylheptane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[20278-84-6]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
YMBNRMDSLJNNPF-UHFFFAOYSA-N	1.1×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	9.0×10^{-7}		Yao et al. (2002)	Q	230, 268
	1.1×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
2,4,6-trimethylheptane	1.3×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[2613-61-8]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
YNLBBDHDNIXQNL-UHFFFAOYSA-N	7.5×10^{-7}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.0×10^{-6}		Yao et al. (2002)	Q	230
	1.3×10^{-6}		Yaws (1999)	?	21
	1.8×10^{-6}		Yaws and Yang (1992)	?	21
2,5,5-trimethylheptane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[1189-99-7]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
SOYLPZSOEXZMLE-UHFFFAOYSA-N	1.1×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.2×10^{-6}		Yao et al. (2002)	Q	230
	1.1×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
3,3,4-trimethylheptane	9.0×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[20278-87-9]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
WRBHKVWLEIYLDZ-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	7.6×10^{-7}		Yao et al. (2002)	Q	230
	9.0×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21
3,3,5-trimethylheptane	9.9×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[7154-80-5]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
VRVRZZWPKABUOE-UHFFFAOYSA-N	1.2×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	8.3×10^{-7}		Yao et al. (2002)	Q	230
	1.0×10^{-6}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4,4-trimethylheptane	9.0×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[20278-88-0]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
BLNBSBLKPFFJKQ-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	7.7×10^{-7}		Yao et al. (2002)	Q	230
	9.0×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21
3,4,5-trimethylheptane	9.4×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[20278-89-1]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
LJIIBBYARMPSMT-UHFFFAOYSA-N	2.3×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	8.9×10^{-7}		Yao et al. (2002)	Q	230
	9.4×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2-methylheptane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[14676-29-0]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
NKMJCVVUYDKHAV-UHFFFAOYSA-N	2.0×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.4×10^{-6}		Yao et al. (2002)	Q	230
	1.0×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
4-ethyl-2-methylheptane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[52896-88-5]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
OJDKRASKNKPYDH-UHFFFAOYSA-N	1.4×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.5×10^{-6}		Yao et al. (2002)	Q	230
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
5-ethyl-2-methylheptane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[13475-78-0]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
DGEMPTLPTFNEHJ-UHFFFAOYSA-N	1.4×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	1.5×10^{-6}		Yao et al. (2002)	Q	230
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-3-methylheptane	9.1×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-01-1]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
HSOMNBKXPGCNBH-UHFFFAOYSA-N	2.2×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.3×10^{-6}		Yao et al. (2002)	Q	230, 268
	9.2×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
4-ethyl-3-methylheptane	9.8×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[52896-89-6]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
BTGGSWBKRYMHQK-UHFFFAOYSA-N	2.2×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	1.2×10^{-6}		Yao et al. (2002)	Q	230
	9.8×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-5-methylheptane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[52896-90-9]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
VXARVYMIZCGZGG-UHFFFAOYSA-N	1.3×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.6×10^{-6}		Yao et al. (2002)	Q	230
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-4-methylheptane	9.7×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[52896-91-0]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
JZBKRUIGSVOOIC-UHFFFAOYSA-N	2.2×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.1×10^{-6}		Yao et al. (2002)	Q	230
	9.8×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
4-ethyl-4-methylheptane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-04-4]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
MPYQJQDSICRCJJ-UHFFFAOYSA-N	2.4×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.0×10^{-6}		Yao et al. (2002)	Q	230
	9.5×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-propylheptane	1.2×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[3178-29-8]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
ABYGSZMCWVXFCQ-UHFFFAOYSA-N	1.6×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	2.6×10^{-6}		Yao et al. (2002)	Q	230
	1.2×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
4-(1-methylethyl)-heptane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
(4-isopropylheptane)	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
[52896-87-4]	2.1×10^{-6}		Hilal et al. (2008)	Q	
AZLAWGCUDHUQDB-UHFFFAOYSA-N	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	2.0×10^{-6}		Yao et al. (2002)	Q	230
	1.0×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3,3-tetramethylhexane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[13475-81-5]	9.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
RMQHJMMCLSJULX-UHFFFAOYSA-N	1.8×10^{-6}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	248
	4.9×10^{-7}		Yao et al. (2002)	Q	230
	8.4×10^{-7}		Yaws (1999)	?	21
	1.2×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3,4-tetramethylhexane	8.7×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-08-2]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
MHPSPNGWFAGBNH-UHFFFAOYSA-N	1.2×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	5.9×10^{-7}		Yao et al. (2002)	Q	230
	8.7×10^{-7}		Yaws (1999)	?	21
	1.2×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3,5-tetramethylhexane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-09-3]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
GCFKTDRTZYDRBI-UHFFFAOYSA-N	8.4×10^{-7}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	6.6×10^{-7}		Yao et al. (2002)	Q	230, 268
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,4,4-tetramethylhexane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[51750-65-3]	9.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
PXHNHTBJHHSVPT-UHFFFAOYSA-N	8.8×10^{-7}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	6.5×10^{-7}		Yao et al. (2002)	Q	230
	8.3×10^{-7}		Yaws (1999)	?	21
	1.1×10^{-6}		Yaws and Yang (1992)	?	21
2,2,4,5-tetramethylhexane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-42-5]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
KDRZICOOQNIJDN-UHFFFAOYSA-N	8.0×10^{-7}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	7.3×10^{-7}		Yao et al. (2002)	Q	230
	1.1×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
2,2,5,5-tetramethylhexane	1.4×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	8.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[1071-81-4]	9.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
HXQDUXXBVMMIKL-UHFFFAOYSA-N	4.6×10^{-7}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	248
	1.1×10^{-6}		Yao et al. (2002)	Q	230
	1.4×10^{-6}		Yaws (1999)	?	21
	1.8×10^{-6}		Yaws and Yang (1992)	?	21
2,3,3,4-tetramethylhexane	7.9×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-10-6]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
HIHSOGFAVTVMCY-UHFFFAOYSA-N	1.4×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	6.0×10^{-7}		Yao et al. (2002)	Q	230
	7.9×10^{-7}		Yaws (1999)	?	21
	1.2×10^{-6}		Yaws and Yang (1992)	?	21
2,3,3,5-tetramethylhexane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-11-7]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
GCGFXFIPOBRMQT-UHFFFAOYSA-N	9.2×10^{-7}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	5.9×10^{-7}		Yao et al. (2002)	Q	230
	1.0×10^{-6}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4,4-tetramethylhexane	8.2×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-12-8]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
XDRDDPSGUQMOBO-UHFFFAOYSA-N	1.3×10^{-6}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	248
	6.3×10^{-7}		Yao et al. (2002)	Q	230
	8.3×10^{-7}		Yaws (1999)	?	21
	1.2×10^{-6}		Yaws and Yang (1992)	?	21
2,3,4,5-tetramethylhexane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-15-1]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
BHGNYYIOYPFWKC-UHFFFAOYSA-N	1.2×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	6.6×10^{-7}		Yao et al. (2002)	Q	230, 268
	1.0×10^{-6}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
3,3,4,4-tetramethylhexane	6.6×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[5171-84-6]	9.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
MCEYLFHKATVXLN-UHFFFAOYSA-N	2.2×10^{-6}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	248
	6.2×10^{-7}		Yao et al. (2002)	Q	230
	6.7×10^{-7}		Yaws (1999)	?	21
	1.0×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,2-dimethylhexane	9.8×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[20291-91-2]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
XYDYODCWVCBIOQ-UHFFFAOYSA-N	1.8×10^{-6}		Hilal et al. (2008)	Q	
	1.8×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	7.1×10^{-7}		Yao et al. (2002)	Q	230
	9.8×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
4-ethyl-2,2-dimethylhexane	1.2×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[52896-99-8]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
QHLDBFLIDFTHQI-UHFFFAOYSA-N	1.1×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	9.9×10^{-7}		Yao et al. (2002)	Q	230
	1.2×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-2,3-dimethylhexane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-00-4]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
PJIFKODHGMUPFH-UHFFFAOYSA-N	2.0×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	6.6×10^{-7}		Yao et al. (2002)	Q	230
	8.6×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21
4-ethyl-2,3-dimethylhexane	9.4×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-01-5]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
RHMRCCBCYFAZIK-UHFFFAOYSA-N	1.6×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	7.2×10^{-7}		Yao et al. (2002)	Q	230
	9.5×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,4-dimethylhexane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[7220-26-0]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
OSKIMJMPFNLVOU-UHFFFAOYSA-N	1.6×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	7.1×10^{-7}		Yao et al. (2002)	Q	230, 268
	9.5×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
4-ethyl-2,4-dimethylhexane	9.1×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-03-7]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
SIKFMUYSQCEQOO-UHFFFAOYSA-N	1.3×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	7.2×10^{-7}		Yao et al. (2002)	Q	230
	9.1×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,5-dimethylhexane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-04-8]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
UJEUVDLASLOZIV-UHFFFAOYSA-N	1.1×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.1×10^{-6}		Yao et al. (2002)	Q	230
	1.1×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-ethyl-3,3-dimethylhexane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-05-9]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
ZRTXVJYJVBTXHE-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	7.3×10^{-7}		Yao et al. (2002)	Q	230
	8.6×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-3,4-dimethylhexane	8.6×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-06-0]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
ZGJCTUKRTSBTIQ-UHFFFAOYSA-N	2.2×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	7.7×10^{-7}		Yao et al. (2002)	Q	230
	8.6×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21
3,3-diethylhexane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-02-2]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
WWNGLKDLYKNGGT-UHFFFAOYSA-N	3.4×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	7.7×10^{-7}		Yao et al. (2002)	Q	230
	8.5×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21
3,4-diethylhexane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[19398-77-7]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
VBZCRMTUDYIWIH-UHFFFAOYSA-N	1.8×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	7.9×10^{-7}		Yao et al. (2002)	Q	230
	9.3×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
2-methyl-3-(1-methylethyl)-hexane	7.5×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.2×10^{-6}		Gharagheizi et al. (2012)	Q	
(3-isopropyl-2-methylhexane)	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
[62016-13-1]	1.5×10^{-6}		Hilal et al. (2008)	Q	
YBOXGRMAQIYMGV-UHFFFAOYSA-N	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	8.5×10^{-7}		Yao et al. (2002)	Q	230, 268
	7.5×10^{-7}		Yaws (1999)	?	21
	1.1×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,3,3,4-pentamethylpentane	6.8×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-44-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
WKQBIIUOSATALN-UHFFFAOYSA-N	1.3×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	8.8×10^{-7}		Yao et al. (2002)	Q	230, 268
	6.8×10^{-7}		Yaws (1999)	?	21
	1.0×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3,4,4-pentamethylpentane	7.2×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-45-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
OWFKEHICSVOVAC-UHFFFAOYSA-N	8.6×10^{-7}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	1.0×10^{-6}		Yao et al. (2002)	Q	230
	7.2×10^{-7}		Yaws (1999)	?	21
	1.0×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,2,3-trimethylpentane	6.6×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-17-3]	9.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
AJDIFHIHSYVDGP-UHFFFAOYSA-N	2.1×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	9.2×10^{-7}		Yao et al. (2002)	Q	230
	6.6×10^{-7}		Yaws (1999)	?	21
	1.0×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,2,4-trimethylpentane	9.2×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-18-4]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
VLIZIVHXZXQRDE-UHFFFAOYSA-N	1.2×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	1.1×10^{-6}		Yao et al. (2002)	Q	230
	9.2×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,3,4-trimethylpentane	7.0×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-19-5]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
OHZNMGSGEFVFTI-UHFFFAOYSA-N	1.5×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.0×10^{-6}		Yao et al. (2002)	Q	230
	7.0×10^{-7}		Yaws (1999)	?	21
	1.1×10^{-6}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3-diethyl-2-methylpentane	7.5×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	2.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-16-2]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
DSSAZLXYIQIXGW-UHFFFAOYSA-N	2.3×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	248
	1.2×10^{-6}		Yao et al. (2002)	Q	230
	7.5×10^{-7}		Yaws (1999)	?	21
	1.1×10^{-6}		Yaws and Yang (1992)	?	21
2,4-dimethyl-3-(1-methylethyl)-pentane	9.1×10^{-7}		Yaws (2003)	X	238
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
(2,4-dimethyl-3-isopropylpentane)	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
[13475-79-1]	1.0×10^{-6}		Hilal et al. (2008)	Q	
YVYHOOYMDHZALB-UHFFFAOYSA-N	1.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.2×10^{-6}		Yao et al. (2002)	Q	230
	9.2×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21
undecane	4.5×10^{-7}		Plyasunov and Shock (2000)	L	
$C_{11}H_{24}$	5.4×10^{-7}		Mackay and Shiu (1981)	L	
[1120-21-4]	5.1×10^{-6}		Duchowicz et al. (2020)	V	187
RSJKGSCJYJTIGS-UHFFFAOYSA-N	5.2×10^{-6}		HSDB (2015)	V	
	4.9×10^{-7}		Mackay et al. (2006a)	V	
	5.4×10^{-6}		Eastcott et al. (1988)	V	
	4.9×10^{-7}		Abraham (1984)	V	
	5.1×10^{-6}		Yaws (2003)	X	238
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	2.1×10^{-5}		Wang et al. (2017)	Q	81, 239
	1.2×10^{-6}		Wang et al. (2017)	Q	81, 240
	1.1×10^{-5}		Wang et al. (2017)	Q	81, 241
	4.4×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
	1.5×10^{-6}		Hilal et al. (2008)	Q	
	3.6×10^{-6}		Modarresi et al. (2007)	Q	68
	5.4×10^{-7}		Yaffe et al. (2003)	Q	249, 250
	3.4×10^{-6}		Yao et al. (2002)	Q	230, 268
	5.1×10^{-6}		Yaws (1999)	?	21
	5.4×10^{-6}		Yaws and Yang (1992)	?	21
2-methyldecane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	3.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[6975-98-0]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
CNPVJWYWYZMPDS-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyldecane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	2.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[13151-34-3]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
JJRUZTXRDDMYGM-UHFFFAOYSA-N					
4-methyldecane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	2.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[2847-72-5]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
DVWZNKLWPILULD-UHFFFAOYSA-N					
5-methyldecane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	2.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[13151-35-4]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
QUYFPNWYGLFQQU-UHFFFAOYSA-N					
2,2-dimethylnonane	9.7×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-14-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
WDSBVMLUILIJOW-UHFFFAOYSA-N					
2,3-dimethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[2884-06-2]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
IGJRNTLDWLTHCQ-UHFFFAOYSA-N					
2,4-dimethylnonane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-24-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
JZUUOAUSQCXSTN-UHFFFAOYSA-N					
2,5-dimethylnonane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-27-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
NQUMJENPNGXAIH-UHFFFAOYSA-N					
2,6-dimethylnonane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-28-2]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
MGNGOEWESNDQAN-UHFFFAOYSA-N					
2,7-dimethylnonane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-29-3]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
QYQSPINNJUXEDY-UHFFFAOYSA-N					
2,8-dimethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-30-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
FZFRYQHIQUEAAV-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3-dimethylnonane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-15-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
HTRYNYZYFGHKDV-UHFFFAOYSA-N					
3,4-dimethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-22-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
PAXLEVPLFYBSQJ-UHFFFAOYSA-N					
3,5-dimethylnonane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-25-9]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
BAFVBVRBYKSWCE-UHFFFAOYSA-N					
3,6-dimethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-31-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
YHLBUWVGPXILSW-UHFFFAOYSA-N					
3,7-dimethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-32-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
YGPVLXJHRFZYJJ-UHFFFAOYSA-N					
4,4-dimethylnonane	9.9×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-18-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
HARRKRKVTQABSF-UHFFFAOYSA-N					
4,5-dimethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-23-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
JDNGDDOTBYZAGS-UHFFFAOYSA-N					
4,6-dimethylnonane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-26-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
JZKWOUUZMBTBDO-UHFFFAOYSA-N					
5,5-dimethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[6414-96-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
BEPKYSJVUZWKMP-UHFFFAOYSA-N					
3-ethylnonane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-11-3]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
FKJSIWPQZCKMIL-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-ethylnonane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[5911-05-7]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
UGCQDCMVAKKTQG-UHFFFAOYSA-N					
5-ethylnonane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-12-4]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
QPOVZYGNFWRMJE-UHFFFAOYSA-N					
2,2,3-trimethyloctane	9.0×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-26-6]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
XZPXMWMVWDSEMY-UHFFFAOYSA-N					
2,2,4-trimethyloctane	9.9×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[18932-14-4]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
IKMGZPRUMVFYBK-UHFFFAOYSA-N					
2,2,5-trimethyloctane	9.9×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62016-27-7]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
CSVNISDVBYGXME-UHFFFAOYSA-N					
2,2,6-trimethyloctane	9.6×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-28-8]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
NBIHFQKVSFKHGH-UHFFFAOYSA-N					
2,2,7-trimethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62016-29-9]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
QGQAHVJOBYNMFN-UHFFFAOYSA-N					
2,3,3-trimethyloctane	8.7×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-30-2]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
KFYWDCDWVPXXCA-UHFFFAOYSA-N					
2,3,4-trimethyloctane	9.7×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-31-3]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
SJQAEXCGOLTHPG-UHFFFAOYSA-N					
2,3,5-trimethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-32-4]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
CEOHXVQAHFSSEG-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,6-trimethyloctane	9.7×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-33-5]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
MNFBUNLEXRMWOY-UHFFFAOYSA-N					
2,3,7-trimethyloctane	9.8×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-34-6]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
XJKKSYAVEVAGFX-UHFFFAOYSA-N					
2,4,4-trimethyloctane	9.9×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62016-35-7]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
CJXXTMYWNCYKHU-UHFFFAOYSA-N					
2,4,5-trimethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-36-8]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
UJYGOBMOHSFJQP-UHFFFAOYSA-N					
2,4,6-trimethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-37-9]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
XHNIFDXYGLPJLP-UHFFFAOYSA-N					
2,4,7-trimethyloctane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62016-38-0]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
DUHKHXHIPOGMOW-UHFFFAOYSA-N					
2,5,5-trimethyloctane	9.8×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62016-39-1]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
DZKJZWAIBSEZKB-UHFFFAOYSA-N					
2,5,6-trimethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-14-2]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
VHBZECSWMWWTMQ-UHFFFAOYSA-N					
2,6,6-trimethyloctane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[54166-32-4]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
RUPXAIGHLDMSOL-UHFFFAOYSA-N					
3,3,4-trimethyloctane	8.7×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-40-4]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
IJVIFYHTPQSPSW-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3,5-trimethyloctane	9.6×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-41-5]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
BEFCOJKHEMBPSK-UHFFFAOYSA-N					
3,3,6-trimethyloctane	9.2×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-42-6]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
CFESHXNQRRYSED-UHFFFAOYSA-N					
3,4,4-trimethyloctane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-43-7]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
WWCBWKZBTINVDE-UHFFFAOYSA-N					
3,4,5-trimethyloctane	9.6×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-44-8]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
BPFOUTQNEVQSFR-UHFFFAOYSA-N					
3,4,6-trimethyloctane	9.8×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-45-9]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
RMGAENUTYIFEJO-UHFFFAOYSA-N					
3,5,5-trimethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-94-8]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
FVYNWISHVUNIOZ-UHFFFAOYSA-N					
4,4,5-trimethyloctane	8.9×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-95-9]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
QGCXVKCDWOOWTQ-UHFFFAOYSA-N					
2-methyl-3-ethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-16-4]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
ITDXDXCBDQBZEB-UHFFFAOYSA-N					
2-methyl-4-ethyloctane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-17-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
ZYEQSLLHBOITAM-UHFFFAOYSA-N					
2-methyl-5-ethyloctane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-18-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
CQCKNPUKBOITAX-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-6-ethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-19-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
AZXGABNJUBNOHW-UHFFFAOYSA-N					
3-methyl-3-ethyloctane	9.1×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-16-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
DQNINFLTCGTQGU-UHFFFAOYSA-N					
3-methyl-4-ethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-20-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
BTRAURWAFYPYMW-UHFFFAOYSA-N					
3-methyl-5-ethyloctane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-21-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
LZFCEXJTLLKGPW-UHFFFAOYSA-N					
3-methyl-6-ethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-22-2]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
FTQLPWORENXYAZ-UHFFFAOYSA-N					
4-methyl-3-ethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-23-3]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
LXRSBMFQRZTMNK-UHFFFAOYSA-N					
4-methyl-4-ethyloctane	9.7×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-19-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
IXZULXYHNRHENR-UHFFFAOYSA-N					
4-methyl-5-ethyloctane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-24-4]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
DTSHQAHKLUTGAR-UHFFFAOYSA-N					
4-methyl-6-ethyloctane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-25-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
NXUUVZOGBPCPDV-UHFFFAOYSA-N					
4-propyloctane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-13-5]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
VFAMBAFLNKONTN-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-isopropyloctane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-15-3]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
VSJAVEFYQMREHJ-UHFFFAOYSA-N					
2,2,3,3-tetramethylheptane	7.5×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-40-4]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
YPGGGWSLWOECQF-UHFFFAOYSA-N					
2,2,3,4-tetramethylheptane	8.6×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-41-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
HPKDRGPKZGWSND-UHFFFAOYSA-N					
2,2,3,5-tetramethylheptane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-42-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
KXNFNEAZTWCHIL-UHFFFAOYSA-N					
2,2,3,6-tetramethylheptane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-43-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
AQHGQPHAJYTMDJ-UHFFFAOYSA-N					
2,2,4,4-tetramethylheptane	8.6×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-44-8]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
JMRHVFQTDSCACD-UHFFFAOYSA-N					
2,2,4,5-tetramethylheptane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-45-9]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
MPDBIZNQOUSUIN-UHFFFAOYSA-N					
2,2,4,6-tetramethylheptane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	7.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-46-0]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
XSMHBEAIQLABAO-UHFFFAOYSA-N					
2,2,5,5-tetramethylheptane	9.1×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-47-1]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
VQJNSRPWQMPDDO-UHFFFAOYSA-N					
2,2,5,6-tetramethylheptane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-48-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
ZYJXKOJVCNGFSL-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,6,6-tetramethylheptane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	7.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[40117-45-1]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
GKNMBVVJQTWDRT-UHFFFAOYSA-N					
2,3,3,4-tetramethylheptane	8.0×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-49-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
OHIUILFTBGSFAG-UHFFFAOYSA-N					
2,3,3,5-tetramethylheptane	8.6×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-50-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
XGCFPCZVDOZHLT-UHFFFAOYSA-N					
2,3,3,6-tetramethylheptane	8.7×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-51-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
ZVRALCAHDAJURU-UHFFFAOYSA-N					
2,3,4,4-tetramethylheptane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-52-8]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
SXHQWTUVNZIMTP-UHFFFAOYSA-N					
2,3,4,5-tetramethylheptane	9.1×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-53-9]	9.6×10^{-7}		Gharagheizi et al. (2010)	Q	247
LGUFKOOYNDNVNP-UHFFFAOYSA-N					
2,3,4,6-tetramethylheptane	9.6×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-54-0]	9.6×10^{-7}		Gharagheizi et al. (2010)	Q	247
WOHJQOFSYZPITE-UHFFFAOYSA-N					
2,3,5,5-tetramethylheptane	9.1×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-55-1]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
QSBIXVGCKCYBBL-UHFFFAOYSA-N					
2,3,5,6-tetramethylheptane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[52670-32-3]	9.6×10^{-7}		Gharagheizi et al. (2010)	Q	247
RAHGVMDMAJFLTP-UHFFFAOYSA-N					
2,4,4,5-tetramethylheptane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-56-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
QALMSCCHYDFGLF-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4,4,6-tetramethylheptane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-57-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
DTMSZIVVBLZFEV-UHFFFAOYSA-N					
2,4,5,5-tetramethylheptane	8.6×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-58-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
JVYVKEOAYQAABU-UHFFFAOYSA-N					
3,3,4,4-tetramethylheptane	7.2×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-59-5]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
CFNIIBCZVLNKPV-UHFFFAOYSA-N					
3,3,4,5-tetramethylheptane	8.1×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-60-8]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
QVCSKDHUHWRVTA-UHFFFAOYSA-N					
3,3,5,5-tetramethylheptane	7.5×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-61-9]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
GALDMESQGNRJGE-UHFFFAOYSA-N					
3,4,4,5-tetramethylheptane	7.8×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-62-0]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
CXIAIMLBUJNNJR-UHFFFAOYSA-N					
2,2-dimethyl-3-ethylheptane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61869-03-2]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
SBWMIVQVGGUMCE-UHFFFAOYSA-N					
2,2-dimethyl-4-ethylheptane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	8.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62016-46-0]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
BJOUMNMMNSZESV-UHFFFAOYSA-N					
2,2-dimethyl-5-ethylheptane	9.8×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62016-47-1]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
HVVFIKMZXFNXKA-UHFFFAOYSA-N					
2,3-dimethyl-3-ethylheptane	8.9×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-21-1]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
KQUHXOYVQZYOOF-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-dimethyl-4-ethylheptane	9.8×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-22-2]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
CNEPAGDSOHLVRW-UHFFFAOYSA-N					
2,3-dimethyl-5-ethylheptane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-23-3]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
BFCKNSGKYWMUNP-UHFFFAOYSA-N					
2,4-dimethyl-3-ethylheptane	9.8×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-24-4]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
OBCGEYFMJYXFJV-UHFFFAOYSA-N					
2,4-dimethyl-4-ethylheptane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-25-5]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
OETKSNKIFXLJDO-UHFFFAOYSA-N					
2,4-dimethyl-5-ethylheptane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-26-6]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
RZHNOEUMKYRHIX-UHFFFAOYSA-N					
2,5-dimethyl-3-ethylheptane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-27-7]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
DEZOXTLNRYCKNK-UHFFFAOYSA-N					
2,5-dimethyl-4-ethylheptane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-28-8]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
CUHCBWKQRDWQMN-UHFFFAOYSA-N					
2,5-dimethyl-5-ethylheptane	9.1×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-29-9]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
GPZDEXDVXFJVLH-UHFFFAOYSA-N					
2,6-dimethyl-3-ethylheptane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-30-2]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
BFXHSWDHLPKFSH-UHFFFAOYSA-N					
2,6-dimethyl-4-ethylheptane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-31-3]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
GBSGJLJGXHBTQQ-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3-dimethyl-4-ethylheptane	8.9×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-32-4]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
QXJXAHFNWHEQEU-UHFFFAOYSA-N					
3,3-dimethyl-5-ethylheptane	9.4×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-33-5]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
FLLHBJKGZIOYAA-UHFFFAOYSA-N					
3,4-dimethyl-3-ethylheptane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-34-6]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
HKSCZRRMBTUZLO-UHFFFAOYSA-N					
3,4-dimethyl-4-ethylheptane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-35-7]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
RMVWUAZCGGWZKA-UHFFFAOYSA-N					
3,4-dimethyl-5-ethylheptane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-36-8]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
PCRCVFLPWIQGNJ-UHFFFAOYSA-N					
3,5-dimethyl-3-ethylheptane	8.9×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-37-9]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
FQOCKNRDCVODKW-UHFFFAOYSA-N					
3,5-dimethyl-4-ethylheptane	9.6×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-38-0]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
IKVNPWSSYMJDKE-UHFFFAOYSA-N					
4,4-dimethyl-3-ethylheptane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-39-1]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
YMWPSGKMCMMFSS-UHFFFAOYSA-N					
2-methyl-4-propylheptane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-96-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
AXOUMHTUGUFOKF-UHFFFAOYSA-N					
3-methyl-4-propylheptane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-97-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
WAMROSASDOIVDE-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methyl-4-propylheptane	9.9×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-20-4]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
RDZFGBZTNOYNAH-UHFFFAOYSA-N					
2-methyl-3-isopropylheptane	9.9×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[6876-18-2]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
GECZBVJYUAPYFD-UHFFFAOYSA-N					
2-methyl-4-isopropylheptane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-98-2]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
ADLZFTVQXMDTCY-UHFFFAOYSA-N					
3-methyl-4-isopropylheptane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-99-3]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
SRECVVXQFXRBNI-UHFFFAOYSA-N					
4-methyl-4-isopropylheptane	8.9×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61869-00-9]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
LSJZMBVEVGYTAG-UHFFFAOYSA-N					
3,3-diethylheptane	9.1×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-17-9]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
XATIZWAWQAIMQJ-UHFFFAOYSA-N					
3,4-diethylheptane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61869-01-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
UWOPVDFSBGDRJR-UHFFFAOYSA-N					
3,5-diethylheptane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61869-02-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
OBHTWTQZINRNAB-UHFFFAOYSA-N					
4,4-diethylheptane	9.6×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-21-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
WDTMGYSKSAMSPF-UHFFFAOYSA-N					
4-*tert*-butylheptane	9.6×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[60302-21-8]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
MDOHZJRFNISIIH-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,3,3,4-pentamethylhexane	6.6×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-85-7]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
RSEBTOONCGVAKN-UHFFFAOYSA-N					
2,2,3,3,5-pentamethylhexane	7.9×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-86-8]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
QGVXFIIZUSICQO-UHFFFAOYSA-N					
2,2,3,4,4-pentamethylhexane	6.5×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-87-9]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
HBVQLCKOFAUQGY-UHFFFAOYSA-N					
2,2,3,4,5-pentamethylhexane	8.2×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-88-0]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
LDUJDGROUWHEKU-UHFFFAOYSA-N					
2,2,3,5,5-pentamethylhexane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[14739-73-2]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
UKYAYXXQXKPIBL-UHFFFAOYSA-N					
2,2,4,4,5-pentamethylhexane	7.3×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[60302-23-0]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
JQFZWBZEZYOCQL-UHFFFAOYSA-N					
2,3,3,4,4-pentamethylhexane	6.4×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-89-1]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
GHRPCKCGHFDDOH-UHFFFAOYSA-N					
2,3,3,4,5-pentamethylhexane	7.5×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[52670-33-4]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
STMIMOZUYGUOQZ-UHFFFAOYSA-N					
2,2,3-trimethyl-3-ethylhexane	7.5×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-72-2]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
HUAYVWMWWLHZAB-UHFFFAOYSA-N					
2,2,3-trimethyl-4-ethylhexane	8.6×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-73-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
ZSUMTZIXJNZKBI-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,4-trimethyl-3-ethylhexane	8.7×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-74-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
UDUTWNYTAVENNO-UHFFFAOYSA-N					
2,2,4-trimethyl-4-ethylhexane	7.7×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-75-5]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
YFQDCXGMLYJDSG-UHFFFAOYSA-N					
2,2,5-trimethyl-3-ethylhexane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-76-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
GJVFOLLEVKEKMU-UHFFFAOYSA-N					
2,2,5-trimethyl-4-ethylhexane	9.9×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-77-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
UKTBERWYLDSZDQ-UHFFFAOYSA-N					
2,3,3-trimethyl-4-ethylhexane	7.9×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-78-8]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
DNDCULLMOLSZER-UHFFFAOYSA-N					
2,3,4-trimethyl-3-ethylhexane	7.6×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-79-9]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
XCNOKZUAQAZTAJ-UHFFFAOYSA-N					
2,3,4-trimethyl-4-ethylhexane	8.2×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-80-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
HNNSQDJQJRTMMW-UHFFFAOYSA-N					
2,3,5-trimethyl-3-ethylhexane	8.6×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-81-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
VYVPEEFLIYVOTH-UHFFFAOYSA-N					
2,3,5-trimethyl-4-ethylhexane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-82-4]	9.6×10^{-7}		Gharagheizi et al. (2010)	Q	247
LDKMZLRIVWGQRW-UHFFFAOYSA-N					
2,4,4-trimethyl-3-ethylhexane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-83-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
MTYPKDRKJRWXKB-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3,4-trimethyl-4-ethylhexane	6.8×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-84-6]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
ADDYWUNUHVKQGT-UHFFFAOYSA-N					
2,2-dimethyl-3-isopropylhexane	9.1×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-63-1]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
VKABOTNMFKIVDN-UHFFFAOYSA-N					
2,3-dimethyl-3-isopropylhexane	8.2×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-64-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
XVWGUCNHEXRNJU-UHFFFAOYSA-N					
2,4-dimethyl-3-isopropylhexane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-65-3]	9.6×10^{-7}		Gharagheizi et al. (2010)	Q	247
QRNSQXWPYPLHTL-UHFFFAOYSA-N					
2,5-dimethyl-3-isopropylhexane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-66-4]	9.6×10^{-7}		Gharagheizi et al. (2010)	Q	247
QKICRGDGSLQROM-UHFFFAOYSA-N					
2-methyl-3,3-diethylhexane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-67-5]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
QNRHKXCWHYUEKP-UHFFFAOYSA-N					
2-methyl-3,4-diethylhexane	9.8×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-68-6]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
MWHIPTVSAPEYPC-UHFFFAOYSA-N					
2-methyl-4,4-diethylhexane	9.0×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-69-7]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
UNPXTJSCIHOMKB-UHFFFAOYSA-N					
3-methyl-3,4-diethylhexane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-70-0]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
ZFMWIWWLOKHXHC-UHFFFAOYSA-N					
3-methyl-4,4-diethylhexane	8.1×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-71-1]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
CUHCCZRBXHOAMW-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,3,3,4,4-hexamethylpentane	5.0×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[60302-27-4]	7.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
JKJQSSSRSKPVEM-UHFFFAOYSA-N					
2,2,3,4-tetramethyl-3-ethylpentane	6.5×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-93-7]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
HBSINJYUKWVYBC-UHFFFAOYSA-N					
2,2,4,4-tetramethyl-3-ethylpentane	6.9×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[3178-30-1]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
FNWCWFQEEKFGHB-UHFFFAOYSA-N					
2,2,4-trimethyl-3-isopropylpentane	8.7×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	9.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-90-4]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
SZPCILWZDHUKLW-UHFFFAOYSA-N					
2,3,4-trimethyl-3-isopropylpentane	7.1×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-91-5]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
FHBFVPOXLRZZPP-UHFFFAOYSA-N					
2,2-dimethyl-3,3-diethylpentane	6.8×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[60302-28-5]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
KCQSYGZVYTYSLG-UHFFFAOYSA-N					
2,4-dimethyl-3,3-diethylpentane	7.5×10^{-7}		Yaws (2003)	X	238
$C_{11}H_{24}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-92-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
VVQOQVXGUMJNET-UHFFFAOYSA-N					
dodecane	1.2×10^{-6}		Plyasunov and Shock (2000)	L	
$C_{12}H_{26}$	1.3×10^{-6}		Mackay and Shiu (1981)	L	
[112-40-3]	1.2×10^{-6}		Duchowicz et al. (2020)	V	187
SNRUBQQJIBEYMU-UHFFFAOYSA-N	1.2×10^{-6}		HSDB (2015)	V	
	1.2×10^{-6}		Mackay et al. (2006a)	V	
	1.3×10^{-6}		Eastcott et al. (1988)	V	
	1.2×10^{-6}		Abraham (1984)	V	
	1.2×10^{-6}		Yaws (2003)	X	259
	1.2×10^{-6}		Yaws (2003)	X	238
	3.0×10^{-6}		Dupeux et al. (2022)	Q	260
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	1.7×10^{-5}		Wang et al. (2017)	Q	81, 239
	8.5×10^{-7}		Wang et al. (2017)	Q	81, 240
	5.3×10^{-6}		Wang et al. (2017)	Q	81, 241
	5.1×10^{-6}		Gharagheizi et al. (2012)	Q	

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-6}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-7}		Raventos-Duran et al. (2010)	Q	246
	1.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
	1.1×10^{-6}		Hilal et al. (2008)	Q	
	3.1×10^{-6}		Modarresi et al. (2007)	Q	68
	1.2×10^{-6}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
2-methylundecane $C_{12}H_{26}$ [31807-55-3] GTJOHISYCKPIMT-UHFFFAOYSA-N	1.1×10^{-6}		Yaws (2003)	X	238
	4.2×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
3-methylundecane $C_{12}H_{26}$ [1002-43-3] HTZWVZNRDDOFEI-UHFFFAOYSA-N	1.1×10^{-6}		Yaws (2003)	X	238
	4.2×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
4-methylundecane $C_{12}H_{26}$ [2980-69-0] KNMXZGDUJVOTOC-UHFFFAOYSA-N	1.1×10^{-6}		Yaws (2003)	X	238
	2.7×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
5-methylundecane $C_{12}H_{26}$ [1632-70-8] QULNVKABFWNUCW-UHFFFAOYSA-N	1.1×10^{-6}		Yaws (2003)	X	238
	2.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
6-methylundecane $C_{12}H_{26}$ [17302-33-9] VPYZCUCKYWHJGX-UHFFFAOYSA-N	1.1×10^{-6}		Yaws (2003)	X	238
	2.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
2,2-dimethyldecane $C_{12}H_{26}$ [17302-37-3] WBWYXWILSHQILH-UHFFFAOYSA-N	9.1×10^{-7}		Yaws (2003)	X	238
	3.3×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
2,3-dimethyldecane $C_{12}H_{26}$ [17312-44-6] ZCTGYLNFWOQVHV-UHFFFAOYSA-N	1.0×10^{-6}		Yaws (2003)	X	238
	2.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
2,4-dimethyldecane $C_{12}H_{26}$ [2801-84-5] OJAFXEXESSNPMH-UHFFFAOYSA-N	1.0×10^{-6}		Yaws (2003)	X	238
	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,5-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-50-4]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
DQHKBYZSYRJBMD-UHFFFAOYSA-N					
2,6-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[13150-81-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
DHJGXZWEQBKLNV-UHFFFAOYSA-N					
2,7-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	2.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-51-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
RVQIXUWWPOTVNP-UHFFFAOYSA-N					
2,8-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	2.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-52-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
KSRGGHUVCVWVDW-UHFFFAOYSA-N					
2,9-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	5.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[1002-17-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
HWISDPDDDUZJAW-UHFFFAOYSA-N					
3,3-dimethyldecane	9.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-38-4]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
URERYYDSQOIHQK-UHFFFAOYSA-N					
3,4-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-45-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
NRBMEEDORZDRIT-UHFFFAOYSA-N					
3,5-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-48-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
XXSUEVGKGOUJMD-UHFFFAOYSA-N					
3,6-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-53-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
NQWFSCYWTXQNGG-UHFFFAOYSA-N					
3,7-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-54-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
VDAVEASVPZDNQB-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,8-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-55-9]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
KMAHIPNGGSOJSM-UHFFFAOYSA-N					
4,4-dimethyldecane	9.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-39-9]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
WZCACTKWHXCWFZ-UHFFFAOYSA-N					
4,5-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-46-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
QZFIIEYSHODCSV-UHFFFAOYSA-N					
4,6-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-49-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
TVGNRLXIJXKVGD-UHFFFAOYSA-N					
4,7-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-56-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
GCKWUFQALHAZDH-UHFFFAOYSA-N					
5,5-dimethyldecane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17453-92-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
RNXSOUOIPAWOAC-UHFFFAOYSA-N					
5,6-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[1636-43-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
NCJIZIYQFWXMFZ-UHFFFAOYSA-N					
3-ethyldecane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	2.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[17085-96-0]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
ZBDDVSBBCGZQDV-UHFFFAOYSA-N					
4-ethyldecane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[1636-44-8]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
IGTKVLJTIZALGL-UHFFFAOYSA-N					
5-ethyldecane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-36-2]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
BCQLAHKMMOGIIS-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,3-trimethylnonane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[55499-04-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
XXNUJUNKYOZLAJ-UHFFFAOYSA-N					
2,2,4-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-50-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
YYYAICGYFLHBIN-UHFFFAOYSA-N					
2,2,5-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-51-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
ZIXRFABUOOUIMA-UHFFFAOYSA-N					
2,2,6-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-52-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
BUTMZMIZSWINDK-UHFFFAOYSA-N					
2,2,7-trimethylnonane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-53-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
PXOURNMYVAOUML-UHFFFAOYSA-N					
2,2,8-trimethylnonane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-54-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
WXUAVABOZJOELJ-UHFFFAOYSA-N					
2,3,3-trimethylnonane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-55-8]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
RSUFJUIYLXRYFG-UHFFFAOYSA-N					
2,3,4-trimethylnonane	9.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-56-9]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
RRZRZLRUYPZYEH-UHFFFAOYSA-N					
2,3,5-trimethylnonane	9.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-57-0]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
IESSJVKAXJWJFD-UHFFFAOYSA-N					
2,3,6-trimethylnonane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-58-1]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
AUXUELQPRQTQBE-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,7-trimethylnonane	9.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-59-2]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
GGUGBCMHEULHJS-UHFFFAOYSA-N					
2,3,8-trimethylnonane	9.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-60-5]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
GQHCJRDJABETBJ-UHFFFAOYSA-N					
2,4,4-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-61-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
RRLKOZCPQXMIIJ-UHFFFAOYSA-N					
2,4,5-trimethylnonane	9.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-62-7]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
NZAPYIGNIYRJNJ-UHFFFAOYSA-N					
2,4,6-trimethylnonane	9.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-10-5]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
QCQMRLDBNMVKOZ-UHFFFAOYSA-N					
2,4,7-trimethylnonane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-11-6]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
OHBDIVOYUFLOTO-UHFFFAOYSA-N					
2,4,8-trimethylnonane	9.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[49542-74-7]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
PZXMOJBYRFSNJH-UHFFFAOYSA-N					
2,5,5-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-12-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
ZRRKWMYBHUMSTG-UHFFFAOYSA-N					
2,5,6-trimethylnonane	9.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-13-8]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
KXHDWXIQHWSOHI-UHFFFAOYSA-N					
2,5,7-trimethylnonane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-14-9]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
KMBPYTMBXFKXON-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,5,8-trimethylnonane	9.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[49557-09-7]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
YYZRNFMGAQMLJJ-UHFFFAOYSA-N					
2,6,6-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-15-0]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
MTPVPWZHWOHMQT-UHFFFAOYSA-N					
2,6,7-trimethylnonane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-16-1]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
PGLYQCHTCUBASV-UHFFFAOYSA-N					
2,7,7-trimethylnonane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-17-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
RCTMUTWYOMEASD-UHFFFAOYSA-N					
3,3,4-trimethylnonane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-18-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
RNCRKMFELJSFRA-UHFFFAOYSA-N					
3,3,5-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-19-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
KRWQPUYFIGHZNF-UHFFFAOYSA-N					
3,3,6-trimethylnonane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-20-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
GPSMOBMYMZBKGT-UHFFFAOYSA-N					
3,3,7-trimethylnonane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-21-8]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
NZYGFHSHEQXPFT-UHFFFAOYSA-N					
3,4,4-trimethylnonane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-22-9]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
UYNWXBDPBKCTRS-UHFFFAOYSA-N					
3,4,5-trimethylnonane	9.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-23-0]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
PFVDUOFPBLPHEQ-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4,6-trimethylnonane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-24-1]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
VSRUKIVBXBGRDU-UHFFFAOYSA-N					
3,4,7-trimethylnonane	9.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[27802-85-3]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
HQIBDLHPQGDJEW-UHFFFAOYSA-N					
3,5,5-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-25-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
MUVSDRJGHVLJQX-UHFFFAOYSA-N					
3,5,6-trimethylnonane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-26-3]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
HMCPPWBQUPZETF-UHFFFAOYSA-N					
3,5,7-trimethylnonane	9.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-27-4]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
LLVWEFHXQBAEJX-UHFFFAOYSA-N					
3,6,6-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-28-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
CBDYLMAJISNHBH-UHFFFAOYSA-N					
4,4,5-trimethylnonane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-29-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
QLJZSYCAASGFGU-UHFFFAOYSA-N					
4,4,6-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-30-9]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
KBTTWWLCACXOSV-UHFFFAOYSA-N					
4,5,5-trimethylnonane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-31-0]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
QVDLUCCOJXIINS-UHFFFAOYSA-N					
4,5,6-trimethylnonane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62211-85-2]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
BBEKERHGCOZOIX-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-3-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-73-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
NVCDNLWOUSWNRQ-UHFFFAOYSA-N					
2-methyl-4-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-37-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
GRYPXYDXCQOVAY-UHFFFAOYSA-N					
2-methyl-5-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-38-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
WZWWJMDOQQIPJZ-UHFFFAOYSA-N					
2-methyl-6-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-39-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
GBMUYXDAAUUNLY-UHFFFAOYSA-N					
2-methyl-7-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-40-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
PHPGTUZXJVCCKP-UHFFFAOYSA-N					
3-methyl-3-ethylnonane	9.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-39-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
MJZXPSBAAXOUJF-UHFFFAOYSA-N					
3-methyl-4-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-41-2]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
ZELDGOVWPZHVJS-UHFFFAOYSA-N					
3-methyl-5-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-42-3]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
GDUZVOIDJDZQBC-UHFFFAOYSA-N					
3-methyl-6-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-43-4]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
WSMCXXNPFLZSMY-UHFFFAOYSA-N					
3-methyl-7-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-44-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
FSGFZSLYTXQNCW-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methyl-3-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-45-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
AUMKRFNJSTUECA-UHFFFAOYSA-N					
4-methyl-4-ethylnonane	9.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[17312-40-2]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
LXQCGRFCISXKCQ-UHFFFAOYSA-N					
4-methyl-5-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-46-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
BDJIXOFXGLDYLN-UHFFFAOYSA-N					
4-methyl-6-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-47-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
SULZKBWLMOBACQ-UHFFFAOYSA-N					
4-methyl-7-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-48-9]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
HYIBWPIYSSTZLB-UHFFFAOYSA-N					
5-methyl-3-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-49-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
ZBALIHDUORTBQR-UHFFFAOYSA-N					
5-methyl-4-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[1632-71-9]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
HKUUNAOHRKAJIY-UHFFFAOYSA-N					
5-methyl-5-ethylnonane	9.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[14531-16-9]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
DZSBQMNPPIKBNF-UHFFFAOYSA-N					
4-propylnonane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[6165-37-3]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
QLKPGWNXMMBQMG-UHFFFAOYSA-N					
5-propylnonane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[998-35-6]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
ISHSSTRAYNPQFX-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-isopropylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-71-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
BXYKZQOGHMLDIE-UHFFFAOYSA-N					
5-isopropylnonane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-72-9]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
ALZCRHWYCQKCQK-UHFFFAOYSA-N					
2,2,3,3-tetramethyloctane	6.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-74-8]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
UXQAEOWCSOPBLF-UHFFFAOYSA-N					
2,2,3,4-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-75-9]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
HEJULKHHKGYPNT-UHFFFAOYSA-N					
2,2,3,5-tetramethyloctane	8.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-76-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
MRBTZFDZTJYCAO-UHFFFAOYSA-N					
2,2,3,6-tetramethyloctane	7.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-77-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
YRSBZJIBIXVOME-UHFFFAOYSA-N					
2,2,3,7-tetramethyloctane	7.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-78-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
CPEHPCZXBBEYOL-UHFFFAOYSA-N					
2,2,4,4-tetramethyloctane	7.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-79-3]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
TYUFTNSABIBNRY-UHFFFAOYSA-N					
2,2,4,5-tetramethyloctane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-80-6]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
SNJCVPBJFQJMFW-UHFFFAOYSA-N					
2,2,4,6-tetramethyloctane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-81-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
ODZRFEPMTHWMBK-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,4,7-tetramethyloctane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-82-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
QHDQKPZLRKHEHV-UHFFFAOYSA-N					
2,2,5,5-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	5.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-83-9]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
RJJMZKVKQLGGDK-UHFFFAOYSA-N					
2,2,5,6-tetramethyloctane	8.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-84-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
BQUVPJLOJUCQGM-UHFFFAOYSA-N					
2,2,5,7-tetramethyloctane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-19-3]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
ISTINYWNHRBEDQ-UHFFFAOYSA-N					
2,2,6,6-tetramethyloctane	7.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-20-6]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
BANZIZHQGFRTMI-UHFFFAOYSA-N					
2,2,6,7-tetramethyloctane	8.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-21-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
ZSXJNQURTCJFGP-UHFFFAOYSA-N					
2,2,7,7-tetramethyloctane	7.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[1071-31-4]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
QZUFNKONEPLWBC-UHFFFAOYSA-N					
2,3,3,4-tetramethyloctane	7.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-22-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
ITTRGXLKGDMYDX-UHFFFAOYSA-N					
2,3,3,5-tetramethyloctane	7.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-23-9]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
RVOIBAZQSHFKMM-UHFFFAOYSA-N					
2,3,3,6-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-24-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
MBJHOSHYIFXEPL-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3,7-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-25-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
WWQBXZREQWIXFF-UHFFFAOYSA-N					
2,3,4,4-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-26-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
MELCVUZPHQRNTK-UHFFFAOYSA-N					
2,3,4,5-tetramethyloctane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-27-3]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
AMIZVDCCXDQOHL-UHFFFAOYSA-N					
2,3,4,6-tetramethyloctane	8.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-28-4]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
OYZWSGWTBSWCLN-UHFFFAOYSA-N					
2,3,4,7-tetramethyloctane	8.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-29-5]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
YUCNZDFGMLKYFT-UHFFFAOYSA-N					
2,3,5,5-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-30-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
RQOLUXQWYAKKTG-UHFFFAOYSA-N					
2,3,5,6-tetramethyloctane	8.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-31-9]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
IPYLOMHOPWIUFA-UHFFFAOYSA-N					
2,3,5,7-tetramethyloctane	8.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-32-0]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
AIUMUUQTYGQPMV-UHFFFAOYSA-N					
2,3,6,6-tetramethyloctane	7.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-33-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
CVRMZIOMFWYAPV-UHFFFAOYSA-N					
2,3,6,7-tetramethyloctane	8.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[52670-34-5]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
FZCGYGCYZRXLDY-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4,4,5-tetramethyloctane	8.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-34-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
OBWRJGVWBWXXAO-UHFFFAOYSA-N					
2,4,4,6-tetramethyloctane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-35-3]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
UQCGTRPILZWACX-UHFFFAOYSA-N					
2,4,4,7-tetramethyloctane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	5.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[35866-96-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
QYUWMFZODNLLRJ-UHFFFAOYSA-N					
2,4,5,5-tetramethyloctane	8.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-36-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
OMFWIGPPTXTQHH-UHFFFAOYSA-N					
2,4,5,6-tetramethyloctane	8.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-37-5]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
YJMGKHXCSVEVKG-UHFFFAOYSA-N					
2,4,5,7-tetramethyloctane	9.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[2217-17-6]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
PWYLDJLMYGOPSR-UHFFFAOYSA-N					
2,4,6,6-tetramethyloctane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-38-6]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
VVEPRQWGSASPPP-UHFFFAOYSA-N					
2,5,5,6-tetramethyloctane	7.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-39-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
DLCPMTDXNVOOLU-UHFFFAOYSA-N					
2,5,6,6-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-40-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
SQOVOQLOSFZJGI-UHFFFAOYSA-N					
3,3,4,4-tetramethyloctane	6.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-41-1]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
VXEUNQVVVNDDTL-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3,4,5-tetramethyloctane	7.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-42-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
FATMBSLXTUXZBP-UHFFFAOYSA-N					
3,3,4,6-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-43-3]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
VCXMKRQQDPQALS-UHFFFAOYSA-N					
3,3,5,5-tetramethyloctane	7.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-44-4]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
UJLDJWNVZROTLS-UHFFFAOYSA-N					
3,3,5,6-tetramethyloctane	7.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-45-5]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
AQPSWWWUVHSZJK-UHFFFAOYSA-N					
3,3,6,6-tetramethyloctane	7.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-46-6]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
PAEUGKMMSQUAGH-UHFFFAOYSA-N					
3,4,4,5-tetramethyloctane	7.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-47-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
HWNTXBYEGXKWKG-UHFFFAOYSA-N					
3,4,4,6-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-19-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
LNRFUGUGPGLBLV-UHFFFAOYSA-N					
3,4,5,5-tetramethyloctane	7.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-20-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
NCNZUEBQNGRARF-UHFFFAOYSA-N					
3,4,5,6-tetramethyloctane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-21-1]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
NADJQGPTQSFIHB-UHFFFAOYSA-N					
4,4,5,5-tetramethyloctane	6.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-22-2]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
INTYEXUWOYUVGJ-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2-dimethyl-3-ethyloctane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-95-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
LIZQPVRBTUZZCL-UHFFFAOYSA-N					
2,2-dimethyl-4-ethyloctane	9.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-96-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
PEGJIJFSOTZJFH-UHFFFAOYSA-N					
2,2-dimethyl-5-ethyloctane	8.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-97-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
ACWGGQUVVQOZPJ-UHFFFAOYSA-N					
2,2-dimethyl-6-ethyloctane	8.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-98-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
SHNILIMSRTWRKG-UHFFFAOYSA-N					
2,3-dimethyl-3-ethyloctane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-99-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
NDFHPGVSCVJNFR-UHFFFAOYSA-N					
2,3-dimethyl-4-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-00-3]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
DCBIYDZULXWXTQ-UHFFFAOYSA-N					
2,3-dimethyl-5-ethyloctane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-01-4]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
NPUNZBBVZZNRNS-UHFFFAOYSA-N					
2,3-dimethyl-6-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-02-5]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
BWSXPPUMTZVKPA-UHFFFAOYSA-N					
2,4-dimethyl-3-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-03-6]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
QYHDQDAUJCPVFJ-UHFFFAOYSA-N					
2,4-dimethyl-4-ethyloctane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-04-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
XAKSPVTVTMAMDT-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4-dimethyl-5-ethyloctane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-05-8]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
JHDZOLPKXSWZKD-UHFFFAOYSA-N					
2,4-dimethyl-6-ethyloctane	9.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-06-9]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
VGDSKYYXZZCASQ-UHFFFAOYSA-N					
2,5-dimethyl-3-ethyloctane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-07-0]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
BCQWMBQACXNHGP-UHFFFAOYSA-N					
2,5-dimethyl-4-ethyloctane	9.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-08-1]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
IMMDGMKEESKIQT-UHFFFAOYSA-N					
2,5-dimethyl-5-ethyloctane	8.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-09-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
BVAIFAWSJOPLJD-UHFFFAOYSA-N					
2,5-dimethyl-6-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-50-0]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
CYTDZGRTFHXLQS-UHFFFAOYSA-N					
2,6-dimethyl-3-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-51-1]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
WAFCPUFGSNTFSP-UHFFFAOYSA-N					
2,6-dimethyl-4-ethyloctane	9.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-52-2]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
JIOQMQLJPQDNFA-UHFFFAOYSA-N					
2,6-dimethyl-5-ethyloctane	9.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-53-3]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
ZBMWKURVBLDBAH-UHFFFAOYSA-N					
2,6-dimethyl-6-ethyloctane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-54-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
DGFWFJRTTJTVEQ-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,7-dimethyl-3-ethyloctane	9.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-55-5]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
XEMFRSYZKNPRTA-UHFFFAOYSA-N					
2,7-dimethyl-4-ethyloctane	9.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-56-6]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
KSVMIUVYLYZDMT-UHFFFAOYSA-N					
3,3-dimethyl-4-ethyloctane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-57-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
BKNJDUXGYCILJT-UHFFFAOYSA-N					
3,3-dimethyl-5-ethyloctane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-58-8]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
GQTCKTISADWVNV-UHFFFAOYSA-N					
3,3-dimethyl-6-ethyloctane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-59-9]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
DDRNTRVXHMVVLA-UHFFFAOYSA-N					
3,4-dimethyl-3-ethyloctane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62212-28-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
AOQVLRSMPNHJPF-UHFFFAOYSA-N					
3,4-dimethyl-4-ethyloctane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-60-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
WBKPODGAYHVUMM-UHFFFAOYSA-N					
3,4-dimethyl-5-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-61-3]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
LEPWFUNEXVKPDO-UHFFFAOYSA-N					
3,4-dimethyl-6-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-62-4]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
DPDGQUDZYGOBAM-UHFFFAOYSA-N					
3,5-dimethyl-3-ethyloctane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-63-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
QYJKERUDQYOWRC-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,5-dimethyl-4-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-64-6]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
OMAJEXDENFMCIN-UHFFFAOYSA-N					
3,5-dimethyl-5-ethyloctane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-65-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
OLBJDMSGRVKJMF-UHFFFAOYSA-N					
3,5-dimethyl-6-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-66-8]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
LLHGAWREVJAITE-UHFFFAOYSA-N					
3,6-dimethyl-3-ethyloctane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-67-9]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
MNXPIOFJFYQCKE-UHFFFAOYSA-N					
3,6-dimethyl-4-ethyloctane	9.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-68-0]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
RTVRGBUFZDOPIH-UHFFFAOYSA-N					
4,4-dimethyl-3-ethyloctane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-69-1]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
RHSANRLUOZFJDW-UHFFFAOYSA-N					
4,4-dimethyl-5-ethyloctane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-70-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
BETVNWPSZXTJLK-UHFFFAOYSA-N					
4,4-dimethyl-6-ethyloctane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-71-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
UGEWSKWSWHZABT-UHFFFAOYSA-N					
4,5-dimethyl-3-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-72-6]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
MNDPOEACQSQPCJ-UHFFFAOYSA-N					
4,5-dimethyl-4-ethyloctane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-73-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
MOEUNMMPAYEJOZ-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3-diethyloctane	9.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-40-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
DGJISSKLLWWXTG-UHFFFAOYSA-N					
3,4-diethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-92-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
HILZBOWVGZXYGQ-UHFFFAOYSA-N					
3,5-diethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-93-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
DSYIMNMBWBEOHY-UHFFFAOYSA-N					
3,6-diethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-94-2]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
UTCTYSTYZOAAOS-UHFFFAOYSA-N					
4,4-diethyloctane	9.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[17312-42-4]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
FTEQKVNFZNDQJG-UHFFFAOYSA-N					
4,5-diethyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[1636-41-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
XRVCHXCONYJHLU-UHFFFAOYSA-N					
2-methyl-4-propyloctane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-33-2]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
FJPVBTBEYVNWCA-UHFFFAOYSA-N					
2-methyl-5-propyloctane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-34-3]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
NYBDGQCIJCAIJL-UHFFFAOYSA-N					
3-methyl-4-propyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-35-4]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
CTXPEFTVFFFIBQ-UHFFFAOYSA-N					
3-methyl-5-propyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-36-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
VOSHMCRSZWNTLJ-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methyl-4-propyloctane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[17312-41-3]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
RNKCZSBPRRHTOZ-UHFFFAOYSA-N					
4-methyl-5-propyloctane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-85-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
MVUWSCFPURGAJF-UHFFFAOYSA-N					
2-methyl-3-isopropyloctane	9.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[13287-19-9]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
KBIUKRVYBYJVSS-UHFFFAOYSA-N					
2-methyl-4-isopropyloctane	9.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-86-2]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
NRRICFUUPCDSKW-UHFFFAOYSA-N					
2-methyl-5-isopropyloctane	9.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-87-3]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
OPKVPKXVSDEXOZ-UHFFFAOYSA-N					
3-methyl-4-isopropyloctane	9.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-88-4]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
UXTHXSNAZBLVOD-UHFFFAOYSA-N					
3-methyl-5-isopropyloctane	9.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-89-5]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
VEJPAYNPRZYJNN-UHFFFAOYSA-N					
4-methyl-4-isopropyloctane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-90-8]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
KCNISWXEVSJYRS-UHFFFAOYSA-N					
4-methyl-5-isopropyloctane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-91-9]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
HEFVKUUZAXCMQX-UHFFFAOYSA-N					
4-*tert*-butyloctane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-32-1]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
RWILNGDOCMDMJW-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,4,6,6-pentamethylheptane	7.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	4.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[13475-82-6]	1.1×10^{-6}		Zhang et al. (2010)	Q	288, 289
VKPSKYDESGTTFR-UHFFFAOYSA-N	2.3×10^{-7}		Zhang et al. (2010)	Q	288, 290
	2.4×10^{-5}		Zhang et al. (2010)	Q	288, 291
	5.1×10^{-6}		Zhang et al. (2010)	Q	288, 292
	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
2,2,3,3,4-pentamethylheptane	6.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-80-5]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
NTDYBHYVUCYILC-UHFFFAOYSA-N					
2,2,3,3,5-pentamethylheptane	6.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-81-6]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
ZLCPPJIFAFIYPV-UHFFFAOYSA-N					
2,2,3,3,6-pentamethylheptane	6.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-82-7]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
LYTFNNQFUUFUDH-UHFFFAOYSA-N					
2,2,3,4,4-pentamethylheptane	6.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-83-8]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
SUFPUVGFEWPIFA-UHFFFAOYSA-N					
2,2,3,4,5-pentamethylheptane	7.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-84-9]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
XYDYIKVIGCXDLV-UHFFFAOYSA-N					
2,2,3,4,6-pentamethylheptane	7.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-85-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
XRJGBYMRUIWAJP-UHFFFAOYSA-N					
2,2,3,5,5-pentamethylheptane	6.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-86-1]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
OSZLORKBJVWZNT-UHFFFAOYSA-N					
2,2,3,5,6-pentamethylheptane	7.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-87-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
MHJUEZDXDYXCPA-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,3,6,6-pentamethylheptane	7.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-88-3]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
SLGYOGBODYIQGW-UHFFFAOYSA-N					
2,2,4,4,5-pentamethylheptane	6.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-61-5]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
XRGPEBQZXVFCRE-UHFFFAOYSA-N					
2,2,4,4,6-pentamethylheptane	7.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-62-6]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
NOFQKTWPZFUCOO-UHFFFAOYSA-N					
2,2,4,5,5-pentamethylheptane	7.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-63-7]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
JGOKXUSMFJOVQT-UHFFFAOYSA-N					
2,2,4,5,6-pentamethylheptane	7.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-64-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
JVESFBBBMJIZLO-UHFFFAOYSA-N					
2,2,5,5,6-pentamethylheptane	7.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-65-9]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
FMJMMNPKKCFHTH-UHFFFAOYSA-N					
2,3,3,4,4-pentamethylheptane	6.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62199-66-0]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
VBOBCKMZHQJDQA-UHFFFAOYSA-N					
2,3,3,4,5-pentamethylheptane	7.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-67-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
OLZJEASBDLLWCY-UHFFFAOYSA-N					
2,3,3,4,6-pentamethylheptane	7.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-68-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
YENAHMOHMFYKPC-UHFFFAOYSA-N					
2,3,3,5,5-pentamethylheptane	6.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-69-3]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
DTLBRJVRUQMSQN-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3,5,6-pentamethylheptane	7.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[52670-35-6]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
SZQDOCSTKXRXAR-UHFFFAOYSA-N					
2,3,4,4,5-pentamethylheptane	7.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-70-6]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
CHHJLGDSEYTKKE-UHFFFAOYSA-N					
2,3,4,4,6-pentamethylheptane	7.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-71-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
DHXWMADSONSWTL-UHFFFAOYSA-N					
2,3,4,5,5-pentamethylheptane	7.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-72-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
BDFJISGXUJUYCX-UHFFFAOYSA-N					
2,3,4,5,6-pentamethylheptane	7.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[27574-98-7]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
YIKFFSNUOIJPSI-UHFFFAOYSA-N					
2,4,4,5,5-pentamethylheptane	6.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-73-9]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
TXGUYEKSMHZHSB-UHFFFAOYSA-N					
3,3,4,4,5-pentamethylheptane	6.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62199-74-0]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
YFXNIDIHYOGTEN-UHFFFAOYSA-N					
3,3,4,5,5-pentamethylheptane	6.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62199-75-1]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
NZIFKVSORPBQSX-UHFFFAOYSA-N					
2,2,3-trimethyl-3-ethylheptane	6.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-04-6]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
CVXGCQXACVZXQR-UHFFFAOYSA-N					
2,2,3-trimethyl-4-ethylheptane	7.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-05-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
COHRBFNOOUABCT-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,3-trimethyl-5-ethylheptane	8.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-06-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
OOIGDPTZPWRGHN-UHFFFAOYSA-N					
2,2,4-trimethyl-3-ethylheptane	8.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-07-9]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
TYGUUZVWCBYDKW-UHFFFAOYSA-N					
2,2,4-trimethyl-4-ethylheptane	7.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-08-0]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
XMUXASPVOBQLPC-UHFFFAOYSA-N					
2,2,4-trimethyl-5-ethylheptane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-09-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
QADOHJKDWMLCQT-UHFFFAOYSA-N					
2,2,5-trimethyl-3-ethylheptane	8.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-10-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
SUDWTPMZYLBGKW-UHFFFAOYSA-N					
2,2,5-trimethyl-4-ethylheptane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-11-5]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
GDPLKYYKURLRKJ-UHFFFAOYSA-N					
2,2,5-trimethyl-5-ethylheptane	7.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-12-6]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
KJWMMFYTYSUWMH-UHFFFAOYSA-N					
2,2,6-trimethyl-3-ethylheptane	8.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-13-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
RIIDJOQRWGTQEN-UHFFFAOYSA-N					
2,2,6-trimethyl-4-ethylheptane	8.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	5.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-14-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
QGYSVVWKEDKPTP-UHFFFAOYSA-N					
2,2,6-trimethyl-5-ethylheptane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-15-9]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
LYZRWXZZVRWJHX-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3-trimethyl-4-ethylheptane	7.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-16-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
VIIXOXRHJWHIBP-UHFFFAOYSA-N					
2,3,3-trimethyl-5-ethylheptane	7.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-17-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
JHGOLBUJAIJLCX-UHFFFAOYSA-N					
2,3,4-trimethyl-3-ethylheptane	7.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62199-18-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
YZXMDESZKHUODO-UHFFFAOYSA-N					
2,3,4-trimethyl-4-ethylheptane	7.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-55-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
QDWZIZQKVLESDK-UHFFFAOYSA-N					
2,3,4-trimethyl-5-ethylheptane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-56-5]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
URFFXJPJMCMXFR-UHFFFAOYSA-N					
2,3,5-trimethyl-3-ethylheptane	7.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-57-6]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
QHACFORXSGHTJG-UHFFFAOYSA-N					
2,3,5-trimethyl-4-ethylheptane	8.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-58-7]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
UEZAASCWBAVHRO-UHFFFAOYSA-N					
2,3,5-trimethyl-5-ethylheptane	7.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-59-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
LTSLSBVPXXAMBM-UHFFFAOYSA-N					
2,3,6-trimethyl-3-ethylheptane	7.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-60-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
KOVQAKVRXODFNL-UHFFFAOYSA-N					
2,3,6-trimethyl-4-ethylheptane	8.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-61-2]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
RBVKVRIWSQSXPO-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,6-trimethyl-5-ethylheptane	8.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-62-3]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
JXCQTSFHNKTOLJ-UHFFFAOYSA-N					
2,4,4-trimethyl-3-ethylheptane	7.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-63-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
BNFUBMCCIACHFX-UHFFFAOYSA-N					
2,4,4-trimethyl-5-ethylheptane	8.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-64-5]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
YSCJXRHNKUXHLH-UHFFFAOYSA-N					
2,4,5-trimethyl-3-ethylheptane	8.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-65-6]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
JFKSTTDMBQAPCT-UHFFFAOYSA-N					
2,4,5-trimethyl-4-ethylheptane	7.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-66-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
HSVLOEWHJNAWLC-UHFFFAOYSA-N					
2,4,5-trimethyl-5-ethylheptane	7.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-67-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
JAUBFUIZENVVAG-UHFFFAOYSA-N					
2,4,6-trimethyl-3-ethylheptane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-68-9]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
KQBJYFJWQOUHCI-UHFFFAOYSA-N					
2,4,6-trimethyl-4-ethylheptane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-69-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
LPNPQCHEMXFBSW-UHFFFAOYSA-N					
2,5,5-trimethyl-3-ethylheptane	8.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-70-3]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
MARFNXCIPCRAJU-UHFFFAOYSA-N					
2,5,5-trimethyl-4-ethylheptane	8.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-71-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
HGYOEMXZYDBOKQ-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3,4-trimethyl-4-ethylheptane	6.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62198-72-5]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
QLOXTBGCIUOWIG-UHFFFAOYSA-N					
3,3,4-trimethyl-5-ethylheptane	7.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-73-6]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
CUWOOQVXUDOHOC-UHFFFAOYSA-N					
3,3,5-trimethyl-4-ethylheptane	7.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-74-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
QXCHZKHHIUTBOU-UHFFFAOYSA-N					
3,3,5-trimethyl-5-ethylheptane	6.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-75-8]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
GCWLDOMARVHVOZ-UHFFFAOYSA-N					
3,4,4-trimethyl-3-ethylheptane	6.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62198-76-9]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
SIIFYRMARKBLER-UHFFFAOYSA-N					
3,4,4-trimethyl-5-ethylheptane	7.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-77-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
XSLWCLUAFIVTLD-UHFFFAOYSA-N					
3,4,5-trimethyl-3-ethylheptane	7.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-78-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
ZHILUIHUWKDTTM-UHFFFAOYSA-N					
3,4,5-trimethyl-4-ethylheptane	7.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62198-79-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
SZOKDASFURUJDF-UHFFFAOYSA-N					
2,2-dimethyl-4-propylheptane	9.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	5.8×10^{-7}		Gharagheizi et al. (2012)	Q	
DWEXNJRCPKKJBQ-UHFFFAOYSA-N	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
2,3-dimethyl-4-propylheptane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-30-2]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
AZUDVOIXPNEOLR-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4-dimethyl-4-propylheptane $C_{12}H_{26}$ [62185-31-3] FDVJFPZZPSPQAO-UHFFFAOYSA-N	8.9×10^{-7} 6.7×10^{-7} 8.7×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
2,5-dimethyl-4-propylheptane $C_{12}H_{26}$ [62185-32-4] PJXVVWKRCASATD-UHFFFAOYSA-N	9.7×10^{-7} 6.8×10^{-7} 9.2×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
2,6-dimethyl-4-propylheptane $C_{12}H_{26}$ [62185-33-5] UFJZYHSURMZROL-UHFFFAOYSA-N	1.0×10^{-6} 5.9×10^{-7} 9.2×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
3,3-dimethyl-4-propylheptane $C_{12}H_{26}$ [62185-34-6] XVWBLUKOUJTCDO-UHFFFAOYSA-N	8.5×10^{-7} 8.2×10^{-7} 8.7×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
3,4-dimethyl-4-propylheptane $C_{12}H_{26}$ [62185-35-7] UGSAJWKYCFFZRD-UHFFFAOYSA-N	8.4×10^{-7} 8.6×10^{-7} 8.7×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
3,5-dimethyl-4-propylheptane $C_{12}H_{26}$ [62185-36-8] GKVRDSIZILZQJE-UHFFFAOYSA-N	9.4×10^{-7} 8.1×10^{-7} 9.2×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
2,2-dimethyl-3-isopropylheptane $C_{12}H_{26}$ [62185-37-9] XPOSVKCTMHOWTN-UHFFFAOYSA-N	8.1×10^{-7} 6.9×10^{-7} 8.0×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
2,2-dimethyl-4-isopropylheptane $C_{12}H_{26}$ [62185-38-0] HFRVMJCEWUXCMP-UHFFFAOYSA-N	8.7×10^{-7} 5.5×10^{-7} 8.0×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
2,3-dimethyl-3-isopropylheptane $C_{12}H_{26}$ [62185-39-1] IAWDNHPMOJTEEN-UHFFFAOYSA-N	7.6×10^{-7} 9.5×10^{-7} 8.0×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
2,3-dimethyl-4-isopropylheptane $C_{12}H_{26}$ [62185-40-4] GEQDAUMUCVOARW-UHFFFAOYSA-N	8.8×10^{-7} 7.3×10^{-7} 8.9×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4-dimethyl-3-isopropylheptane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-41-5]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
MWVRZCOXSIAHLW-UHFFFAOYSA-N					
2,4-dimethyl-4-isopropylheptane	8.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-42-6]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
MTPOSRQPOBWFQC-UHFFFAOYSA-N					
2,5-dimethyl-3-isopropylheptane	8.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-43-7]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
XSKMFUBSJXETFW-UHFFFAOYSA-N					
2,5-dimethyl-4-isopropylheptane	9.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-44-8]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
OOYWQZAQFKOCKA-UHFFFAOYSA-N					
2,6-dimethyl-3-isopropylheptane	8.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-45-9]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
NOAGKIODSFDOTA-UHFFFAOYSA-N					
2,6-dimethyl-4-isopropylheptane	9.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	5.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[35866-89-8]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
BIBHNAJLMRUJLS-UHFFFAOYSA-N					
3,3-dimethyl-4-isopropylheptane	7.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-46-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
MACIOLXBYDNTTI-UHFFFAOYSA-N					
3,4-dimethyl-4-isopropylheptane	7.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-47-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
QFKXRROMVRXZIF-UHFFFAOYSA-N					
3,5-dimethyl-4-isopropylheptane	8.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-89-4]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
XJRRTENBDSNHQB-UHFFFAOYSA-N					
2-methyl-3,3-diethylheptane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62198-90-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
VBKOVPDJLQIMSZ-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-3,4-diethylheptane	9.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-91-8]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
PRSHREOBBOOUSO-UHFFFAOYSA-N					
2-methyl-3,5-diethylheptane	9.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-92-9]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
KZTGLPPJUZINLQ-UHFFFAOYSA-N					
2-methyl-4,4-diethylheptane	8.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-93-0]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
VJTVFYMTOXDIID-UHFFFAOYSA-N					
2-methyl-4,5-diethylheptane	9.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-94-1]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
SRLQJPCYGKMUSM-UHFFFAOYSA-N					
2-methyl-5,5-diethylheptane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-95-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
XPAWKGLXSPHNAN-UHFFFAOYSA-N					
3-methyl-3,4-diethylheptane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-96-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
VRVVWJIPKQWWJB-UHFFFAOYSA-N					
3-methyl-3,5-diethylheptane	8.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-97-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
RGRSPNWZJFXFAN-UHFFFAOYSA-N					
3-methyl-4,4-diethylheptane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62198-98-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
WSBKWCXGZHVUHW-UHFFFAOYSA-N					
3-methyl-4,5-diethylheptane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-99-6]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
NVBVLQDXCRDBBU-UHFFFAOYSA-N					
3-methyl-5,5-diethylheptane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-00-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
JOJSCBROPYJHJX-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methyl-3,3-diethylheptane	8.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62199-01-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
KGSWPEXUAXYDMO-UHFFFAOYSA-N					
4-methyl-3,4-diethylheptane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-02-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
RAFABRWSQNCWEY-UHFFFAOYSA-N					
4-methyl-3,5-diethylheptane	9.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-03-5]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
XUVBJZPYCGZQDK-UHFFFAOYSA-N					
2-methyl-4-*tert*-butylheptane	8.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-23-3]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
HIHQJZLWJQHTEJ-UHFFFAOYSA-N					
3-methyl-4-*tert*-butylheptane	8.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-24-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
IKKVFRPBQQTTKP-UHFFFAOYSA-N					
4-methyl-4-*tert*-butylheptane	7.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-25-5]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
JABLMQZBFVBNBS-UHFFFAOYSA-N					
3-ethyl-4-propylheptane	1.0×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-26-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
FPODIYZXVCXXQE-UHFFFAOYSA-N					
4-ethyl-4-propylheptane	9.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[17312-43-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
JTZJHTZCYBYCSZ-UHFFFAOYSA-N					
3-ethyl-4-isopropylheptane	9.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-27-7]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
VENQCMDSFBOTMS-UHFFFAOYSA-N					
4-ethyl-4-isopropylheptane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-28-8]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
IKRHMKIYGHBTGZ-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,3,3,4,4-hexamethylhexane	4.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[62185-11-9]	6.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
ACZDZCRQHVWGEF-UHFFFAOYSA-N					
2,2,3,3,4,5-hexamethylhexane	5.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-12-0]	7.4×10^{-7}		Gharagheizi et al. (2010)	Q	247
IFHVEHXJQMYGHH-UHFFFAOYSA-N					
2,2,3,3,5,5-hexamethylhexane	5.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[60302-24-1]	6.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
YFGLJPQISFJQSO-UHFFFAOYSA-N					
2,2,3,4,4,5-hexamethylhexane	5.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62185-13-1]	7.4×10^{-7}		Gharagheizi et al. (2010)	Q	247
QJVUKMHIEDVCDT-UHFFFAOYSA-N					
2,2,3,4,5,5-hexamethylhexane	6.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-14-2]	7.4×10^{-7}		Gharagheizi et al. (2010)	Q	247
NXZMBOYMQLHOPD-UHFFFAOYSA-N					
2,3,3,4,4,5-hexamethylhexane	5.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[52670-36-7]	7.4×10^{-7}		Gharagheizi et al. (2010)	Q	247
GRVNDHRZJGSRDC-UHFFFAOYSA-N					
2,2,3,3-tetramethyl-4-ethylhexane	6.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-98-9]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
CRTTYRRLFPCOTC-UHFFFAOYSA-N					
2,2,3,4-tetramethyl-3-ethylhexane	6.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62184-99-0]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
SYWRGACXWPDDMM-UHFFFAOYSA-N					
2,2,3,4-tetramethyl-4-ethylhexane	6.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62185-00-6]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
WVLMCSYUMSZJQJ-UHFFFAOYSA-N					
2,2,3,5-tetramethyl-3-ethylhexane	6.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-01-7]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
CHURHVBNTYCJDL-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,3,5-tetramethyl-4-ethylhexane	7.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-02-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
GYAMSLKQDQYJGT-UHFFFAOYSA-N					
2,2,4,4-tetramethyl-3-ethylhexane	6.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-03-9]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
HWHADLCAKCOTRI-UHFFFAOYSA-N					
2,2,4,5-tetramethyl-3-ethylhexane	7.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-04-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
KZHIDSBQFJFWDV-UHFFFAOYSA-N					
2,2,4,5-tetramethyl-4-ethylhexane	6.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-05-1]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
HAVVVIZEMKFOFL-UHFFFAOYSA-N					
2,2,5,5-tetramethyl-3-ethylhexane	7.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	5.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-06-2]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
GJJUHGLRQQDIFN-UHFFFAOYSA-N					
2,3,3,4-tetramethyl-4-ethylhexane	6.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62185-07-3]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
YVKQGHGRZXUTNK-UHFFFAOYSA-N					
2,3,3,5-tetramethyl-4-ethylhexane	7.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-08-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
AMMSTTMNZHWREI-UHFFFAOYSA-N					
2,3,4,4-tetramethyl-3-ethylhexane	6.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62185-09-5]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
VYCKEOSFJUAFGK-UHFFFAOYSA-N					
2,3,4,5-tetramethyl-3-ethylhexane	6.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-10-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
IBPLCPRMAQRHHK-UHFFFAOYSA-N					
2,2,3-trimethyl-3-isopropylhexane	6.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-79-5]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
UTCSLOLKGOKPGW-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,4-trimethyl-3-isopropylhexane	7.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-80-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
VEMACPZMOMAUAN-UHFFFAOYSA-N					
2,2,5-trimethyl-3-isopropylhexane	8.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	5.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-81-9]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
GZFAXOCUKPGWEA-UHFFFAOYSA-N					
2,2,5-trimethyl-4-isopropylhexane	8.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	5.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-82-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
QFLYTOVYLBZBJC-UHFFFAOYSA-N					
2,3,4-trimethyl-3-isopropylhexane	6.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62199-83-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
SXELEUFFBZGXIC-UHFFFAOYSA-N					
2,3,5-trimethyl-3-isopropylhexane	7.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-84-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
GUMUKRVQSSIBJO-UHFFFAOYSA-N					
2,3,5-trimethyl-4-isopropylhexane	8.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-85-3]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
VBRDSJSWPGXVIR-UHFFFAOYSA-N					
2,4,4-trimethyl-3-isopropylhexane	7.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-86-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
UGPHXQWIHGYHOH-UHFFFAOYSA-N					
2,2-dimethyl-3,4-diethylhexane	8.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-89-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
ZAKPEOVUOZWBNO-UHFFFAOYSA-N					
2,2-dimethyl-4,4-diethylhexane	6.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-89-8]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
CYPRMBGQWCLJBN-UHFFFAOYSA-N					
2,3-dimethyl-3,4-diethylhexane	7.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62184-90-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
BUUBMKJJLVCTKU-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-dimethyl-4,4-diethylhexane	7.5×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62184-91-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
YNHBDJNMYMZVLM-UHFFFAOYSA-N					
2,4-dimethyl-3,3-diethylhexane	7.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-92-3]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
OXAROVXPKXMTIV-UHFFFAOYSA-N					
2,4-dimethyl-3,4-diethylhexane	7.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-93-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
AUVJTUXGNKLTIN-UHFFFAOYSA-N					
2,5-dimethyl-3,3-diethylhexane	8.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-94-5]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
XHDPVTDRZGCNFV-UHFFFAOYSA-N					
2,5-dimethyl-3,4-diethylhexane	8.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-95-6]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
WCPAKUFSQFCWTQ-UHFFFAOYSA-N					
3,3-dimethyl-4,4-diethylhexane	6.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62184-96-7]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
XFUAJHJJXMVZCQ-UHFFFAOYSA-N					
3,4-dimethyl-3,4-diethylhexane	6.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62184-97-8]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	247
NTQKWVJMJSYRDX-UHFFFAOYSA-N					
2,2-dimethyl-3-*tert*-butylhexane	6.4×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-76-2]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
VZAYJUSYQVNGBC-UHFFFAOYSA-N					
2-methyl-3-ethyl-3-isopropylhexane	8.3×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-77-3]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
TXYYDQJNRQJTOW-UHFFFAOYSA-N					
2-methyl-4-ethyl-3-isopropylhexane	9.7×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	6.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-78-4]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	247
JXHSGKIMXDNKIS-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3,4-triethylhexane	8.2×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62199-87-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
YGNQREHYYJPYLX-UHFFFAOYSA-N					
2,2,3,4,4-pentamethyl-3-ethylpentane	4.9×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[66576-21-4]	6.7×10^{-7}		Gharagheizi et al. (2010)	Q	247
IZNAUALMSCRPBS-UHFFFAOYSA-N					
2,2,3,4-tetramethyl-3-isopropylpentane	5.6×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62185-17-5]	7.4×10^{-7}		Gharagheizi et al. (2010)	Q	247
OKGFCJOAXUYCBG-UHFFFAOYSA-N					
2,2,4,4-tetramethyl-3-isopropylpentane	6.0×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-18-6]	7.4×10^{-7}		Gharagheizi et al. (2010)	Q	247
BYIFHEDQKBAFSW-UHFFFAOYSA-N					
2,2,4-trimethyl-3,3-diethylpentane	6.1×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62185-15-3]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	247
GIKXQMPMOJVRDN-UHFFFAOYSA-N					
2,4-dimethyl-3-ethyl-3-isopropylpentane	6.8×10^{-7}		Yaws (2003)	X	238
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62185-16-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
ASDDXPPGGPFNIL-UHFFFAOYSA-N					
tridecane	3.4×10^{-6}		Duchowicz et al. (2020)	V	187
$C_{13}H_{28}$	1.4×10^{-6}		Yaws (2003)	X	238
[629-50-5]	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
IIYFAKIEWZDVMP-UHFFFAOYSA-N	5.9×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
	7.9×10^{-7}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Yaws (1999)	?	21
	4.3×10^{-6}		Yaws and Yang (1992)	?	21
2-methyldodecane	1.5×10^{-6}		Yaws (2003)	X	238
$C_{13}H_{28}$	4.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[1560-97-0]	1.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
HGEMCUOAMCILCP-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyldodecane	1.5×10^{-6}		Yaws (2003)	X	238
$C_{13}H_{28}$	4.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-57-1]	1.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
GRJUENNHVNYCHD-UHFFFAOYSA-N					
2,2-dimethylundecane	1.1×10^{-6}		Yaws (2003)	X	238
$C_{13}H_{28}$	3.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-64-0]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
QDKSGHXRHXVMPF-UHFFFAOYSA-N					
2,3-dimethylundecane	1.3×10^{-6}		Yaws (2003)	X	238
$C_{13}H_{28}$	4.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-77-5]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
QSSUTSOGIQHRIU-UHFFFAOYSA-N					
2,4-dimethylundecane	1.2×10^{-6}		Yaws (2003)	X	238
$C_{13}H_{28}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-80-0]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
WMZNFELFMFOGCC-UHFFFAOYSA-N					
tetradecane	9.3×10^{-7}		Plyasunov and Shock (2000)	L	
$C_{14}H_{30}$	1.1×10^{-6}		Duchowicz et al. (2020)	V	187
[629-59-4]	1.1×10^{-6}		HSDB (2015)	V	
BGHCVCJVXZWKCC-UHFFFAOYSA-N	2.6×10^{-6}		Eastcott et al. (1988)	V	
	7.4×10^{-6}		Abraham (1984)	V	
	7.2×10^{-6}		Yaws (2003)	X	238
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	6.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	3.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
	5.6×10^{-7}		Hilal et al. (2008)	Q	
	2.9×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	2.2×10^{-6}		Yao et al. (2002)	Q	230
	7.2×10^{-6}		Yaws (1999)	?	21
	8.7×10^{-6}		Yaws and Yang (1992)	?	21
2-methyltridecane	2.4×10^{-6}		Yaws (2003)	X	238
$C_{14}H_{30}$	5.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[1560-96-9]	2.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
CJBFZKZYIPBBTO-UHFFFAOYSA-N					
3-methyltridecane	2.5×10^{-6}		Yaws (2003)	X	238
$C_{14}H_{30}$	5.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[6418-41-3]	2.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
NLHRRMKILFRDGV-UHFFFAOYSA-N					
2,2-dimethyldodecane	1.6×10^{-6}		Yaws (2003)	X	238
$C_{14}H_{30}$	4.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[49598-54-1]	1.8×10^{-6}		Gharagheizi et al. (2010)	Q	247
ATWISEHEXAEGKB-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-dimethyldodecane	2.1×10^{-6}		Yaws (2003)	X	238
$C_{14}H_{30}$	5.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[6117-98-2]	1.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
QBIXLGJCVGNDBJ-UHFFFAOYSA-N					
2,4-dimethyldodecane	1.6×10^{-6}		Yaws (2003)	X	238
$C_{14}H_{30}$	3.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[6117-99-3]	1.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
AFELDWXNIFIYOC-UHFFFAOYSA-N					
pentadecane	7.8×10^{-7}		Duchowicz et al. (2020)	V	187
$C_{15}H_{32}$	7.6×10^{-7}		HSDB (2015)	V	
[629-62-9]	1.1×10^{-5}		Yaws (2003)	X	238
YCOZIPAWZNQLMR-UHFFFAOYSA-N	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	7.1×10^{-6}		Gharagheizi et al. (2012)	Q	
	7.9×10^{-6}		Gharagheizi et al. (2010)	Q	247
	4.0×10^{-7}		Hilal et al. (2008)	Q	
	1.1×10^{-5}		Yaws (1999)	?	21
	2.1×10^{-5}		Yaws and Yang (1992)	?	21
2-methyltetradecane	4.9×10^{-6}		Yaws (2003)	X	238
$C_{15}H_{32}$	5.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[1560-95-8]	4.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
KUVMKLCGXIYSNH-UHFFFAOYSA-N					
3-methyltetradecane	5.1×10^{-6}		Yaws (2003)	X	238
$C_{15}H_{32}$	5.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[18435-22-8]	4.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
HXUYUZCPGPKNGS-UHFFFAOYSA-N					
2,2-dimethyltridecane	2.9×10^{-6}		Yaws (2003)	X	238
$C_{15}H_{32}$	4.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61869-04-3]	3.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
NVEUWWMNWPNXOC-UHFFFAOYSA-N					
2,3-dimethyltridecane	4.3×10^{-6}		Yaws (2003)	X	238
$C_{15}H_{32}$	5.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[18435-20-6]	3.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
SWUJSLXRUPXTQB-UHFFFAOYSA-N					
2,4-dimethyltridecane	2.6×10^{-6}		Yaws (2003)	X	238
$C_{15}H_{32}$	3.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-05-1]	3.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
JDFJCABQSZLDMZ-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexadecane	2.1×10^{-5}		Duchowicz et al. (2020)	V	187
$C_{16}H_{34}$	2.6×10^{-6}		Eastcott et al. (1988)	V	
[544-76-3]	2.7×10^{-5}		Abraham (1984)	V	
DCAYPVUWAIABOU-UHFFFAOYSA-N	2.1×10^{-5}		Yaws (2003)	X	238
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	7.2×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
	2.9×10^{-7}		Hilal et al. (2008)	Q	
	2.1×10^{-5}		Yaws (1999)	?	21
	4.3×10^{-5}		Yaws and Yang (1992)	?	21
2-methylpentadecane	1.2×10^{-5}		Yaws (2003)	X	238
$C_{16}H_{34}$	5.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[1560-93-6]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
BANXPJUEBPWEOT-UHFFFAOYSA-N					
3-methylpentadecane	1.2×10^{-5}		Yaws (2003)	X	238
$C_{16}H_{34}$	6.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[2882-96-4]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
FWXKCXJPHSAYMK-UHFFFAOYSA-N					
2,2-dimethyltetradecane	6.5×10^{-6}		Yaws (2003)	X	238
$C_{16}H_{34}$	4.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[59222-86-5]	7.9×10^{-6}		Gharagheizi et al. (2010)	Q	247
VCAMXEBNASZVEZ-UHFFFAOYSA-N					
2,3-dimethyltetradecane	1.1×10^{-5}		Yaws (2003)	X	238
$C_{16}H_{34}$	6.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[18435-23-9]	7.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
ZQRVEWIJXCRTFW-UHFFFAOYSA-N					
2,4-dimethyltetradecane	5.1×10^{-6}		Yaws (2003)	X	238
$C_{16}H_{34}$	3.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-06-2]	7.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
NWTLFDYNCLTSAR-UHFFFAOYSA-N					
heptadecane	2.2×10^{-7}		Hilal et al. (2008)	Q	
$C_{17}H_{36}$	2.1×10^{-4}		Yaws (1999)	?	21
[629-78-7]	1.8×10^{-4}		Yaws and Yang (1992)	?	21
NDJKXXJCMXVBJW-UHFFFAOYSA-N					
octadecane	1.6×10^{-6}		Eastcott et al. (1988)	V	
$C_{18}H_{38}$	7.8×10^{-4}		Abraham (1984)	V	
[593-45-3]	1.5×10^{-7}		Hilal et al. (2008)	Q	
RZJRJXONCZWCBN-UHFFFAOYSA-N	6.1×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	3.6×10^{-4}		Yaws (1999)	?	21
	1.1×10^{-3}		Yaws and Yang (1992)	?	21

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
nonadecane	1.3×10^{-7}		Hilal et al. (2008)	Q	
$C_{19}H_{40}$	9.3×10^{-4}		Yaws (1999)	?	21
[629-92-5]	3.4×10^{-3}		Yaws and Yang (1992)	?	21
LQERIDTXQFOHKA-UHFFFAOYSA-N					
eicosane	5.0×10^{-6}		Eastcott et al. (1988)	V	
$C_{20}H_{42}$	1.4×10^{-2}		Abraham (1984)	V	
[112-95-8]	9.7×10^{-8}		Hilal et al. (2008)	Q	
CBFCDTFDPHXCNY-UHFFFAOYSA-N	2.3×10^{-3}		Yaws (1999)	?	21
	3.0×10^{-2}		Yaws and Yang (1992)	?	21
heneicosane	7.3×10^{-8}		Hilal et al. (2008)	Q	
$C_{21}H_{44}$					
[629-94-7]					
FNAZRRHPUDJQCJ-UHFFFAOYSA-N					
docosane	5.4×10^{-8}		Hilal et al. (2008)	Q	
$C_{22}H_{46}$					
[629-97-0]					
HOWGUJZVBDQJKV-UHFFFAOYSA-N					
tricosane	4.1×10^{-8}		Hilal et al. (2008)	Q	
$C_{23}H_{48}$					
[638-67-5]					
FIGVVZUWCLSUEI-UHFFFAOYSA-N					
tetracosane	3.1×10^{-8}		Hilal et al. (2008)	Q	
$C_{24}H_{50}$					
[646-31-1]					
POOSGDOYLQNASK-UHFFFAOYSA-N					
pentacosane	1.5×10^{-8}		Hilal et al. (2008)	Q	
$C_{25}H_{52}$					
[629-99-2]					
YKNWIILGEFFOPE-UHFFFAOYSA-N					
hexacosane	5.0×10^{-5}		Eastcott et al. (1988)	V	
$C_{26}H_{54}$	1.3×10^{2}		Abraham (1984)	V	
[630-01-3]	1.1×10^{-8}		Hilal et al. (2008)	Q	
HMSWAIKSFDFLKN-UHFFFAOYSA-N					
heptacosane	7.7×10^{-9}		Hilal et al. (2008)	Q	
$C_{27}H_{56}$					
[593-49-7]					
BJQWYEJQWHSSCJ-UHFFFAOYSA-N					
octacosane	5.6×10^{-9}		Hilal et al. (2008)	Q	
$C_{28}H_{58}$					
[630-02-4]					
ZYURHZPYMFLWSH-UHFFFAOYSA-N					

Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
nonacosane $C_{29}H_{60}$ [630-03-5] IGGUPRCHHJZPBS-UHFFFAOYSA-N	4.0×10^{-9}		Hilal et al. (2008)	Q	
triacontane $C_{30}H_{62}$ [638-68-6] JXTPJDDICSTXJX-UHFFFAOYSA-N	2.9×10^{-9}		Hilal et al. (2008)	Q	
dotriacontane $C_{32}H_{66}$ [544-85-4] QHMGJGNTMQDRQA-UHFFFAOYSA-N	1.5×10^{-9}		Hilal et al. (2008)	Q	
pentatriacontane $C_{35}H_{72}$ [630-07-9] VHQQPFLOGSTQPC-UHFFFAOYSA-N	5.8×10^{-10}		Hilal et al. (2008)	Q	
hexatriacontane $C_{36}H_{74}$ [630-06-8] YDLYQMBWCWFRAI-UHFFFAOYSA-N	8.6×10^{8}		Abraham (1984)	V	
octatriacontane $C_{38}H_{78}$ [7194-85-6] BVKCQBBZBGYNOP-UHFFFAOYSA-N	2.2×10^{-10}		Hilal et al. (2008)	Q	

A2.2 Cycloalkanes

Table A2.2: Cycloalkanes

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyclopropane	1.2×10^{-4}	2800	Plyasunov and Shock (2000)	L	
C_3H_6	1.1×10^{-4}	1600	Wilhelm et al. (1977)	L	
[75-19-4]	8.1×10^{-5}		Steward et al. (1973)	L	14
LVZWSLJZHVFIQJ-UHFFFAOYSA-N	1.1×10^{-4}	2300	Allott et al. (1973)	L	
	7.8×10^{-5}		Guitart et al. (1989)	M	14
	1.1×10^{-4}	2000	Saidman et al. (1966)	M	
	1.2×10^{-5}		Duchowicz et al. (2020)	V	187
	1.2×10^{-5}		HSDB (2015)	V	
	1.3×10^{-4}		Irmann (1965)	V	
	1.3×10^{-4}		Yaws (2003)	X	238, 295
	1.1×10^{-4}		Hayer et al. (2022)	Q	20
	3.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.6×10^{-5}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-5}		Raventos-Duran et al. (2010)	Q	272, 244
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-4}		Gharagheizi et al. (2010)	Q	247
	1.4×10^{-4}		Hilal et al. (2008)	Q	
	2.3×10^{-5}		Modarresi et al. (2007)	Q	68
		2500	Kühne et al. (2005)	Q	
	1.2×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	7.3×10^{-5}		English and Carroll (2001)	Q	231, 232
	3.9×10^{-5}		Katritzky et al. (1998)	Q	
	9.0×10^{-5}		Nirmalakhandan et al. (1997)	Q	
		2200	Kühne et al. (2005)	?	
	1.3×10^{-4}		Yaws (1999)	?	21, 295
	1.1×10^{-4}	1600	Yaws et al. (1999)	?	21
	1.3×10^{-4}		Yaws and Yang (1992)	?	21, 295
	1.1×10^{-4}		Abraham et al. (1990)	?	
cyclobutane	1.3×10^{-6}		Hayer et al. (2022)	Q	20
C_4H_8	7.0×10^{-5}		HSDB (2015)	Q	100
[287-23-0]					
PMPVIKIVABFJJI-UHFFFAOYSA-N					
cyclopentane	5.8×10^{-5}	3500	Brockbank (2013)	L	1
C_5H_{10}	5.5×10^{-5}	3200	Plyasunov and Shock (2000)	L	
[287-92-3]	5.4×10^{-5}		Mackay and Shiu (1981)	L	
RGSFGYAAUTVSQA-UHFFFAOYSA-N	6.5×10^{-5}	3400	Hansen et al. (1993)	M	282
	5.6×10^{-5}		Mackay et al. (2006a)	V	
	5.2×10^{-5}		Mackay et al. (1993)	V	
	5.5×10^{-5}		Hwang et al. (1992)	V	
	5.4×10^{-5}		Eastcott et al. (1988)	V	
	5.3×10^{-5}		Hine and Mookerjee (1975)	V	
	5.6×10^{-5}		McAuliffe (1963)	V	

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.3×10^{-5}		Yaws (2003)	X	259
	5.2×10^{-5}		Yaws (2003)	X	238
	6.2×10^{-5}		Dupeux et al. (2022)	Q	260
	4.9×10^{-5}		Keshavarz et al. (2022)	Q	
	3.6×10^{-3}		Duchowicz et al. (2020)	Q	185
	5.2×10^{-5}		HSDB (2015)	Q	100
	3.0×10^{-5}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	5.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
	1.1×10^{-4}		Hilal et al. (2008)	Q	
	1.2×10^{-5}		Modarresi et al. (2007)	Q	68
		3200	Kühne et al. (2005)	Q	
	3.1×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	4.8×10^{-5}		Yao et al. (2002)	Q	230
	3.8×10^{-5}		English and Carroll (2001)	Q	231, 232
	3.5×10^{-5}		Katritzky et al. (1998)	Q	
	4.3×10^{-5}		Suzuki et al. (1992)	Q	233
	5.7×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	6.5×10^{-5}		Duchowicz et al. (2020)	?	186, 21
		4300	Kühne et al. (2005)	?	
	5.3×10^{-5}		Yaws (1999)	?	21
	5.2×10^{-5}		Yaws and Yang (1992)	?	21
	5.3×10^{-5}		Abraham et al. (1990)	?	
	5.3×10^{-5}		Abraham (1979)	?	
cyclohexane C_6H_{12} [110-82-7] XDTMQSROBMDMFD-UHFFFAOYSA-N	5.1×10^{-5}	3900	Brockbank (2013)	L	1, 296
	5.3×10^{-5}	4000	Plyasunov and Shock (2000)	L	
	5.6×10^{-5}		Mackay and Shiu (1981)	L	
	3.2×10^{-4}	5400	Hiatt (2013)	M	
	8.0×10^{-5}		Helburn et al. (2008)	M	
	5.2×10^{-5}	4500	Dewulf et al. (1999)	M	297
	6.0×10^{-5}		Hansen et al. (1993)	M	298
	5.4×10^{-5}	3800	Kolb et al. (1992)	M	278
	3.4×10^{-5}		Guitart et al. (1989)	M	14
	5.5×10^{-5}	3200	Ashworth et al. (1988)	M	279
	5.4×10^{-5}	3400	Tsonopoulos and Wilson (1983)	M	1
	5.4×10^{-5}	3800	Tucker et al. (1981)	M	
	5.3×10^{-5}		Mackay et al. (2006a)	V	
	5.1×10^{-5}		Mackay et al. (1993)	V	
	6.0×10^{-5}		Hwang et al. (1992)	V	
	5.4×10^{-5}		Eastcott et al. (1988)	V	
	5.1×10^{-5}		Hine and Mookerjee (1975)	V	
	5.6×10^{-5}		McAuliffe (1963)	V	
	5.4×10^{-5}	4000	Plyasunov et al. (2001)	T	

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		4000	Gill et al. (1976)	T	
	5.0×10^{-5}		Yaws (2003)	X	259
	5.1×10^{-5}		Yaws (2003)	X	238
	6.2×10^{-5}	710	Goldstein (1982)	X	299
	6.7×10^{-5}		Dupeux et al. (2022)	Q	260
	6.6×10^{-5}		Keshavarz et al. (2022)	Q	
	3.6×10^{-3}		Duchowicz et al. (2020)	Q	300
	1.6×10^{-4}		Wang et al. (2017)	Q	81, 239
	9.6×10^{-5}		Wang et al. (2017)	Q	81, 240
	1.5×10^{-4}		Wang et al. (2017)	Q	81, 241
	2.7×10^{-5}		Gharagheizi et al. (2012)	Q	
	5.0×10^{-5}		Gharagheizi et al. (2010)	Q	247
	9.5×10^{-5}		Hilal et al. (2008)	Q	
	2.3×10^{-5}		Modarresi et al. (2007)	Q	68
		3600	Kühne et al. (2005)	Q	
	5.8×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	3.4×10^{-5}		Yao et al. (2002)	Q	230
	2.7×10^{-5}		English and Carroll (2001)	Q	231, 275
	3.4×10^{-5}		Katritzky et al. (1998)	Q	
	3.4×10^{-5}		Suzuki et al. (1992)	Q	233
	4.5×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	6.6×10^{-5}		Duchowicz et al. (2020)	?	186, 21
		3900	Kühne et al. (2005)	?	
	5.1×10^{-5}		Yaws (1999)	?	21
	3.1×10^{-5}		Abraham and Weathersby (1994)	?	21
	5.1×10^{-5}		Yaws and Yang (1992)	?	21
	5.1×10^{-5}		Abraham et al. (1990)	?	
	5.1×10^{-5}		Abraham (1979)	?	
methylcyclopentane	2.8×10^{-5}		Brockbank (2013)	L	
$C_5H_9CH_3$	2.8×10^{-5}	5500	Plyasunov and Shock (2000)	L	
[96-37-7]	2.7×10^{-5}		Mackay and Shiu (1981)	L	
GDOPTJXRTPNYNR-UHFFFAOYSA-N	2.7×10^{-5}		Duchowicz et al. (2020)	V	187
	2.7×10^{-5}		HSDB (2015)	V	
	2.8×10^{-5}		Mackay et al. (2006a)	V	
	2.7×10^{-5}		Mackay et al. (1993)	V	
	2.7×10^{-5}		Eastcott et al. (1988)	V	
	2.7×10^{-5}		Hine and Mookerjee (1975)	V	
	2.9×10^{-5}		McAuliffe (1963)	V	
	2.8×10^{-5}		Yaws (2003)	X	238
	1.4×10^{-3}		Duchowicz et al. (2020)	Q	
	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	272, 244
	4.9×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	3.2×10^{-5}		Gharagheizi et al. (2010)	Q	247

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.4×10^{-5}		Hilal et al. (2008)	Q	
	1.1×10^{-5}		Modarresi et al. (2007)	Q	68
	2.9×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	2.6×10^{-5}		Yao et al. (2002)	Q	230
	2.7×10^{-5}		English and Carroll (2001)	Q	231, 232
	3.6×10^{-5}		Katritzky et al. (1998)	Q	
	3.1×10^{-5}		Suzuki et al. (1992)	Q	233
	3.9×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	2.8×10^{-5}		Yaws (1999)	?	21
	1.7×10^{-5}		Abraham and Weathersby (1994)	?	21
	2.8×10^{-5}		Yaws and Yang (1992)	?	21
cycloheptane	6.7×10^{-5}		Brockbank (2013)	L	
C_7H_{14}	1.0×10^{-4}	3100	Plyasunov and Shock (2000)	L	
[291-64-5]	1.1×10^{-4}		Duchowicz et al. (2020)	V	187
DMEGYFMYUHOHGS-UHFFFAOYSA-N	8.2×10^{-5}		Mackay et al. (2006a)	V	
	1.0×10^{-4}		Mackay et al. (1993)	V	
	1.1×10^{-4}		Cabani et al. (1981)	V	
	1.1×10^{-4}		Yaws (2003)	X	259
	1.1×10^{-4}		Yaws (2003)	X	238
	1.2×10^{-4}		Dupeux et al. (2022)	Q	260
	3.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.5×10^{-5}		HSDB (2015)	Q	100
	3.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	5.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
	5.1×10^{-5}		Hilal et al. (2008)	Q	
	8.3×10^{-6}		Modarresi et al. (2007)	Q	68
	1.1×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	3.2×10^{-5}		Katritzky et al. (1998)	Q	
	1.1×10^{-4}		Yaws (1999)	?	21
	1.6×10^{-3}		Hoff et al. (1993)	?	21
	1.1×10^{-4}		Yaws and Yang (1992)	?	21
methylcyclohexane	2.6×10^{-5}	4500	Brockbank (2013)	L	1
$C_6H_{11}CH_3$	2.4×10^{-5}		Plyasunov and Shock (2000)	L	
[108-87-2]	2.5×10^{-5}		Mackay and Shiu (1981)	L	
UAEPNZWRGJTJPN-UHFFFAOYSA-N	3.2×10^{-4}	5300	Hiatt (2013)	M	
	1.5×10^{-4}		Ramachandran et al. (1996)	M	
	9.6×10^{-5}	9400	Hansen et al. (1993)	M	282
	5.0×10^{-6}		Abraham and Acree (2007)	V	
	2.5×10^{-5}		Mackay et al. (2006a)	V	
	2.3×10^{-5}		Mackay et al. (1993)	V	
	2.3×10^{-5}		Meylan and Howard (1991)	V	
	2.6×10^{-5}		Eastcott et al. (1988)	V	

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.3×10^{-5}		Hine and Mookerjee (1975)	V	
	2.7×10^{-5}		McAuliffe (1963)	V	
	2.3×10^{-5}		Yaws (2003)	X	238
	8.9×10^{-5}		Keshavarz et al. (2022)	Q	
	1.4×10^{-3}		Duchowicz et al. (2020)	Q	300
	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	272, 244
	3.9×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	2.4×10^{-5}		Gharagheizi et al. (2010)	Q	247
	3.5×10^{-5}		Hilal et al. (2008)	Q	
	2.1×10^{-5}		Modarresi et al. (2007)	Q	68
		3900	Kühne et al. (2005)	Q	
	2.5×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	2.7×10^{-5}		Yao et al. (2002)	Q	230
	1.9×10^{-5}		English and Carroll (2001)	Q	231, 261
	3.5×10^{-5}		Katritzky et al. (1998)	Q	
	8.6×10^{-5}		Russell et al. (1992)	Q	280
	2.3×10^{-5}		Suzuki et al. (1992)	Q	233
	2.9×10^{-5}		Meylan and Howard (1991)	Q	
	3.1×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	2.3×10^{-5}		Duchowicz et al. (2020)	?	186, 21
		3100	Kühne et al. (2005)	?	
	2.3×10^{-5}		Yaws (1999)	?	21
	2.3×10^{-5}		Yaws and Yang (1992)	?	21
methylcyclohexane-d14 $C_6D_{11}CD_3$ [10120-28-2] UAEPNZWRGJTJPN-OBYKGMMLSA-N	3.1×10^{-4}	5600	Hiatt (2013)	M	
ethylcyclopentane C_7H_{14} [1640-89-7] IFTRQJLVEBNKJK-UHFFFAOYSA-N	1.8×10^{-5}		Yaws (2003)	X	238
	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
	2.4×10^{-5}		Yao et al. (2002)	Q	230
	1.8×10^{-5}		Yaws (1999)	?	21
1,1-dimethylcyclopentane C_7H_{14} [1638-26-2] QWHNJUXXYKPLQM-UHFFFAOYSA-N	2.3×10^{-5}		Yaws (2003)	X	238
	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
	1.7×10^{-5}		Yao et al. (2002)	Q	230
	2.3×10^{-5}		Yaws (1999)	?	21
cis-1,2-dimethylcyclopentane C_7H_{14} [1192-18-3] RIRARCHMRDHZAR-KNVOCYPGSA-N	1.9×10^{-5}		Yaws (2003)	X	238
	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
	1.9×10^{-5}		Yaws (1999)	?	21

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cis-1,3-dimethylcyclopentane	2.2×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[2532-58-3]	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
XAZKFISIRYLAEE-KNVOCYPGSA-N	2.2×10^{-5}		Yaws (1999)	?	21
trans-1,2-dimethylcyclopentane	2.2×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[822-50-4]	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
RIRARCHMRDHZAR-RNFRBKRXSA-N	2.2×10^{-5}		Yaws (1999)	?	21
trans-1,3-dimethylcyclopentane	2.2×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[1759-58-6]	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
XAZKFISIRYLAEE-RNFRBKRXSA-N	2.2×10^{-5}		Yaws (1999)	?	21
cyclooctane	7.3×10^{-5}	4800	Brockbank (2013)	L	1
C_8H_{16}	9.3×10^{-5}	3800	Plyasunov and Shock (2000)	L	
[292-64-8]	6.9×10^{-5}	4700	Dohányosová et al. (2004)	M	301
WJTCGQSWYFHTAC-UHFFFAOYSA-N	6.9×10^{-5}		Mackay et al. (2006a)	V	
	9.3×10^{-5}		Mackay et al. (1993)	V	
	9.5×10^{-5}		Cabani et al. (1981)	V	
	9.7×10^{-5}		Yaws (2003)	X	238
	3.1×10^{-5}		Gharagheizi et al. (2012)	Q	
	9.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
	7.5×10^{-5}		Hilal et al. (2008)	Q	
	7.4×10^{-6}		Modarresi et al. (2007)	Q	68
		4300	Kühne et al. (2005)	Q	
		5000	Kühne et al. (2005)	?	
	9.8×10^{-5}		Hoff et al. (1993)	?	21
	9.5×10^{-5}		Yaws and Yang (1992)	?	21
methylcycloheptane C_8H_{16} [4126-78-7] GYNNXHKOJHMOHS-UHFFFAOYSA-N	2.1×10^{-5}		Hilal et al. (2008)	Q	
1,1-dimethylcyclohexane	1.8×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	8.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[590-66-9]	1.6×10^{-5}		Gharagheizi et al. (2010)	Q	247
QEGNUYASOUJEHD-UHFFFAOYSA-N	2.0×10^{-5}		Yao et al. (2002)	Q	230
	1.8×10^{-5}		Yaws (1999)	?	21
1,2-dimethylcyclohexane	2.8×10^{-5}		Duchowicz et al. (2020)	V	187
$C_6H_{10}(CH_3)_2$	2.1×10^{-5}		Mackay et al. (1993)	V	
[583-57-3]	5.5×10^{-4}		Duchowicz et al. (2020)	Q	
KVZJLSYJROEPSQ-UHFFFAOYSA-N	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	272, 244
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	1.4×10^{-5}		Hilal et al. (2008)	Q	

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.1×10^{-5}		Katritzky et al. (1998)	Q	
	1.7×10^{-5}		Suzuki et al. (1992)	Q	233
	2.3×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
cis-1,2-dimethylcyclohexane	2.6×10^{-5}	4600	Brockbank (2013)	L	1
$C_6H_{10}(CH_3)_2$	2.8×10^{-5}		Plyasunov and Shock (2000)	L	
[2207-01-4]	2.8×10^{-5}		Mackay and Shiu (1981)	L	
KVZJLSYJROEPSQ-OCAPTIKFSA-N	2.7×10^{-5}	4600	Dohányosová et al. (2004)	M	302
	2.8×10^{-5}		Duchowicz et al. (2020)	V	187
	4.6×10^{-6}		Abraham and Acree (2007)	V	
	2.8×10^{-5}		Mackay et al. (2006a)	V	
	2.8×10^{-5}		Meylan and Howard (1991)	V	
	2.8×10^{-5}		Eastcott et al. (1988)	V	
	2.8×10^{-5}		Hine and Mookerjee (1975)	V	
	2.8×10^{-5}		Yaws (2003)	X	238
	5.5×10^{-4}		Duchowicz et al. (2020)	Q	
	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	247
	2.3×10^{-5}		Modarresi et al. (2007)	Q	68
		4300	Kühne et al. (2005)	Q	
	2.9×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	1.4×10^{-5}		English and Carroll (2001)	Q	231, 232
	4.3×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	2.2×10^{-5}		Meylan and Howard (1991)	Q	
		4900	Kühne et al. (2005)	?	
	2.8×10^{-5}		Yaws (1999)	?	21
	2.8×10^{-5}		Yaws and Yang (1992)	?	21
trans-1,2-dimethylcyclohexane	1.6×10^{-5}	4000	Brockbank (2013)	L	1
$C_6H_{10}(CH_3)_2$	1.6×10^{-5}	4300	Dohányosová et al. (2004)	M	303
[6876-23-9]	1.8×10^{-5}		Duchowicz et al. (2020)	V	187
KVZJLSYJROEPSQ-HTQZYQBOSA-N	5.7×10^{-6}		Abraham and Acree (2007)	V	
	1.3×10^{-5}		Mackay et al. (1993)	V	
	1.6×10^{-5}		Yaws (2003)	X	238
	5.5×10^{-4}		Duchowicz et al. (2020)	Q	
	9.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	247
		4300	Kühne et al. (2005)	Q	
		4600	Kühne et al. (2005)	?	
	1.6×10^{-5}		Yaws (1999)	?	21
	2.1×10^{-5}		Yaws and Yang (1992)	?	21
			Haynes (2014)	W	304
cis-1,3-dimethylcyclohexane	1.8×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	8.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[638-04-0]	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	247
SGVUHPSBDNVHKL-OCAPTIKFSA-N	1.8×10^{-5}		Yaws (1999)	?	21

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
trans-1,3-dimethylcyclohexane	1.7×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	9.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[2207-03-6]	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	247
SGVUHPSBDNVHKL-HTQZYQBOSA-N	1.7×10^{-5}		Yaws (1999)	?	21
1,4-dimethylcyclohexane	1.5×10^{-5}		Hilal et al. (2008)	Q	
$C_6H_{10}(CH_3)_2$					
[589-90-2]					
QRMPKOFEUHIBNM-UHFFFAOYSA-N					
cis-1,4-dimethylcyclohexane	1.7×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	9.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[624-29-3]	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	247
QRMPKOFEUHIBNM-OCAPTIKFSA-N	1.7×10^{-5}		Yaws (1999)	?	21
trans-1,4-dimethylcyclohexane	1.1×10^{-5}		Plyasunov and Shock (2000)	L	
$C_6H_{10}(CH_3)_2$	1.1×10^{-5}		Mackay and Shiu (1981)	L	
[2207-04-7]	1.1×10^{-5}		Duchowicz et al. (2020)	V	187
QRMPKOFEUHIBNM-ZKCHVHJHSA-N	1.1×10^{-5}		Mackay et al. (2006a)	V	
	1.1×10^{-5}		Mackay et al. (1993)	V	
	1.1×10^{-5}		Eastcott et al. (1988)	V	
	1.1×10^{-5}		Yaws (2003)	X	238
	5.5×10^{-4}		Duchowicz et al. (2020)	Q	
	8.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	247
	2.9×10^{-5}		Yaffe et al. (2003)	Q	249, 273
	1.4×10^{-5}		English and Carroll (2001)	Q	231, 232
	2.2×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	1.1×10^{-5}		Yaws (1999)	?	21
	1.1×10^{-5}		Yaws and Yang (1992)	?	21
ethylcyclohexane	2.1×10^{-5}	4100	Brockbank (2013)	L	1, 305
C_8H_{16}	2.0×10^{-5}	4400	Dohányosová et al. (2004)	M	306
[1678-91-7]	3.1×10^{-5}	4600	Heidman et al. (1985)	M	1
IIEWJVIFRVWJOD-UHFFFAOYSA-N	3.3×10^{-5}		Duchowicz et al. (2020)	V	187
	7.3×10^{-6}		Abraham and Acree (2007)	V	
	1.5×10^{-5}		Yaws (2003)	X	238
	1.4×10^{-3}		Duchowicz et al. (2020)	Q	
	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
	2.3×10^{-5}		Hilal et al. (2008)	Q	
		4300	Kühne et al. (2005)	Q	

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.3×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	3.5×10^{-5}		Yao et al. (2002)	Q	230, 268
	3.4×10^{-5}		Katritzky et al. (1998)	Q	
		4700	Kühne et al. (2005)	?	
	1.5×10^{-5}		Yaws (1999)	?	21
1,1,2-trimethylcyclopentane	1.3×10^{-5}		Yaws (2003)	X	238
$C_5H_7(CH_3)_3$	8.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[4259-00-1]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
WINCSBAYCULVDU-UHFFFAOYSA-N	6.9×10^{-6}		Hilal et al. (2008)	Q	
1,1,3-trimethylcyclopentane	6.2×10^{-6}		Plyasunov and Shock (2000)	L	
$C_5H_7(CH_3)_3$	6.3×10^{-6}		Mackay and Shiu (1981)	L	
[4516-69-2]	6.3×10^{-6}		Mackay et al. (2006a)	V	
OBKHYUIZSOIEPG-UHFFFAOYSA-N	6.3×10^{-6}		Mackay et al. (1993)	V	
	6.3×10^{-6}		Eastcott et al. (1988)	V	
	1.5×10^{-5}		Yaws (2003)	X	238
	6.2×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	272, 244
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
	6.2×10^{-6}		Yaffe et al. (2003)	Q	249, 250
1,*cis*-2,*cis*-3-trimethylcyclopentane	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	8.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[2613-69-6]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
VCWNHOPGKQCXIQ-RNLVFQAGSA-N					
1,*cis*-2,*trans*-3-trimethylcyclopentane	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	7.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[15890-40-1]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
VCWNHOPGKQCXIQ-JIGDXULJSA-N					
1,*trans*-2,*cis*-3-trimethylcyclopentane	1.4×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	6.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[19374-46-0]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
VCWNHOPGKQCXIQ-RNFRBKRXSA-N					
1,*cis*-2,*cis*-4-trimethylcyclopentane	1.3×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	7.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[2613-72-1]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
PNUFYSGVPVMNRN-RNLVFQAGSA-N					

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,*cis*-2,*trans*-4-trimethylcyclopentane	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	7.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[4850-28-6]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
PNUFYSGVPVMNRN-WHUPJOBBSA-N					
1,*trans*-2,*cis*-4-trimethylcyclopentane	1.4×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	6.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[16883-48-0]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
PNUFYSGVPVMNRN-HTQZYQBOSA-N					
1-methyl-1-ethylcyclopentane	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	9.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-50-5]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
LETYIFNDQBJGPJ-UHFFFAOYSA-N	1.5×10^{-5}		Yao et al. (2002)	Q	230
	1.1×10^{-5}		Yaws (1999)	?	21
1-methyl-*cis*-2-ethylcyclopentane	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[930-89-2]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
BSKOLJVTLRLTHE-SFYZADRCSA-N					
1-methyl-*trans*-2-ethylcyclopentane	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	9.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[930-90-5]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
BSKOLJVTLRLTHE-HTQZYQBOSA-N					
1-methyl-*cis*-3-ethylcyclopentane	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	9.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[2613-66-3]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
PQXAPVOKLYINEI-SFYZADRCSA-N					
1-methyl-*trans*-3-ethylcyclopentane	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	9.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[2613-65-2]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
PQXAPVOKLYINEI-HTQZYQBOSA-N					
propylcyclopentane	1.1×10^{-5}		Plyasunov and Shock (2000)	L	
$C_5H_9C_3H_7$	1.1×10^{-5}		Mackay and Shiu (1981)	L	
[2040-96-2]	1.1×10^{-5}		Duchowicz et al. (2020)	V	187
KDIAMAVWIJYWHN-UHFFFAOYSA-N	1.1×10^{-5}		Mackay et al. (2006a)	V	
	1.1×10^{-5}		Mackay et al. (1993)	V	
	1.1×10^{-5}		Eastcott et al. (1988)	V	
	1.1×10^{-5}		Yaws (2003)	X	238
	1.4×10^{-3}		Duchowicz et al. (2020)	Q	
	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
	2.0×10^{-5}		Hilal et al. (2008)	Q	
	1.1×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	2.5×10^{-5}		Yao et al. (2002)	Q	230
	3.2×10^{-5}		Katritzky et al. (1998)	Q	
	2.5×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	1.1×10^{-5}		Yaws (1999)	?	21
	1.1×10^{-5}		Yaws and Yang (1992)	?	21
isopropylcyclopentane	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[3875-51-2]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
TVSBRLGQVHJIKT-UHFFFAOYSA-N					
5,5-dimethylbicyclo[2.1.1]hexane	3.1×10^{-4}		Wang et al. (2017)	Q	81, 239
C_8H_{14}	1.7×10^{-5}		Wang et al. (2017)	Q	81, 240
(MCM:C8BC)	2.1×10^{-4}		Wang et al. (2017)	Q	81, 241
WZXMVFMYGAOEAT-UHFFFAOYSA-N					
1,1,2-trimethylcyclohexane	9.0×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	8.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[7094-26-0]	9.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
MEBONNVPKOBPEA-UHFFFAOYSA-N					
1,1,3-trimethylcyclohexane	9.3×10^{-6}		Plyasunov and Shock (2000)	L	
C_9H_{18}	9.5×10^{-6}		Mackay et al. (2006a)	V	
[3073-66-3]	9.5×10^{-6}		Mackay et al. (1993)	V	
PYOLJOJPIPCRDP-UHFFFAOYSA-N	1.2×10^{-5}		Yaws (2003)	X	238
	6.2×10^{-6}		Gharagheizi et al. (2012)	Q	
	9.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
1,1,4-trimethylcyclohexane	1.1×10^{-5}		Yaws (2003)	X	238
C_9H_{18}	5.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[7094-27-1]	9.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
UIWORXHEVNIOJG-UHFFFAOYSA-N					
1,*cis*-2,*cis*-3-trimethylcyclohexane	5.6×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	8.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[1839-88-9]	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	247
DQTVJLHNWPRPPH-AYMMMOKOSA-N					
1,*cis*-2,*trans*-3-trimethylcyclohexane	6.2×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	8.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[7667-55-2]	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	247
DQTVJLHNWPRPPH-BRPSZJMVSA-N					

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,*cis*-2,*cis*-4-trimethylcyclohexane	6.2×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	7.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[1678-80-4]	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	247
VCJPCEVERINRSG-YIZRAAEISA-N					
1,*cis*-2,*trans*-4-trimethylcyclohexane	6.7×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	7.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[7667-58-5]	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	247
VCJPCEVERINRSG-HLTSFMKQSA-N					
cis,*cis*-1,3,5-trimethylcyclohexane	1.7×10^{-5}		Yaws (2003)	X	238
C_9H_{18}	5.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[1795-27-3]	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	247
ODNRTOSCFYDTKF-AYMMMOKOSA-N					
cis,*trans*-1,3,5-trimethylcyclohexane	1.6×10^{-5}		Yaws (2003)	X	238
C_9H_{18}	6.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[1795-26-2]	6.1×10^{-6}		Gharagheizi et al. (2012)	Q	
ODNRTOSCFYDTKF-FBJIGQNJSA-N	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	247
1,*trans*-2,*cis*-3-trimethylcyclohexane	7.8×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	6.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[1678-81-5]	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	247
DQTVJLHNWPRPPH-HTQZYQBOSA-N					
1,*trans*-2,*cis*-4-trimethylcyclohexane	7.1×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	6.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[7667-59-6]	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	247
VCJPCEVERINRSG-DJLDLDEBSA-N					
1,*trans*-2,*trans*-4-trimethylcyclohexane	7.8×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	6.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[7667-60-9]	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	247
VCJPCEVERINRSG-IWSPIJDZSA-N					
1-methyl-1-ethylcyclohexane	8.1×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[4926-90-3]	1.0×10^{-5}		Gharagheizi et al. (2010)	Q	247
YPJRYQGOKHKNKZ-UHFFFAOYSA-N					
1-methyl-*cis*-2-ethylcyclohexane	9.7×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[4923-77-7]	8.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
XARGIVYWQPXRTC-BDAKNGLRSA-N					

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methyl-*cis*-3-ethylcyclohexane	1.1×10^{-5}		Yaws (2003)	X	238
C_9H_{18}	7.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[19489-10-2]	8.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
UDDVMPHNQKRNNS-BDAKNGLRSA-N					
1-methyl-*cis*-4-ethylcyclohexane	1.2×10^{-5}		Yaws (2003)	X	238
C_9H_{18}	8.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[4926-78-7]	8.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
CYISMTMRBPPERU-DTORHVGOSA-N					
1-methyl-*trans*-2-ethylcyclohexane	1.0×10^{-5}		Yaws (2003)	X	238
C_9H_{18}	8.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[4923-78-8]	8.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
XARGIVYWQPXRTC-RKDXNWHRSA-N					
1-methyl-*trans*-3-ethylcyclohexane	1.1×10^{-5}		Yaws (2003)	X	238
C_9H_{18}	8.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[4926-76-5]	8.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
UDDVMPHNQKRNNS-RKDXNWHRSA-N					
1-methyl-*trans*-4-ethylcyclohexane	8.4×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	7.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[6236-88-0]	8.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
CYISMTMRBPPERU-KYZUINATSA-N					
propylcyclohexane	9.6×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[1678-92-8]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
DEDZSLCZHWTGOR-UHFFFAOYSA-N	4.9×10^{-5}		Yao et al. (2002)	Q	230
	9.6×10^{-6}		Yaws (1999)	?	21
isopropylcyclohexane	9.4×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[696-29-7]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
GWESVXSMPKAFAS-UHFFFAOYSA-N	2.7×10^{-5}		Yao et al. (2002)	Q	230, 268
	9.4×10^{-6}		Yaws (1999)	?	21
1,1,2,2-tetramethylcyclopentane	8.0×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	5.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[52688-89-8]	8.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
YXDMSFJDVHXFCV-UHFFFAOYSA-N					
cis-1,1,2,3-tetramethylcyclopentane	7.2×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	5.8×10^{-6}		Gharagheizi et al. (2012)	Q	
CXCBKSYSKZEEJB-YUMQZZPRSA-N	8.6×10^{-6}		Gharagheizi et al. (2010)	Q	247

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
trans-1,1,2,3- tetramethylcyclopentane	8.4×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	4.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-70-0]	8.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
CXCBKSYSKZEEJB-SFYZADRCSA-N					
cis-1,1,2,4- tetramethylcyclopentane	8.4×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	4.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-71-1]	8.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
AVBGIJNNMIBMQG-SFYZADRCSA-N					
trans-1,1,2,4- tetramethylcyclopentane	8.4×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	4.6×10^{-6}		Gharagheizi et al. (2012)	Q	
AVBGIJNNMIBMQG-YUMQZZPRSA-N	8.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
1,1,3,3-tetramethylcyclopentane	1.1×10^{-5}		Yaws (2003)	X	238
C_9H_{18}	3.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[50876-33-0]	8.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
YWYCGTZNHWYQBD-UHFFFAOYSA-N					
cis-1,1,3,4- tetramethylcyclopentane	8.0×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	5.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[53907-60-1]	8.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
OWHFMVURUNNXMJ-OCAPTIKFSA-N					
trans-1,1,3,4- tetramethylcyclopentane	9.9×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	3.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[20309-77-7]	8.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
OWHFMVURUNNXMJ-HTQZYQBOSA-N					
cis-1,2,2,3- tetramethylcyclopentane	7.2×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	5.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[18938-68-6]	8.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
DHLYDHNCPUAVHP-OCAPTIKFSA-N					
trans-1,2,2,3- tetramethylcyclopentane	7.2×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	5.8×10^{-6}		Gharagheizi et al. (2012)	Q	
DHLYDHNCPUAVHP-YUMQZZPRSA-N	8.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
1,*cis*-2,*cis*-3,*cis*-4- tetramethylcyclopentane	6.3×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	6.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[2532-65-2]	7.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
INYXDKODFMWKER-FNCVBFRFSA-N					

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,*cis*-2,*cis*-3,*trans*-4-tetramethylcyclopentane	7.2×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	7.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
[2532-69-6]					
INYXDKODFMWKER-BGZDPUMWSA-N					
1,*cis*-2,*trans*-3,*cis*-4-tetramethylcyclopentane	8.2×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	4.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[2532-68-5]	7.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
INYXDKODFMWKER-BZNPZCIMSA-N					
1,*trans*-2,*cis*-3,*trans*-4-tetramethylcyclopentane	8.8×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	3.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[2532-67-4]	7.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
INYXDKODFMWKER-HXFLIBJXSA-N					
1,*trans*-2,*trans*-3,*cis*-4-tetramethylcyclopentane	8.2×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	4.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[19907-40-5]	7.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
INYXDKODFMWKER-OJOKCITNSA-N					
1,1-dimethyl-2-ethylcyclopentane	7.7×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	6.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[54549-80-3]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
RXPIHZJWAFCHEJ-UHFFFAOYSA-N					
1,1-dimethyl-3-ethylcyclopentane	8.3×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	5.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-61-9]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
WXHYOGXBESCULU-UHFFFAOYSA-N					
1,*cis*-2-dimethyl-1-ethylcyclopentane	6.9×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	7.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-63-1]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
DRWDWIMYUGHJBR-DTWKUNHWSA-N					
1,*trans*-2-dimethyl-1-ethylcyclopentane	6.9×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	7.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-62-0]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
DRWDWIMYUGHJBR-RKDXNWHRSA-N					

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,*cis*-2-dimethyl-*cis*-3-ethylcyclopentane	6.0×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	8.0×10^{-6}		Gharagheizi et al. (2012)	Q	
UMUGNPFWQJAOJI-HLTSFMKQSA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
1,*trans*-2-dimethyl-*trans*-3-ethylcyclopentane	6.7×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	6.6×10^{-6}		Gharagheizi et al. (2012)	Q	
UMUGNPFWQJAOJI-HRDYMLBCSA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
1,*cis*-2-dimethyl-*trans*-3-ethylcyclopentane	6.7×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	6.6×10^{-6}		Gharagheizi et al. (2012)	Q	
UMUGNPFWQJAOJI-IWSPIJDZSA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
1,*trans*-2-dimethyl-*cis*-3-ethylcyclopentane	7.7×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	5.4×10^{-6}		Gharagheizi et al. (2012)	Q	
UMUGNPFWQJAOJI-VGMNWLOBSA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
1,*cis*-2-dimethyl-*cis*-4-ethylcyclopentane	6.5×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	7.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-64-2]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
QKXQNQVXTYSGKS-BRPSZJMVSA-N					
1,*cis*-2-dimethyl-*trans*-4-ethylcyclopentane	6.5×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	7.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-65-3]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
QKXQNQVXTYSGKS-AYMMMOKOSA-N					
1,*trans*-2-dimethyl-*cis*-4-ethylcyclopentane	7.4×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	5.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-66-4]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
QKXQNQVXTYSGKS-HTQZYQBOSA-N					
1,*cis*-3-dimethyl-1-ethylcyclopentane	8.0×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	5.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-68-6]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
OAWOMHRJVJMDLZ-DTWKUNHWSA-N					
1,*trans*-3-dimethyl-1-ethylcyclopentane	8.0×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	5.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-67-5]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
OAWOMHRJVJMDLZ-RKDXNWHRSA-N					

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,*cis*-3-dimethyl-*cis*-2-ethylcyclopentane	6.0×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	8.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[19903-00-5]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
JREISGVVJTVFBL-AYMMMOKOSA-N					
1,*cis*-3-dimethyl-*trans*-2-ethylcyclopentane	7.8×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	5.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[19902-98-8]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
JREISGVVJTVFBL-BRPSZJMVSA-N					
1,*trans*-3-dimethyl-*cis*-2-ethylcyclopentane	6.9×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	6.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[19902-99-9]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
JREISGVVJTVFBL-HTQZYQBOSA-N					
1,*cis*-3-dimethyl-*cis*-4-ethylcyclopentane	6.7×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	6.6×10^{-6}		Gharagheizi et al. (2012)	Q	
VMCXXGFUCWAIIN-YIZRAAEISA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
1,*cis*-3-dimethyl-*trans*-4-ethylcyclopentane	7.8×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	5.2×10^{-6}		Gharagheizi et al. (2012)	Q	
VMCXXGFUCWAIIN-DJLDLDEBSA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
1,*trans*-3-dimethyl-*cis*-4-ethylcyclopentane	3.5×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	2.5×10^{-5}		Gharagheizi et al. (2012)	Q	
VMCXXGFUCWAIIN-CIUDSAMLSA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
1,*trans*-3-dimethyl-*trans*-4-ethylcyclopentane	6.7×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	6.6×10^{-6}		Gharagheizi et al. (2012)	Q	
VMCXXGFUCWAIIN-XHNCKOQMSA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
1-methyl-1-propylcyclopentane	7.2×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	8.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[16631-63-3]	7.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
HICYLMKNNFKEMK-UHFFFAOYSA-N					
1-methyl-*cis*-2-propylcyclopentane	6.4×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	8.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[932-43-4]	6.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
ADQJFBQXLAAVQA-BDAKNGLRSA-N					

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methyl-*trans*-2-propylcyclopentane	7.1×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	7.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[932-44-5]	6.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
ADQJFBQXLAAVQA-RKDXNWHRSA-N					
1-methyl-*cis*-3-propylcyclopentane	6.9×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	7.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[2443-04-1]	6.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
HRSBIYASWAILIF-BDAKNGLRSA-N					
1-methyl-*trans*-3-propylcyclopentane	6.9×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	7.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[2443-03-0]	6.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
HRSBIYASWAILIF-RKDXNWHRSA-N					
1-methyl-1-isopropylcyclopentane	6.5×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	8.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[61828-00-0]	7.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
XFMQGDWBNOQLEG-UHFFFAOYSA-N					
1-methyl-*cis*-2-isopropylcyclopentane	6.5×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	7.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-01-7]	7.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
CGWXYEIWDQDFIU-RKDXNWHRSA-N					
1-methyl-*trans*-2-isopropylcyclopentane	7.3×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	6.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[61828-01-1]	7.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
CGWXYEIWDQDFIU-BDAKNGLRSA-N					
1-methyl-*cis*-3-isopropylcyclopentane	7.2×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	6.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61828-02-2]	7.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
CDTDMKCVKCGRPD-BDAKNGLRSA-N					
1-methyl-*trans*-3-isopropylcyclopentane	7.2×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	6.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61828-03-3]	7.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
CDTDMKCVKCGRPD-RKDXNWHRSA-N					
1,1-diethylcyclopentane	6.7×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	9.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[2721-38-2]	7.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
DPGQSDLGKGLNHC-UHFFFAOYSA-N					

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,*cis*-2-diethylcyclopentane	6.3×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	8.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[932-39-8]	6.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
JKMYLSLBFNMSFP-DTORHVGOSA-N					
1,*trans*-2-diethylcyclopentane	6.9×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	7.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[932-40-1]	6.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
JKMYLSLBFNMSFP-RKDXNWHRSA-N					
1,*cis*-3-diethylcyclopentane	6.7×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	8.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-59-5]	6.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
RUUVWUNHERVOAY-DTORHVGOSA-N					
1,*trans*-3-diethylcyclopentane	6.7×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	8.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-60-8]	6.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
RUUVWUNHERVOAY-RKDXNWHRSA-N					
butylcyclopentane	6.5×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[2040-95-1]	8.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
ZAGHKONXGGSVDV-UHFFFAOYSA-N	6.5×10^{-6}		Yaws (1999)	?	21
isobutylcyclopentane	7.2×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	8.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[3788-32-7]	8.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
DPUYDFJBHDYVQM-UHFFFAOYSA-N					
sec-butylcyclopentane	6.5×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	9.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[4850-32-2]	8.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
DCEHVBLXWODXCW-UHFFFAOYSA-N					
tert-butylcyclopentane	6.7×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	7.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[3875-52-3]	7.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
BFWVYBVSRYIDHI-UHFFFAOYSA-N					
octahydro-1H-indene	8.8×10^{-5}		Hilal et al. (2008)	Q	
C_9H_{16}					
[496-10-6]					
BNRNAKTVFSZAFA-UHFFFAOYSA-N					
butylcyclohexane	7.2×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{20}$	8.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[1678-93-9]	9.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
GGBJHURWWWLEQH-UHFFFAOYSA-N	7.2×10^{-6}		Yaws (1999)	?	21

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pentylcyclopentane	5.3×10^{-6}		Plyasunov and Shock (2000)	L	
$C_{10}H_{20}$	5.4×10^{-6}		Mackay and Shiu (1981)	L	
[3741-00-2]	5.4×10^{-6}		Mackay et al. (2006a)	V	
HPQURZRDYMUHJI-UHFFFAOYSA-N	5.4×10^{-6}		Mackay et al. (1993)	V	
	5.4×10^{-6}		Eastcott et al. (1988)	V	
	5.2×10^{-6}		Yaws (2003)	X	238
	8.1×10^{-6}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	7.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
	9.2×10^{-6}		Hilal et al. (2008)	Q	
	5.8×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	1.6×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	5.4×10^{-6}		Yaws and Yang (1992)	?	21
decahydronaphthalene	7.2×10^{-5}	4100	Ashworth et al. (1988)	M	279
$C_{10}H_{18}$	2.1×10^{-5}		Duchowicz et al. (2020)	V	187
(decalin)	2.1×10^{-5}		HSDB (2015)	V	
[91-17-8]	4.4×10^{-3}		Duchowicz et al. (2020)	Q	
NNBZCPXTIHJBJL-UHFFFAOYSA-N	6.5×10^{-5}		Hilal et al. (2008)	Q	
		4500	Kühne et al. (2005)	Q	
	2.1×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	6.5×10^{-5}		Katritzky et al. (1998)	Q	
		4100	Kühne et al. (2005)	?	
(*Z*)-bicyclo[4.4.0]decane	4.3×10^{-4}		Mackay et al. (1993)	V	
$C_{10}H_{18}$	6.1×10^{-5}		Yaws (2003)	X	238
(*cis*-decahydronaphthalene; *cis*-decalin)	4.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[493-01-6]	8.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
NNBZCPXTIHJBJL-AOOOYVTPSA-N	6.1×10^{-5}		Yaws (1999)	?	21
(*E*)-bicyclo[4.4.0]decane	2.7×10^{-4}		Mackay et al. (1993)	V	
$C_{10}H_{18}$	3.9×10^{-5}		Yaws (2003)	X	238
(*trans*-decahydronaphthalene; *trans*-decalin)	2.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[493-02-7]	8.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
NNBZCPXTIHJBJL-MGCOHNPYSA-N	4.0×10^{-5}		Yaws (1999)	?	21
2,6,6-trimethylbicyclo[3.1.1]heptane	2.8×10^{-5}		HSDB (2015)	Q	100
$C_{10}H_{18}$					
(dihydropinene)					
[473-55-2]					
XOKSLPVRUOBDEW-UHFFFAOYSA-N					

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tricyclene $C_{10}H_{16}$ [508-32-7] RRBYUSWBLVXTQN-UHFFFAOYSA-N	4.9×10^{-5}		Plyasunov and Shock (2000)	L	
hexylcyclopentane $C_{11}H_{22}$ [4457-00-5] LKHGKBBAJAFMSQ-UHFFFAOYSA-N	5.1×10^{-6} 6.2×10^{-6} 6.5×10^{-6}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
pentylcyclohexane $C_{11}H_{22}$ [4292-92-6] HLTMUYBTNSVOFY-UHFFFAOYSA-N	7.1×10^{-6} 6.6×10^{-6} 9.2×10^{-6}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
cyclododecane $C_{12}H_{24}$ [294-62-2] DDTBPAQBQHZRDW-UHFFFAOYSA-N	6.4×10^{-6}		HSDB (2015)	Q	100
heptylcyclopentane $C_{12}H_{24}$ [5617-42-5] BOFNAOHMSHEKQL-UHFFFAOYSA-N	6.6×10^{-6} 9.8×10^{-6} 7.3×10^{-6}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
hexylcyclohexane $C_{12}H_{24}$ [4292-75-5] QHWAQXOSHHKCFK-UHFFFAOYSA-N	8.8×10^{-6} 7.4×10^{-6} 1.1×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
1,1'-bicyclohexyl $C_{12}H_{22}$ [92-51-3] WVIIMZNLDWSIRH-UHFFFAOYSA-N	3.1×10^{-5}		Hilal et al. (2008)	Q	
heptylcyclohexane $C_{13}H_{26}$ [5617-41-4] MSTLSCNJAHAQNU-UHFFFAOYSA-N	1.4×10^{-5} 1.3×10^{-5} 1.7×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
octylcyclopentane $C_{13}H_{26}$ [1795-20-6] HARXDULSBROLME-UHFFFAOYSA-N	1.1×10^{-5} 1.8×10^{-5} 1.0×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
octylcyclohexane $C_{14}H_{28}$ [1795-15-9] FBXWCEKQCVOOLT-UHFFFAOYSA-N	3.1×10^{-5} 2.1×10^{-5} 3.3×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247

Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
nonylcyclopentane	2.3×10^{-5}		Yaws (2003)	X	238
$C_{14}H_{28}$	2.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[2882-98-6]	1.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
GDCYEUOAZVKNHT-UHFFFAOYSA-N					
octahydro-1,1,2,3,3-pentamethyl-1H-indene	9.0×10^{-6}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_{26}$	1.1×10^{-6}		Zhang et al. (2010)	Q	288, 290
[33704-60-8]	6.5×10^{-4}		Zhang et al. (2010)	Q	288, 291
TUALLFJCLUYJEN-UHFFFAOYSA-N	3.5×10^{-5}		Zhang et al. (2010)	Q	288, 292
nonylcyclohexane	8.7×10^{-5}		Yaws (2003)	X	238
$C_{15}H_{30}$	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[2883-02-5]	8.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
CLMFECCMAVQYQA-UHFFFAOYSA-N					
decylcyclopentane	6.4×10^{-5}		Yaws (2003)	X	238
$C_{15}H_{30}$	2.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[1795-21-7]	4.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
WOUVLFFZQCUYOL-UHFFFAOYSA-N					
decylcyclohexane	3.7×10^{-4}		Yaws (1999)	?	21
$C_{16}H_{32}$					
[1795-16-0]					
STWFZICHPLEOIC-UHFFFAOYSA-N					
1,1'-(2-methylpentane-2,4-diyl)dicyclohexane	2.9×10^{-6}		Zhang et al. (2010)	Q	288, 289
$C_{18}H_{34}$	2.1×10^{-6}		Zhang et al. (2010)	Q	288, 290
[38970-72-8]	1.1×10^{-3}		Zhang et al. (2010)	Q	288, 291
XUVKLBIJXLIPDZ-UHFFFAOYSA-N	1.9×10^{-5}		Zhang et al. (2010)	Q	288, 292
1,1':3',1"-tercyclohexane	6.7×10^{-6}		Zhang et al. (2010)	Q	288, 289
$C_{18}H_{32}$	1.5×10^{-5}		Zhang et al. (2010)	Q	288, 290
[1706-50-9]	1.7×10^{-3}		Zhang et al. (2010)	Q	288, 291
JBQRJHVXZMSLNH-UHFFFAOYSA-N	9.0×10^{-5}		Zhang et al. (2010)	Q	288, 292

A2.3 Aliphatic alkenes and cycloalkenes

Table A2.3: Aliphatic alkenes and cycloalkenes

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethene	5.9×10^{-5}	2200	Burkholder et al. (2019)	L	1
C_2H_4	5.9×10^{-5}	2200	Burkholder et al. (2015)	L	1
(ethylene)	5.9×10^{-5}	2200	Sander et al. (2011)	L	1
[74-85-1]	5.9×10^{-5}	2200	Sander et al. (2006)	L	1
VGGSQFUCUMXWEO-UHFFFAOYSA-N	4.8×10^{-5}	2000	Plyasunov and Shock (2000)	L	
	4.7×10^{-5}	2000	Hayduk (1994)	L	1
	4.6×10^{-5}		Mackay and Shiu (1981)	L	
	4.7×10^{-5}	1800	Wilhelm et al. (1977)	L	
	3.5×10^{-5}		Steward et al. (1973)	L	14
	4.6×10^{-5}	2200	Allott et al. (1973)	L	
	4.9×10^{-5}	2000	Maaßen (1995)	M	307
	4.8×10^{-5}	1900	Reichl (1995)	M	308
	4.7×10^{-5}		McAuliffe (1966)	M	
	4.7×10^{-5}	2000	Morrison and Billett (1952)	M	309
	4.8×10^{-5}		Orcutt and Seevers (1937a)	M	
	3.4×10^{-5}		Grollman (1929)	M	59
	4.8×10^{-5}	2300	Winkler (1906)	M	
	4.6×10^{-5}		Hine and Mookerjee (1975)	V	
	4.7×10^{-5}	1900	Wauchope and Haque (1972)	V	
	3.1×10^{-5}		Pierotti (1965)	T	
	4.7×10^{-5}		Yaws (2003)	X	238
	4.7×10^{-5}		Deno and Berkheimer (1960)	C	
	3.4×10^{-5}		Hayer et al. (2022)	Q	20
	2.0×10^{-5}		Keshavarz et al. (2022)	Q	
	4.0×10^{-3}		Duchowicz et al. (2020)	Q	300
	2.1×10^{-4}		Wang et al. (2017)	Q	81, 239
	2.6×10^{-5}		Wang et al. (2017)	Q	81, 240
	8.3×10^{-5}		Wang et al. (2017)	Q	81, 241
	4.6×10^{-5}		Li et al. (2014)	Q	242
	2.4×10^{-5}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	6.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
	2.9×10^{-5}		Hilal et al. (2008)	Q	
	1.0×10^{-4}		Modarresi et al. (2007)	Q	68
		2700	Kühne et al. (2005)	Q	
	4.7×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	8.2×10^{-5}		English and Carroll (2001)	Q	231, 232
	1.5×10^{-5}		Katritzky et al. (1998)	Q	
	9.5×10^{-5}		Suzuki et al. (1992)	Q	233
	5.2×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	4.3×10^{-5}		Duchowicz et al. (2020)	?	186, 21

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		1900	Kühne et al. (2005)	?	
	4.8×10^{-5}		Yaws (1999)	?	21
	5.1×10^{-5}	2400	Yaws et al. (1999)	?	21
	3.9×10^{-5}		Abraham and Weathersby (1994)	?	21
	4.8×10^{-5}	2000	Dean and Lange (1999)	?	310, 23
	4.7×10^{-5}		Yaws and Yang (1992)	?	21
	4.6×10^{-5}		Abraham et al. (1990)	?	
	4.8×10^{-5}		Seinfeld (1986)	?	21
propene	5.6×10^{-5}	2600	Plyasunov and Shock (2000)	L	
C_3H_6	4.7×10^{-5}		Mackay and Shiu (1981)	L	
(propylene)	7.3×10^{-5}	3400	Wilhelm et al. (1977)	L	
[115-07-1]	5.4×10^{-5}	2700	Maaßen (1995)	M	311
QQONPFPTGQHPMA-UHFFFAOYSA-N	5.4×10^{-5}	2800	Reichl (1995)	M	312
	4.8×10^{-5}		McAuliffe (1966)	M	
	4.7×10^{-5}		Hine and Mookerjee (1975)	V	
	4.4×10^{-5}		Irmann (1965)	V	
	4.8×10^{-5}		Yaws (2003)	X	238
	9.2×10^{-5}		Deno and Berkheimer (1960)	C	
	6.5×10^{-5}		Hayer et al. (2022)	Q	20
	2.7×10^{-5}		Keshavarz et al. (2022)	Q	
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	300
	2.5×10^{-4}		Wang et al. (2017)	Q	81, 239
	2.7×10^{-5}		Wang et al. (2017)	Q	81, 240
	8.5×10^{-5}		Wang et al. (2017)	Q	81, 241
	2.9×10^{-5}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	6.6×10^{-5}		Gharagheizi et al. (2010)	Q	247
	3.4×10^{-5}		Hilal et al. (2008)	Q	
	5.9×10^{-5}		Modarresi et al. (2007)	Q	68
		3100	Kühne et al. (2005)	Q	
	5.1×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	1.0×10^{-4}		Yao et al. (2002)	Q	230
	6.2×10^{-5}		English and Carroll (2001)	Q	231, 232
	4.4×10^{-5}		Katritzky et al. (1998)	Q	
	6.9×10^{-5}		Suzuki et al. (1992)	Q	233
	4.1×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	4.6×10^{-5}		Irmann (1965)	Q	
	5.0×10^{-5}		Duchowicz et al. (2020)	?	186, 21
		3800	Kühne et al. (2005)	?	
	4.8×10^{-5}		Yaws (1999)	?	21
	6.8×10^{-5}	2800	Yaws et al. (1999)	?	21
	4.8×10^{-5}		Yaws and Yang (1992)	?	21
	4.3×10^{-5}		Abraham et al. (1990)	?	

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-butene	4.2×10^{-5}	3000	Plyasunov and Shock (2000)	L	
C_4H_8	1.3×10^{-4}	6400	Wilhelm et al. (1977)	L	
[106-98-9]	4.5×10^{-5}	3000	Serra and Palavra (2003)	M	313
VXNZUUAINFGPBY-UHFFFAOYSA-N	4.0×10^{-5}		McAuliffe (1966)	M	
	3.9×10^{-5}		Mackay et al. (2006a)	V	
	3.9×10^{-5}		Mackay et al. (1993)	V	
	3.9×10^{-5}		Hine and Mookerjee (1975)	V	
	4.1×10^{-5}		Irmann (1965)	V	
	4.0×10^{-5}		Yaws (2003)	X	238
	5.5×10^{-5}		Hayer et al. (2022)	Q	20
	3.6×10^{-5}		Keshavarz et al. (2022)	Q	
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	185
	2.2×10^{-4}		Wang et al. (2017)	Q	81, 239
	3.2×10^{-5}		Wang et al. (2017)	Q	81, 240
	8.5×10^{-5}		Wang et al. (2017)	Q	81, 241
	3.9×10^{-5}		Li et al. (2014)	Q	242
	3.1×10^{-5}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	4.6×10^{-5}		Gharagheizi et al. (2010)	Q	247
	3.4×10^{-5}		Hilal et al. (2008)	Q	
	5.7×10^{-5}		Modarresi et al. (2007)	Q	68
	6.0×10^{-6}		Modarresi et al. (2005)	Q	248
	3.9×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	7.1×10^{-5}		Yao et al. (2002)	Q	230
	4.7×10^{-5}		English and Carroll (2001)	Q	231, 232
	5.6×10^{-5}		Katritzky et al. (1998)	Q	
	5.2×10^{-5}		Suzuki et al. (1992)	Q	233
	3.4×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	4.1×10^{-5}		Irmann (1965)	Q	
	4.2×10^{-5}		Duchowicz et al. (2020)	?	186, 21
	4.0×10^{-5}		Yaws (1999)	?	21
	4.0×10^{-5}		Yaws and Yang (1992)	?	21
	3.9×10^{-5}		Abraham et al. (1990)	?	
			Mackay and Shiu (1981)	W	314
2-butene	5.1×10^{-5}		Hilal et al. (2008)	Q	
C_4H_8					
[107-01-7]					
IAQRGUVFOMOMEM-UHFFFAOYSA-N					

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cis-2-butene	5.5×10^{-5}		Irmann (1965)	V	
C_4H_8	4.1×10^{-5}		Yaws (2003)	X	238
[590-18-1]	3.6×10^{-5}		Keshavarz et al. (2022)	Q	
IAQRGUVFOMOMEM-ARJAWSKDSA-N	5.2×10^{-4}		Duchowicz et al. (2020)	Q	300
	3.2×10^{-4}		Wang et al. (2017)	Q	315, 81, 239
	5.4×10^{-5}		Wang et al. (2017)	Q	315, 81, 240
	6.0×10^{-5}		Wang et al. (2017)	Q	315, 81, 241
	3.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	5.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
	4.5×10^{-5}		Modarresi et al. (2007)	Q	68
	6.9×10^{-6}		Modarresi et al. (2005)	Q	248
	9.1×10^{-5}		Yao et al. (2002)	Q	230
	5.9×10^{-5}		Irmann (1965)	Q	
	4.3×10^{-5}		Duchowicz et al. (2020)	?	186, 21
	4.1×10^{-5}		Yaws (1999)	?	21
trans-2-butene	3.9×10^{-5}		Irmann (1965)	V	
C_4H_8	4.3×10^{-5}		Yaws (2003)	X	238
[624-64-6]	1.0×10^{-4}		Hayer et al. (2022)	Q	20
IAQRGUVFOMOMEM-ONEGZZNKSA-N	3.6×10^{-5}		Keshavarz et al. (2022)	Q	
	5.2×10^{-4}		Duchowicz et al. (2020)	Q	
	3.2×10^{-4}		Wang et al. (2017)	Q	315, 81, 239
	5.4×10^{-5}		Wang et al. (2017)	Q	315, 81, 240
	6.0×10^{-5}		Wang et al. (2017)	Q	315, 81, 241
	2.7×10^{-5}		Gharagheizi et al. (2012)	Q	
	5.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
	4.5×10^{-5}		Modarresi et al. (2007)	Q	68
	8.5×10^{-6}		Modarresi et al. (2005)	Q	248
	7.9×10^{-5}		Yao et al. (2002)	Q	230
	5.4×10^{-5}		Irmann (1965)	Q	
	4.4×10^{-5}		Duchowicz et al. (2020)	?	186, 21
	4.3×10^{-5}		Yaws (1999)	?	21
2-methylpropene	5.7×10^{-5}	3000	Plyasunov and Shock (2000)	L	
C_4H_8	5.6×10^{-5}	3000	Wilhelm et al. (1977)	L	
(isobutene)	4.8×10^{-5}		McAuliffe (1966)	M	
[115-11-7]	4.6×10^{-5}		Mackay et al. (2006a)	V	
VQTUBCCKSQIDNK-UHFFFAOYSA-N	4.6×10^{-5}		Mackay et al. (1993)	V	
	4.6×10^{-5}		Hine and Mookerjee (1975)	V	
	4.8×10^{-5}		Yaws (2003)	X	238
	6.1×10^{-5}		Hayer et al. (2022)	Q	20

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.6×10^{-5}		Keshavarz et al. (2022)	Q	
	5.1×10^{-4}		Duchowicz et al. (2020)	Q	300
	1.6×10^{-4}		Wang et al. (2017)	Q	81, 239
	3.9×10^{-5}		Wang et al. (2017)	Q	81, 240
	9.3×10^{-5}		Wang et al. (2017)	Q	81, 241
	2.0×10^{-5}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	6.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
	8.6×10^{-5}		Hilal et al. (2008)	Q	
	4.6×10^{-5}		Modarresi et al. (2007)	Q	68
		3400	Kühne et al. (2005)	Q	
	8.2×10^{-6}		Modarresi et al. (2005)	Q	248
	4.7×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	6.5×10^{-5}		Yao et al. (2002)	Q	230
	4.8×10^{-5}		English and Carroll (2001)	Q	231, 232
	5.3×10^{-5}		Katritzky et al. (1998)	Q	
	4.5×10^{-5}		Suzuki et al. (1992)	Q	233
	2.8×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	4.5×10^{-5}		Duchowicz et al. (2020)	?	186, 21
		3000	Kühne et al. (2005)	?	
	4.8×10^{-5}		Yaws (1999)	?	21
	5.6×10^{-5}	3000	Yaws et al. (1999)	?	21
	4.8×10^{-5}		Yaws and Yang (1992)	?	21
			Mackay and Shiu (1981)	W	314
1-pentene C_5H_{10} [109-67-1] YWAKXRMUMFPDSH-UHFFFAOYSA-N	3.0×10^{-5}		Brockbank (2013)	L	
	2.4×10^{-5}		Plyasunov and Shock (2000)	L	
	2.5×10^{-5}		Mackay and Shiu (1981)	L	
	2.5×10^{-5}		Duchowicz et al. (2020)	V	187
	2.5×10^{-5}		HSDB (2015)	V	
	2.5×10^{-5}		Mackay et al. (2006a)	V	
	2.5×10^{-5}		Mackay et al. (1993)	V	
	2.5×10^{-5}		Eastcott et al. (1988)	V	
	1.8×10^{-5}		Amoore and Buttery (1978)	V	
	2.4×10^{-5}		Hine and Mookerjee (1975)	V	
	2.7×10^{-5}		McAuliffe (1966)	V	24
	2.5×10^{-5}		Yaws (2003)	X	238
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.7×10^{-4}		Wang et al. (2017)	Q	81, 239
	2.3×10^{-5}		Wang et al. (2017)	Q	81, 240
	7.6×10^{-5}		Wang et al. (2017)	Q	81, 241
	3.0×10^{-5}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-5}		Raventos-Duran et al. (2010)	Q	272, 244
	3.1×10^{-5}		Raventos-Duran et al. (2010)	Q	245

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.9×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	3.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
	2.5×10^{-5}		Hilal et al. (2008)	Q	
	4.7×10^{-5}		Modarresi et al. (2007)	Q	68
	5.4×10^{-6}		Modarresi et al. (2005)	Q	248
	2.5×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	5.1×10^{-5}		Yao et al. (2002)	Q	230
	3.6×10^{-5}		English and Carroll (2001)	Q	231, 261
	6.0×10^{-5}		Katritzky et al. (1998)	Q	
	4.0×10^{-5}		Suzuki et al. (1992)	Q	233
	2.7×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	2.5×10^{-5}		Yaws (1999)	?	21
	2.5×10^{-5}		Yaws and Yang (1992)	?	21
	2.4×10^{-5}		Abraham et al. (1990)	?	
2-pentene	4.1×10^{-5}		Plyasunov and Shock (2000)	L	
C_5H_{10}	4.1×10^{-5}		Duchowicz et al. (2020)	V	187
[109-68-2]	4.4×10^{-5}		Eastcott et al. (1988)	V	
QMMOXUPEWRXHJS-UHFFFAOYSA-N	5.2×10^{-4}		Duchowicz et al. (2020)	Q	
	3.6×10^{-5}		Hilal et al. (2008)	Q	
	4.7×10^{-5}		Yaffe et al. (2003)	Q	249, 273
	6.1×10^{-5}		Katritzky et al. (1998)	Q	
cis-2-pentene	4.4×10^{-5}		Brockbank (2013)	L	
C_5H_{10}	4.4×10^{-5}		Mackay and Shiu (1981)	L	
[627-20-3]	4.4×10^{-5}		Duchowicz et al. (2020)	V	187
QMMOXUPEWRXHJS-HYXAFXHYSA-N	4.4×10^{-5}		Yaws (2003)	X	238
	5.2×10^{-4}		Duchowicz et al. (2020)	Q	
	2.6×10^{-4}		Wang et al. (2017)	Q	315, 81, 239
	3.7×10^{-5}		Wang et al. (2017)	Q	315, 81, 240
	5.8×10^{-5}		Wang et al. (2017)	Q	315, 81, 241
	4.5×10^{-5}		HSDB (2015)	Q	100
	2.7×10^{-5}		Gharagheizi et al. (2012)	Q	
	3.6×10^{-5}		Gharagheizi et al. (2010)	Q	247
	5.4×10^{-6}		Modarresi et al. (2005)	Q	248
	4.7×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	7.3×10^{-5}		Yao et al. (2002)	Q	230
	4.4×10^{-5}		Yaws (1999)	?	21
	4.4×10^{-5}		Yaws and Yang (1992)	?	21

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
trans-2-pentene	4.3×10^{-5}		Brockbank (2013)	L	
C_5H_{10}	4.3×10^{-5}		Duchowicz et al. (2020)	V	187
[646-04-8]	4.2×10^{-5}		Hine and Mookerjee (1975)	V	
QMMOXUPEWRXHJS-HWKANZROSA-N	4.3×10^{-5}		Yaws (2003)	X	238
	5.2×10^{-4}		Duchowicz et al. (2020)	Q	
	2.6×10^{-4}		Wang et al. (2017)	Q	315, 81, 239
	3.7×10^{-5}		Wang et al. (2017)	Q	315, 81, 240
	5.9×10^{-5}		Wang et al. (2017)	Q	315, 81, 241
	3.1×10^{-5}		HSDB (2015)	Q	100
	2.6×10^{-5}		Gharagheizi et al. (2012)	Q	
	3.6×10^{-5}		Gharagheizi et al. (2010)	Q	247
	1.0×10^{-5}		Modarresi et al. (2005)	Q	248
	6.7×10^{-5}		Yao et al. (2002)	Q	230
	3.6×10^{-5}		English and Carroll (2001)	Q	231, 232
	4.0×10^{-5}		Suzuki et al. (1992)	Q	233
	2.7×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	4.3×10^{-5}		Yaws (1999)	?	21
	4.3×10^{-5}		Yaws and Yang (1992)	?	21
2-methyl-1-butene	2.3×10^{-5}		Duchowicz et al. (2020)	V	187
C_5H_{10}	2.3×10^{-5}		HSDB (2015)	V	
[563-46-2]	3.3×10^{-5}		Yaws (2003)	X	238
MHNNAWXXUZQSNM-UHFFFAOYSA-N	5.1×10^{-4}		Duchowicz et al. (2020)	Q	
	1.5×10^{-4}		Wang et al. (2017)	Q	81, 239
	4.6×10^{-5}		Wang et al. (2017)	Q	81, 240
	8.7×10^{-5}		Wang et al. (2017)	Q	81, 241
	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
	3.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
	4.2×10^{-6}		Modarresi et al. (2005)	Q	248
	5.1×10^{-5}		Yao et al. (2002)	Q	230, 268
	3.4×10^{-5}		Yaws (1999)	?	21
2-methyl-2-butene	5.7×10^{-5}	3500	Brockbank (2013)	L	1
C_5H_{10}	6.7×10^{-5}	3600	Plyasunov and Shock (2000)	L	
[513-35-9]	4.4×10^{-5}		Duchowicz et al. (2020)	V	187
BKOOMYPCSUNDGP-UHFFFAOYSA-N	7.4×10^{-5}		Mackay et al. (2006a)	V	
	4.4×10^{-5}		Hine and Mookerjee (1975)	V	
	3.4×10^{-5}		Yaws (2003)	X	238
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	2.1×10^{-4}		Wang et al. (2017)	Q	81, 239
	6.0×10^{-5}		Wang et al. (2017)	Q	81, 240
	6.3×10^{-5}		Wang et al. (2017)	Q	81, 241
	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
	4.3×10^{-5}		Gharagheizi et al. (2010)	Q	247

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.5×10^{-5}		Hilal et al. (2008)	Q	
	9.7×10^{-6}		Modarresi et al. (2005)	Q	248
	4.7×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	5.4×10^{-5}		Yao et al. (2002)	Q	230
	4.8×10^{-5}		English and Carroll (2001)	Q	231, 275
	5.8×10^{-5}		Katritzky et al. (1998)	Q	
	3.6×10^{-5}		Suzuki et al. (1992)	Q	233
	2.3×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	3.5×10^{-5}		Yaws (1999)	?	21
3-methyl-1-butene	1.9×10^{-5}		Plyasunov and Shock (2000)	L	
C_5H_{10}	1.8×10^{-5}		Mackay and Shiu (1981)	L	
[563-45-1]	1.9×10^{-5}		McAuliffe (1966)	M	
YHQXBTXEYZIYOV-UHFFFAOYSA-N	1.8×10^{-5}		HSDB (2015)	V	
	1.8×10^{-5}		Mackay et al. (2006a)	V	
	1.8×10^{-5}		Mackay et al. (1993)	V	
	1.8×10^{-5}		Hine and Mookerjee (1975)	V	
	1.9×10^{-5}		Yaws (2003)	X	238
	2.1×10^{-4}		Wang et al. (2017)	Q	81, 239
	1.4×10^{-5}		Wang et al. (2017)	Q	81, 240
	6.9×10^{-5}		Wang et al. (2017)	Q	81, 241
	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	3.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
	1.5×10^{-5}		Hilal et al. (2008)	Q	
	3.7×10^{-5}		Modarresi et al. (2007)	Q	68
	7.2×10^{-6}		Modarresi et al. (2005)	Q	248
	1.8×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	2.6×10^{-5}		Yao et al. (2002)	Q	230
	3.6×10^{-5}		English and Carroll (2001)	Q	231, 232
	5.7×10^{-5}		Katritzky et al. (1998)	Q	
	3.6×10^{-5}		Suzuki et al. (1992)	Q	233
	2.3×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	1.9×10^{-5}		Yaws (1999)	?	21
	1.9×10^{-5}		Yaws and Yang (1992)	?	21
1-hexene	2.5×10^{-5}		Brockbank (2013)	L	
C_6H_{12}	2.3×10^{-5}	3900	Plyasunov and Shock (2000)	L	
[592-41-6]	2.4×10^{-5}		Mackay and Shiu (1981)	L	
LIKMAJRDDDTEIG-UHFFFAOYSA-N	2.4×10^{-5}		Duchowicz et al. (2020)	V	187
	2.4×10^{-5}		HSDB (2015)	V	
	2.4×10^{-5}		Mackay et al. (2006a)	V	
	2.4×10^{-5}		Mackay et al. (1993)	V	
	2.4×10^{-5}		Hwang et al. (1992)	V	
	2.4×10^{-5}		Eastcott et al. (1988)	V	

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.4×10^{-5}		Hine and Mookerjee (1975)	V	
	2.7×10^{-5}		McAuliffe (1966)	V	24
	2.4×10^{-5}		Yaws (2003)	X	238
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.4×10^{-4}		Wang et al. (2017)	Q	81, 239
	1.7×10^{-5}		Wang et al. (2017)	Q	81, 240
	7.1×10^{-5}		Wang et al. (2017)	Q	81, 241
	2.8×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	2.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
	1.8×10^{-5}		Hilal et al. (2008)	Q	
	3.6×10^{-5}		Modarresi et al. (2007)	Q	68
		4100	Kühne et al. (2005)	Q	
	4.0×10^{-6}		Modarresi et al. (2005)	Q	248
	2.5×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	2.5×10^{-5}		Yao et al. (2002)	Q	230, 268
	2.7×10^{-5}		English and Carroll (2001)	Q	231, 232
	6.1×10^{-5}		Katritzky et al. (1998)	Q	
	3.1×10^{-5}		Suzuki et al. (1992)	Q	233
	2.1×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
		4000	Kühne et al. (2005)	?	
	3.3×10^{-5}		Yaws (1999)	?	21
	3.3×10^{-5}		Yaws and Yang (1992)	?	21
	2.8×10^{-5}		Abraham et al. (1990)	?	
cis-2-hexene	2.6×10^{-5}		Yaws (2003)	X	238
C_6H_{12}	2.3×10^{-4}		Wang et al. (2017)	Q	315, 81, 239
[7688-21-3]	2.4×10^{-5}		Wang et al. (2017)	Q	315, 81, 240
RYPKRALMXUUNKS-HYXAFXHYSA-N	5.0×10^{-5}		Wang et al. (2017)	Q	315, 81, 241
	2.3×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
	5.8×10^{-6}		Modarresi et al. (2005)	Q	248
	3.0×10^{-5}		Yao et al. (2002)	Q	230
	2.6×10^{-5}		Yaws (1999)	?	21

Table A2.3: Aliphatic alkenes and cycloalkenes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
trans-2-hexene	2.6×10^{-5}		Yaws (2003)	X	238
C_6H_{12}	2.3×10^{-4}		Wang et al. (2017)	Q	315, 81, 239
[4050-45-7]	2.4×10^{-5}		Wang et al. (2017)	Q	315, 81, 240
RYPKRALMXUUNKS-HWKANZROSA-N	5.0×10^{-5}		Wang et al. (2017)	Q	315, 81, 241
	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
	5.6×10^{-6}		Modarresi et al. (2005)	Q	248
	3.2×10^{-5}		Yao et al. (2002)	Q	230
	2.7×10^{-5}		Yaws (1999)	?	21
cis-3-hexene	2.6×10^{-5}		Yaws (2003)	X	238
C_6H_{12}	2.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[7642-09-3]	2.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
ZQDPJFUHLCOCRG-WAYWQWQTSA-N	4.5×10^{-6}		Modarresi et al. (2005)	Q	248
	3.3×10^{-5}		Yao et al. (2002)	Q	230
	2.7×10^{-5}		Yaws (1999)	?	21
trans-3-hexene	2.6×10^{-5}		Yaws (2003)	X	238
C_6H_{12}	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[13269-52-8]	2.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
ZQDPJFUHLCOCRG-AATRIKPKSA-N	5.4×10^{-6}		Modarresi et al. (2005)	Q	248
	3.1×10^{-5}		Yao et al. (2002)	Q	230
	2.7×10^{-5}		Yaws (1999)	?	21
2-methyl-1-pentene	3.3×10^{-5}		Plyasunov and Shock (2000)	L	
C_6H_{12}	3.6×10^{-5}		Mackay and Shiu (1981)	L	
[763-29-1]	3.6×10^{-5}		Duchowicz et al. (2020)	V	187
WWUVJRULCWHUSA-UHFFFAOYSA-N	3.6×10^{-5}		Mackay et al. (2006a)	V	
	3.6×10^{-5}		Mackay et al. (1993)	V	
	3.6×10^{-5}		Eastcott et al. (1988)	V	
	3.4×10^{-5}		Cabani et al. (1981)	V	
	3.5×10^{-5}		Yaws (2003)	X	238
	5.1×10^{-4}		Duchowicz et al. (2020)	Q	
	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	272, 244
	3.1×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	2.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
	2.2×10^{-5}		Hilal et al. (2008)	Q	
	5.8×10^{-6}		Modarresi et al. (2005)	Q	248
	3.6×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	4.5×10^{-5}		Yao et al. (2002)	Q	230
	2.1×10^{-5}		English and Carroll (2001)	Q	231, 232
	1.9×10^{-5}		Nirmalakhandan et al. (1997)	Q	

Table A2.3: Aliphatic alkenes and cycloalkenes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.6×10^{-5}		Yaws (1999)	?	21
	3.5×10^{-5}		Yaws and Yang (1992)	?	21
3-methyl-1-pentene	2.8×10^{-5}		Yaws (2003)	X	238
C_6H_{12}	2.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[760-20-3]	2.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
LDTAOIUHUHHCMU-UHFFFAOYSA-N	6.2×10^{-6}		Modarresi et al. (2005)	Q	248
	2.1×10^{-5}		Yao et al. (2002)	Q	230
	2.8×10^{-5}		Yaws (1999)	?	21
4-methyl-1-pentene	1.5×10^{-5}		Plyasunov and Shock (2000)	L	
C_6H_{12}	1.6×10^{-5}		Mackay and Shiu (1981)	L	
[691-37-2]	1.6×10^{-5}		Duchowicz et al. (2020)	V	187
WSSSPWUEQFSQQG-UHFFFAOYSA-N	1.6×10^{-5}		Mackay et al. (2006a)	V	
	1.6×10^{-5}		Mackay et al. (1993)	V	
	1.6×10^{-5}		Eastcott et al. (1988)	V	
	1.6×10^{-5}		Hine and Mookerjee (1975)	V	
	1.6×10^{-5}		Yaws (2003)	X	238
	6.1×10^{-4}		Duchowicz et al. (2020)	Q	
	2.3×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	2.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
	1.2×10^{-5}		Hilal et al. (2008)	Q	
	3.4×10^{-5}		Modarresi et al. (2007)	Q	68
	7.3×10^{-6}		Modarresi et al. (2005)	Q	248
	1.6×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	2.7×10^{-5}		Yao et al. (2002)	Q	230
	2.7×10^{-5}		English and Carroll (2001)	Q	231, 232
	5.8×10^{-5}		Katritzky et al. (1998)	Q	
	2.8×10^{-5}		Suzuki et al. (1992)	Q	233
	1.8×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	1.6×10^{-5}		Yaws (1999)	?	21
	1.6×10^{-5}		Yaws and Yang (1992)	?	21
2-methyl-2-pentene	2.6×10^{-5}		Yaws (2003)	X	238
C_6H_{12}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[625-27-4]	2.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
JMMZCWZIJXAGKW-UHFFFAOYSA-N	7.9×10^{-6}		Modarresi et al. (2005)	Q	248
	4.8×10^{-5}		Yao et al. (2002)	Q	230, 268
	2.7×10^{-5}		Yaws (1999)	?	21
cis-3-methyl-2-pentene	2.6×10^{-5}		Yaws (2003)	X	238
C_6H_{12}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[922-62-3]	2.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
BEQGRRJLJLVQAQ-XQRVVYSFSA-N	2.7×10^{-5}		Yaws (1999)	?	21

Table A2.3: Aliphatic alkenes and cycloalkenes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
trans-3-methyl-2-pentene	2.6×10^{-5}		Yaws (2003)	X	238
C_6H_{12}	1.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[616-12-6]	2.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
BEQGRRJLJLVQAQ-GQCTYLIASA-N	5.5×10^{-6}		Modarresi et al. (2005)	Q	248
	3.9×10^{-5}		Yao et al. (2002)	Q	230
	2.6×10^{-5}		Yaws (1999)	?	21
cis-4-methyl-2-pentene	2.8×10^{-5}		Yaws (2003)	X	238
C_6H_{12}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[691-38-3]	2.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
LGAQJENWWYGFSN-PLNGDYQASA-N	3.7×10^{-6}		Modarresi et al. (2005)	Q	248
	3.3×10^{-5}		Yao et al. (2002)	Q	230
	2.8×10^{-5}		Yaws (1999)	?	21
trans-4-methyl-2-pentene	2.8×10^{-5}		Yaws (2003)	X	238
C_6H_{12}	1.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[674-76-0]	2.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
LGAQJENWWYGFSN-SNAWJCMRSA-N	5.0×10^{-6}		Modarresi et al. (2005)	Q	248
	3.1×10^{-5}		Yao et al. (2002)	Q	230
	2.8×10^{-5}		Yaws (1999)	?	21
3-methylenepentane	2.7×10^{-5}		Yaws (2003)	X	238
C_6H_{12}	2.0×10^{-5}		Gharagheizi et al. (2012)	Q	
(2-ethyl-1-butene)	2.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
[760-21-4]	3.9×10^{-6}		Modarresi et al. (2005)	Q	248
RYKZRKKEYSRDNF-UHFFFAOYSA-N	4.3×10^{-5}		Yao et al. (2002)	Q	230
	2.7×10^{-5}		Yaws (1999)	?	21
2,3-dimethyl-1-butene	2.8×10^{-5}		Yaws (2003)	X	238
C_6H_{12}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[563-78-0]	2.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
OWWIWYDDISJUMY-UHFFFAOYSA-N	1.7×10^{-5}		Hilal et al. (2008)	Q	
	6.0×10^{-6}		Modarresi et al. (2005)	Q	248
	1.9×10^{-5}		Yao et al. (2002)	Q	230
	2.8×10^{-5}		Yaws (1999)	?	21
3,3-dimethyl-1-butene	2.8×10^{-5}		Yaws (2003)	X	238
C_6H_{12}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[558-37-2]	2.6×10^{-5}		Gharagheizi et al. (2010)	Q	247
PKXHXOTZMFCXSH-UHFFFAOYSA-N	5.2×10^{-6}		Modarresi et al. (2005)	Q	248
	1.0×10^{-5}		Yao et al. (2002)	Q	230
	2.9×10^{-5}		Yaws (1999)	?	21

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-dimethyl-2-butene	2.5×10^{-5}		Yaws (2003)	X	238
C_6H_{12}	1.4×10^{-4}		Wang et al. (2017)	Q	81, 239
[563-79-1]	1.1×10^{-4}		Wang et al. (2017)	Q	81, 240
WGLLSSPDPJPLOR-UHFFFAOYSA-N	5.5×10^{-5}		Wang et al. (2017)	Q	81, 241
	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
	4.9×10^{-6}		Modarresi et al. (2005)	Q	248
	2.7×10^{-5}		Yao et al. (2002)	Q	230
	2.6×10^{-5}		Yaws (1999)	?	21
1-heptene	2.0×10^{-5}		Brockbank (2013)	L	
C_7H_{14}	2.5×10^{-5}		Plyasunov and Shock (2000)	L	
[592-76-7]	2.3×10^{-5}		Duchowicz et al. (2020)	V	187
ZGEGCLOFRBLKSE-UHFFFAOYSA-N	2.3×10^{-5}		HSDB (2015)	V	
	2.5×10^{-5}		Mackay et al. (2006a)	V	
	2.5×10^{-5}		Mackay et al. (1993)	V	
	2.5×10^{-5}		Yaws (2003)	X	238
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.6×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-5}		Gharagheizi et al. (2010)	Q	247
	1.3×10^{-5}		Hilal et al. (2008)	Q	
	3.3×10^{-5}		Modarresi et al. (2007)	Q	68
	3.2×10^{-6}		Modarresi et al. (2005)	Q	248
	2.2×10^{-5}		Yao et al. (2002)	Q	230
	2.1×10^{-5}		English and Carroll (2001)	Q	231, 232
	5.8×10^{-5}		Katritzky et al. (1998)	Q	
	1.7×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	2.5×10^{-5}		Yaws (1999)	?	21
	2.5×10^{-5}		Yaws and Yang (1992)	?	21
	2.4×10^{-5}		Abraham et al. (1990)	?	
2-heptene	2.3×10^{-5}		Plyasunov and Shock (2000)	L	
C_7H_{14}	2.4×10^{-5}		Duchowicz et al. (2020)	V	187
[592-77-8]	5.2×10^{-4}		Duchowicz et al. (2020)	Q	
OTTZHAVKAVGASB-UHFFFAOYSA-N	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	272, 244
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	1.7×10^{-5}		Hilal et al. (2008)	Q	
	2.6×10^{-5}		Modarresi et al. (2007)	Q	68
	2.1×10^{-5}		English and Carroll (2001)	Q	231, 275

Table A2.3: Aliphatic alkenes and cycloalkenes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cis-2-heptene	2.4×10^{-5}		Brockbank (2013)	L	
C_7H_{14}	1.5×10^{-5}		Yaws (2003)	X	238
[6443-92-1]	2.0×10^{-5}		Gharagheizi et al. (2012)	Q	
OTTZHAVKAVGASB-HYXAFXHYSA-N	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
	9.1×10^{-6}		Modarresi et al. (2005)	Q	248
	3.0×10^{-5}		Yao et al. (2002)	Q	230, 268
	1.5×10^{-5}		Yaws (1999)	?	21
trans-2-heptene	2.4×10^{-5}		Brockbank (2013)	L	
C_7H_{14}	2.4×10^{-5}		Mackay and Shiu (1981)	L	
[14686-13-6]	2.3×10^{-5}		Duchowicz et al. (2020)	V	187
OTTZHAVKAVGASB-HWKANZROSA-N	2.4×10^{-5}		Mackay et al. (1993)	V	
	2.4×10^{-5}		Eastcott et al. (1988)	V	
	2.4×10^{-5}		Hine and Mookerjee (1975)	V	
	1.5×10^{-5}		Yaws (2003)	X	238
	5.2×10^{-4}		Duchowicz et al. (2020)	Q	
	2.0×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
	2.5×10^{-5}		Modarresi et al. (2007)	Q	68
	4.4×10^{-6}		Modarresi et al. (2005)	Q	248
	2.8×10^{-5}		Yao et al. (2002)	Q	230
	1.7×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	2.4×10^{-5}		Suzuki et al. (1992)	Q	233
	1.5×10^{-5}		Yaws (1999)	?	21
cis-3-heptene	1.6×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[7642-10-6]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
WZHKDGJSXCTSCK-ALCCZGGFSA-N	3.8×10^{-6}		Modarresi et al. (2005)	Q	248
	3.1×10^{-5}		Yao et al. (2002)	Q	230
	1.6×10^{-5}		Yaws (1999)	?	21
trans-3-heptene	1.6×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[14686-14-7]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
WZHKDGJSXCTSCK-FNORWQNLSA-N	4.0×10^{-6}		Modarresi et al. (2005)	Q	248
	2.8×10^{-5}		Yao et al. (2002)	Q	230
	1.6×10^{-5}		Yaws (1999)	?	21
2-methyl-1-hexene	1.7×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[6094-02-6]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
IRUDSQHLKGNCGF-UHFFFAOYSA-N	3.2×10^{-6}		Modarresi et al. (2005)	Q	248
	2.4×10^{-5}		Yao et al. (2002)	Q	230
	1.7×10^{-5}		Yaws (1999)	?	21

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-2-hexene	1.6×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[2738-19-4]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
BWEKDYGHDCHWEN-UHFFFAOYSA-N					
2-methyl-*cis*-3-hexene	1.9×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[15840-60-5]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
IQANHWBWTVLDTP-WAYWQWQTSA-N					
2-methyl-*trans*-3-hexene	1.9×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[692-24-0]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
IQANHWBWTVLDTP-AATRIKPKSA-N					
3-methyl-1-hexene	1.9×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	2.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[3404-61-3]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
RITONZMLZWYPHW-UHFFFAOYSA-N	9.9×10^{-6}		Modarresi et al. (2005)	Q	248
	1.0×10^{-5}		Yao et al. (2002)	Q	230
	1.9×10^{-5}		Yaws (1999)	?	21
3-methyl-*cis*-2-hexene	1.6×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[10574-36-4]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
JZMUUSXQSKCZNO-ALCCZGGFSA-N					
3-methyl-*trans*-2-hexene	1.6×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[20710-38-7]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
JZMUUSXQSKCZNO-FNORWQNLSA-N					
3-methyl-*cis*-3-hexene	1.7×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[4914-89-0]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
FHHSSXNRVNXTBG-SREVYHEPSA-N					
3-methyl-*trans*-3-hexene	1.7×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[3899-36-3]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
FHHSSXNRVNXTBG-VOTSOKGWSA-N					
4-methyl-1-hexene	1.8×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	2.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[3769-23-1]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
SUWJESCICIOQHO-UHFFFAOYSA-N	4.8×10^{-6}		Modarresi et al. (2005)	Q	248
	1.3×10^{-5}		Yao et al. (2002)	Q	230, 268
	1.9×10^{-5}		Yaws (1999)	?	21

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methyl-*cis*-2-hexene	1.9×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[3683-19-0]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
MBNDKEPQUVZHCM-XQRVVYSFSA-N					
4-methyl-*trans*-2-hexene	1.9×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[3683-22-5]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
MBNDKEPQUVZHCM-GQCTYLIASA-N					
5-methyl-1-hexene	1.9×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[3524-73-0]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
JIUFYGIESXPUPL-UHFFFAOYSA-N					
5-methyl-*cis*-2-hexene	1.8×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[13151-17-2]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
GHBKCPRDHLITSE-PLNGDYQASA-N					
5-methyl-*trans*-2-hexene	1.8×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[7385-82-2]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
GHBKCPRDHLITSE-SNAWJCMRSA-N					
2,3-dimethyl-1-pentene	1.9×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[3404-72-6]	1.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
LIMAEKMEXJTSNI-UHFFFAOYSA-N					
2,3-dimethyl-2-pentene	1.5×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[10574-37-5]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
WFHALSLYRWWUGH-UHFFFAOYSA-N					
2,4-dimethyl-1-pentene	1.9×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[2213-32-3]	1.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
LXQPBCHJNIOMQU-UHFFFAOYSA-N					
2,4-dimethyl-2-pentene	2.0×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	9.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[625-65-0]	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
VVCFYASOGFVJFN-UHFFFAOYSA-N					
3,3-dimethyl-1-pentene	2.1×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[3404-73-7]	1.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
TXBZITDWMURSEF-UHFFFAOYSA-N					

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4-dimethyl-1-pentene	2.0×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	2.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[7385-78-6]	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
WFHXQNMTMDKVJG-UHFFFAOYSA-N					
3,4-dimethyl-*cis*-2-pentene	1.8×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[4914-91-4]	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
PPBWEVVDSRKEIK-ALCCZGGFSA-N					
3,4-dimethyl-*trans*-2-pentene	1.7×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[4914-92-5]	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
PPBWEVVDSRKEIK-FNORWQNLSA-N					
4,4-dimethyl-1-pentene	2.1×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[762-62-9]	1.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
KLCNJIQZXOQYTE-UHFFFAOYSA-N					
4,4-dimethyl-*cis*-2-pentene	1.9×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[762-63-0]	1.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
BIDIHFPLDRSAMB-WAYWQWQTSA-N					
4,4-dimethyl-*trans*-2-pentene	2.1×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[690-08-4]	1.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
BIDIHFPLDRSAMB-AATRIKPKSA-N					
2-ethyl-1-pentene	1.6×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[3404-71-5]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
TWCRBBJSQAZZQB-UHFFFAOYSA-N	2.9×10^{-6}		Modarresi et al. (2005)	Q	248
	2.4×10^{-5}		Yao et al. (2002)	Q	230
	1.6×10^{-5}		Yaws (1999)	?	21
3-ethyl-1-pentene	1.9×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[4038-04-4]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
YPVPQMCSLFDIKA-UHFFFAOYSA-N	4.9×10^{-6}		Modarresi et al. (2005)	Q	248
	1.3×10^{-5}		Yao et al. (2002)	Q	230
	1.9×10^{-5}		Yaws (1999)	?	21
3-ethyl-2-pentene	1.6×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[816-79-5]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
XMYFZAWUNVHVGI-UHFFFAOYSA-N					

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-2-ethyl-1-butene	1.9×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[7357-93-9]	1.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
ADHCYQWFCLQBFG-UHFFFAOYSA-N					
2,3,3-trimethyl-1-butene	1.9×10^{-5}		Yaws (2003)	X	238
C_7H_{14}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[594-56-9]	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
AUYRUAVCWOAHQN-UHFFFAOYSA-N	3.0×10^{-6}		Modarresi et al. (2005)	Q	248
	7.8×10^{-6}		Yao et al. (2002)	Q	230
	2.0×10^{-5}		Yaws (1999)	?	21
1-octene	1.6×10^{-5}		Brockbank (2013)	L	
C_8H_{16}	1.1×10^{-5}	4400	Plyasunov and Shock (2000)	L	
[111-66-0]	1.0×10^{-5}		Mackay and Shiu (1981)	L	
KWKAKUADMBZCLK-UHFFFAOYSA-N	1.6×10^{-5}		Duchowicz et al. (2020)	V	187
	1.6×10^{-5}		HSDB (2015)	V	
	1.0×10^{-5}		Mackay et al. (2006a)	V	
	1.0×10^{-5}		Mackay et al. (1993)	V	
	1.0×10^{-5}		Hwang et al. (1992)	V	
	1.0×10^{-5}		Meylan and Howard (1991)	V	
	1.0×10^{-5}		Eastcott et al. (1988)	V	
	1.0×10^{-5}		Hine and Mookerjee (1975)	V	
	1.5×10^{-5}		McAuliffe (1966)	V	24
	1.6×10^{-5}		Yaws (2003)	X	238
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
	9.2×10^{-6}		Hilal et al. (2008)	Q	
	2.6×10^{-5}		Modarresi et al. (2007)	Q	68
	2.1×10^{-6}		Modarresi et al. (2005)	Q	248
	1.1×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	1.9×10^{-5}		Yao et al. (2002)	Q	230
	1.6×10^{-5}		English and Carroll (2001)	Q	231, 232
	5.7×10^{-5}		Katritzky et al. (1998)	Q	
	8.4×10^{-6}		Russell et al. (1992)	Q	280
	1.8×10^{-5}		Suzuki et al. (1992)	Q	233
	1.6×10^{-5}		Meylan and Howard (1991)	Q	
	1.3×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	1.6×10^{-5}		Yaws (1999)	?	21
	1.6×10^{-5}		Yaws and Yang (1992)	?	21
	1.6×10^{-5}		Abraham et al. (1990)	?	

Table A2.3: Aliphatic alkenes and cycloalkenes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cis-2-octene	8.3×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[7642-04-8]	9.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
ILPBINAXDRFYPL-HYXAFXHYSA-N					
trans-2-octene	8.3×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[13389-42-9]	9.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
ILPBINAXDRFYPL-HWKANZROSA-N	8.4×10^{-6}		Yaws (1999)	?	21
cis-3-octene	8.9×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[14850-22-7]	9.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
YCTDZYMMFQCTEO-ALCCZGGFSA-N					
trans-3-octene	8.6×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[14919-01-8]	9.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
YCTDZYMMFQCTEO-FNORWQNLSA-N	8.8×10^{-6}		Yaws (1999)	?	21
cis-4-octene	8.9×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[7642-15-1]	9.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
IRUCBBFNLDIMIK-FPLPWBNLSA-N					
trans-4-octene	8.9×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[14850-23-8]	9.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
IRUCBBFNLDIMIK-BQYQJAHWSA-N	9.1×10^{-6}		Yaws (1999)	?	21
2-methyl-1-heptene	9.6×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[15870-10-7]	9.8×10^{-6}		Gharagheizi et al. (2010)	Q	247
RCBGGJURENJHKV-UHFFFAOYSA-N					
2-methyl-2-heptene	8.9×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[627-97-4]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
WEPNJTDVIIKRIK-UHFFFAOYSA-N					
2-methyl-*cis*-3-heptene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[20488-34-0]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
CYEZJYAMLNTSKN-SREVYHEPSA-N					
2-methyl-*trans*-3-heptene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[692-96-6]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
CYEZJYAMLNTSKN-VOTSOKGWSA-N					

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-1-heptene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[4810-09-7]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
QDMFTFWKTYXBIW-UHFFFAOYSA-N					
3-methyl-*cis*-2-heptene	9.0×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[22768-19-0]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
OFKLSPUVNMOIJB-YVMONPNESA-N					
3-methyl-*trans*-2-heptene	9.0×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[22768-20-3]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
OFKLSPUVNMOIJB-VMPITWQZSA-N					
3-methyl-*cis*-3-heptene	9.2×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[22768-17-8]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
AAUHUDBDDBJONC-FPLPWBNLSA-N					
3-methyl-*trans*-3-heptene	9.2×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[22768-18-9]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
AAUHUDBDDBJONC-BQYQJAHWSA-N					
4-methyl-1-heptene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[13151-05-8]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
BFGOGLKYJXQPJZ-UHFFFAOYSA-N					
4-methyl-*cis*-2-heptene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[66225-16-9]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
SVGLFIBXFVQUQY-XQRVVYSFSA-N					
4-methyl-*trans*-2-heptene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[66225-17-0]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
SVGLFIBXFVQUQY-GQCTYLIASA-N					
4-methyl-*cis*-3-heptene	9.0×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[14255-24-4]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
KKVVJQGDNYIIMN-VURMDHGXSA-N					
4-methyl-*trans*-3-heptene	9.0×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[13714-85-7]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
KKVVJQGDNYIIMN-SOFGYWHQSA-N					

Table A2.3: Aliphatic alkenes and cycloalkenes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5-methyl-1-heptene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[13151-04-7]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
WNEYWVBECXCQRT-UHFFFAOYSA-N					
5-methyl-*cis*-2-heptene	9.9×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[24608-84-2]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
VIHUHUGDEZCPDK-XQRVVYSFSA-N					
5-methyl-*trans*-2-heptene	9.9×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[24608-85-3]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
VIHUHUGDEZCPDK-GQCTYLIASA-N					
5-methyl-*cis*-3-heptene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[50422-80-5]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
YMNTZRCUPAYGLG-SREVYHEPSA-N					
5-methyl-*trans*-3-heptene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[53510-18-2]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
YMNTZRCUPAYGLG-VOTSOKGWSA-N					
6-methyl-1-heptene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[5026-76-6]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
DFVOXRAAHOJJBN-UHFFFAOYSA-N					
6-methyl-*cis*-2-heptene	1.0×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[66225-18-1]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
LXBJRNXXTAWCKU-PLNGDYQASA-N					
6-methyl-*trans*-2-heptene	1.0×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[51065-65-7]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
LXBJRNXXTAWCKU-SNAWJCMRSA-N					
6-methyl-*cis*-3-heptene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[66225-19-2]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
PMPISKBGRHSPEE-WAYWQWQTSA-N					
6-methyl-*trans*-3-heptene	1.0×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[66225-20-5]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
PMPISKBGRHSPEE-AATRIKPKSA-N					

Table A2.3: Aliphatic alkenes and cycloalkenes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2-dimethyl-*cis*-3-hexene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[690-92-6]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
JPLZSSHKQZJYTJ-SREVYHEPSA-N					
2,2-dimethyl-*trans*-3-hexene	1.4×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	9.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[690-93-7]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
JPLZSSHKQZJYTJ-VOTSOKGWSA-N					
2,3-dimethyl-1-hexene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[16746-86-4]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
LVLXQRZPKUFJJQ-UHFFFAOYSA-N					
2,3-dimethyl-2-hexene	9.1×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	7.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[7145-20-2]	9.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
RGYAVZGBAJFMIZ-UHFFFAOYSA-N					
2,3-dimethyl-*cis*-3-hexene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	9.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[59643-75-3]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
PRTXQHCLTIKAAJ-VURMDHGXSA-N					
2,3-dimethyl-*trans*-3-hexene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	9.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[66225-30-7]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
PRTXQHCLTIKAAJ-SOFGYWHQSA-N					
2,4-dimethyl-1-hexene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[16746-87-5]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
PKVDGQHNRICJLA-UHFFFAOYSA-N					
2,4-dimethyl-2-hexene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	8.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[14255-23-3]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
IZSBIPQYBGDXJZ-UHFFFAOYSA-N					
2,4-dimethyl-*cis*-3-hexene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	8.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[37549-89-6]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
VFCHHMABGOYOQI-VURMDHGXSA-N					
2,4-dimethyl-*trans*-3-hexene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	7.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[61847-78-7]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
VFCHHMABGOYOQI-SOFGYWHQSA-N					

Table A2.3: Aliphatic alkenes and cycloalkenes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,5-dimethyl-1-hexene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[6975-92-4]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
ISZWTVCVSJVEOL-UHFFFAOYSA-N					
2,5-dimethyl-2-hexene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	8.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[3404-78-2]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
VFZIUYUUQFYZBR-UHFFFAOYSA-N					
2,5-dimethyl-*cis*-3-hexene	1.3×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	9.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[10557-44-5]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
KNCMKWVOMRUHKZ-WAYWQWQTSA-N					
2,5-dimethyl-*trans*-3-hexene	1.4×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	9.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[692-70-6]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
KNCMKWVOMRUHKZ-AATRIKPKSA-N					
3,3-dimethyl-1-hexene	1.3×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[3404-77-1]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
RXYYKIMRVXDSFR-UHFFFAOYSA-N					
3,4-dimethyl-1-hexene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[16745-94-1]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
OWWRMMIWAOBBFK-UHFFFAOYSA-N					
3,4-dimethyl-*cis*-2-hexene	1.0×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	9.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[19550-81-3]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
FMNLVKMLDPGPRY-ALCCZGGFSA-N					
3,4-dimethyl-*trans*-2-hexene	1.0×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	9.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[19550-82-4]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
FMNLVKMLDPGPRY-FNORWQNLSA-N					
3,4-dimethyl-*cis*-3-hexene	9.0×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	7.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[19550-87-9]	9.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
XTUXVDJHGIEBAA-FPLPWBNLSA-N					
3,4-dimethyl-*trans*-3-hexene	9.0×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	7.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[19550-88-0]	9.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
XTUXVDJHGIEBAA-BQYQJAHWSA-N					

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,5-dimethyl-1-hexene	1.3×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[7423-69-0]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
FEZKAPRRVNNJTK-UHFFFAOYSA-N					
3,5-dimethyl-*cis*-2-hexene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	8.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[66225-31-8]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
BQAZYKYBFAMHPG-YVMONPNESA-N					
3,5-dimethyl-*trans*-2-hexene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	8.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[66225-12-5]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
BQAZYKYBFAMHPG-VMPITWQZSA-N					
4,4-dimethyl-1-hexene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[1647-08-1]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
SUJVAMIXNUAJEY-UHFFFAOYSA-N					
4,4-dimethyl-*cis*-2-hexene	1.3×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
OQEVAISXHCRQGF-ALCCZGGFSA-N	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
4,4-dimethyl-*trans*-2-hexene	1.3×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[19550-83-5]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
OQEVAISXHCRQGF-FNORWQNLSA-N					
4,5-dimethyl-1-hexene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[16106-59-5]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
UFWIBUBEFUNVNI-UHFFFAOYSA-N					
4,5-dimethyl-*cis*-2-hexene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[65036-71-7]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
OAVNNZUEVHDCKP-WAYWQWQTSA-N					
4,5-dimethyl-*trans*-2-hexene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[66225-14-7]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
OAVNNZUEVHDCKP-AATRIKPKSA-N					
5,5-dimethyl-1-hexene	1.4×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[7116-86-1]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
KZJIOVQKSAOPOP-UHFFFAOYSA-N					

Table A2.3: Aliphatic alkenes and cycloalkenes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5,5-dimethyl-*cis*-2-hexene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[39761-61-0]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
NWZJLSKAFZXSQH-WAYWQWQTSA-N					
5,5-dimethyl-*trans*-2-hexene	1.3×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[39782-43-9]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
NWZJLSKAFZXSQH-AATRIKPKSA-N					
2-ethyl-1-hexene	9.2×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	2.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[1632-16-2]	9.8×10^{-6}		Gharagheizi et al. (2010)	Q	247
XTVRLCUJHGUXCP-UHFFFAOYSA-N	9.4×10^{-6}		Yaws (1999)	?	21
3-ethyl-1-hexene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[3404-58-8]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
OLGHJTHQWQKJQQ-UHFFFAOYSA-N					
3-ethyl-3-hexene	1.0×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	9.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[16789-51-8]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
AUJLDZJNMXNESO-UHFFFAOYSA-N					
3-ethyl-*cis*-2-hexene	9.2×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[36880-72-5]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
QEMJIDSLEPYRLM-YVMONPNESA-N					
3-ethyl-*trans*-2-hexene	9.2×10^{-6}		Yaws (2003)	X	238
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[66225-15-8]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
QEMJIDSLEPYRLM-VMPITWQZSA-N					
4-ethyl-1-hexene	1.3×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[16746-85-3]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
OPMUAJRVOWSBTP-UHFFFAOYSA-N					
4-ethyl-*cis*-2-hexene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[54616-49-8]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
STHONQMAWQLWLX-DAXSKMNVSA-N					
4-ethyl-*trans*-2-hexene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[19781-63-6]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
STHONQMAWQLWLX-QPJJXVBHSA-N					

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3-trimethyl-1-pentene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[560-23-6]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
TUSBCMPNIOJUBX-UHFFFAOYSA-N					
2,3,4-trimethyl-1-pentene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[565-76-4]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
FAWUHEYSSPPNSH-UHFFFAOYSA-N					
2,3,4-trimethyl-2-pentene	1.0×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	6.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[565-77-5]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
SZFRZEBLZFTODC-UHFFFAOYSA-N					
2,4,4-trimethyl-1-pentene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.3×10^{-5}		HSDB (2015)	Q	100
[107-39-1]	9.0×10^{-6}		Gharagheizi et al. (2012)	Q	
FXNDIJDIPNCZQJ-UHFFFAOYSA-N	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
	2.6×10^{-6}		Modarresi et al. (2005)	Q	248
	1.1×10^{-5}		Yao et al. (2002)	Q	230
	1.2×10^{-5}		Yaws (1999)	?	21
2,4,4-trimethyl-2-pentene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.1×10^{-5}		HSDB (2015)	Q	100
[107-40-4]	6.8×10^{-6}		Gharagheizi et al. (2012)	Q	
LAAVYEUJEMRIGF-UHFFFAOYSA-N	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
	5.9×10^{-6}		Modarresi et al. (2005)	Q	248
	1.0×10^{-5}		Yao et al. (2002)	Q	230
	1.2×10^{-5}		Yaws (1999)	?	21
3,3,4-trimethyl-1-pentene	1.3×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[560-22-5]	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	247
LLFHCOGPDCJMKY-UHFFFAOYSA-N					
3,4,4-trimethyl-1-pentene	1.3×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[564-03-4]	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	247
BOPVNOMJIDZBQB-UHFFFAOYSA-N					
3,4,4-trimethyl-2-pentene	1.1×10^{-5}		HSDB (2015)	Q	100
C_8H_{16}					
[598-96-9]					
FZQMZRXKWHQJAG-UHFFFAOYSA-N					
3,4,4-trimethyl-*cis*-2-pentene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	8.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[39761-64-3]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
FZQMZRXKWHQJAG-SREVYHEPSA-N					

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4,4-trimethyl-*trans*-2-pentene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	8.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[39761-57-4]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
FZQMZRXKWHQJAG-VOTSOKGWSA-N					
2-methyl-3-ethyl-1-pentene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[19780-66-6]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
HPHHYSWOBXEIRG-UHFFFAOYSA-N					
2-methyl-3-ethyl-2-pentene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	6.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[19780-67-7]	9.0×10^{-6}		Gharagheizi et al. (2010)	Q	247
FQYUGAXHZSQHMU-UHFFFAOYSA-N					
3-methyl-2-ethyl-1-pentene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[3404-67-9]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
YXLCVBVDFKWWRW-UHFFFAOYSA-N					
3-methyl-3-ethyl-1-pentene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[6196-60-7]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
PHHHEKOJKDYRIN-UHFFFAOYSA-N					
4-methyl-2-ethyl-1-pentene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[3404-80-6]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
TVBQWTDYXVGWJL-UHFFFAOYSA-N					
4-methyl-3-ethyl-1-pentene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[61847-80-1]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
DTNALCAUPPLROB-UHFFFAOYSA-N					
4-methyl-3-ethyl-*cis*-2-pentene	1.0×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	9.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[42067-48-1]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
DSTFDBMUTNIZGD-YVMONPNESA-N					
4-methyl-3-ethyl-*trans*-2-pentene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	9.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[42067-49-2]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
DSTFDBMUTNIZGD-VMPITWQZSA-N					
2-propyl-1-pentene	1.0×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[15918-08-8]	9.8×10^{-6}		Gharagheizi et al. (2010)	Q	247
FYUUBXZYRPRIHC-UHFFFAOYSA-N					

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-isopropyl-1-pentene	1.1×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[16746-02-4]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
QOUCFWFZPKWYRE-UHFFFAOYSA-N					
3,3-dimethyl-2-ethyl-1-butene	1.2×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[18231-53-3]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
KQRPZENSXZIOQO-UHFFFAOYSA-N					
3-methyl-2-isopropyl-1-butene	1.3×10^{-5}		Yaws (2003)	X	238
C_8H_{16}	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[111823-35-9]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
GIBPFTYFAOOKOV-UHFFFAOYSA-N					
1-nonene	1.1×10^{-5}		Brockbank (2013)	L	
C_9H_{18}	1.2×10^{-5}		Plyasunov and Shock (2000)	L	
[124-11-8]	1.2×10^{-5}		Duchowicz et al. (2020)	V	187
JRZJOMJEPLMPRA-UHFFFAOYSA-N	1.2×10^{-5}		Mackay et al. (2006a)	V	
	1.2×10^{-5}		Mackay et al. (1993)	V	
	1.2×10^{-5}		Yaws (2003)	X	238
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
	8.9×10^{-6}		Gharagheizi et al. (2010)	Q	247
	6.5×10^{-6}		Hilal et al. (2008)	Q	
	1.1×10^{-5}		Yaffe et al. (2003)	Q	249, 273
	1.7×10^{-5}		Yao et al. (2002)	Q	230
	1.2×10^{-5}		English and Carroll (2001)	Q	231, 232
	1.0×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	1.2×10^{-5}		Yaws (1999)	?	21
	1.2×10^{-5}		Yaws and Yang (1992)	?	21
	1.2×10^{-5}		Abraham et al. (1990)	?	
2-methyl-1-octene	6.2×10^{-6}		Yaws (2003)	X	238
C_9H_{18}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[4588-18-5]	6.9×10^{-6}		Gharagheizi et al. (2010)	Q	247
FBEDQPGLIKZGIN-UHFFFAOYSA-N					
1-decene	8.6×10^{-6}		Brockbank (2013)	L	
$C_{10}H_{20}$	1.8×10^{-5}		Duchowicz et al. (2020)	V	187
[872-05-9]	3.7×10^{-6}		HSDB (2015)	V	
AFFLGGQVNFXPEV-UHFFFAOYSA-N	3.3×10^{-6}		Mackay et al. (1993)	V	
	3.7×10^{-6}		Yaws (2003)	X	238
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.4×10^{-5}		Gharagheizi et al. (2012)	Q	
	7.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
	4.2×10^{-6}		Hilal et al. (2008)	Q	
	4.7×10^{-6}		Yaws (1999)	?	21

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-1-nonene	4.3×10^{-6}		Yaws (2003)	X	238
$C_{10}H_{20}$	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[2980-71-4]	5.2×10^{-6}		Gharagheizi et al. (2010)	Q	247
YLZQHQUVNZVGOK-UHFFFAOYSA-N					
1-undecene	4.5×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{22}$	6.7×10^{-6}		HSDB (2015)	Q	100
[821-95-4]	2.9×10^{-5}		Gharagheizi et al. (2012)	Q	
DCTOHCCUXLBQMS-UHFFFAOYSA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	247
	2.2×10^{-6}		Hilal et al. (2008)	Q	
	1.2×10^{-5}		Yao et al. (2002)	Q	230
	4.6×10^{-6}		Yaws (1999)	?	21
2-methyl-1-decene	3.4×10^{-6}		Yaws (2003)	X	238
$C_{11}H_{22}$	1.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[13151-27-4]	4.4×10^{-6}		Gharagheizi et al. (2010)	Q	247
HLMACKQLXSEXIY-UHFFFAOYSA-N					
1-dodecene	5.1×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{24}$	2.3×10^{-6}		HSDB (2015)	Q	100
[112-41-4]	3.4×10^{-5}		Gharagheizi et al. (2012)	Q	
CRSBERNSMYQZNG-UHFFFAOYSA-N	7.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
	1.5×10^{-6}		Hilal et al. (2008)	Q	
	9.9×10^{-6}		Yao et al. (2002)	Q	230
	5.2×10^{-6}		Yaws (1999)	?	21
2-methyl-1-undecene	3.4×10^{-6}		Yaws (2003)	X	238
$C_{12}H_{24}$	4.3×10^{-6}		Gharagheizi et al. (2010)	Q	247
[18516-37-5]					
SJVKHZYVCVKEGM-UHFFFAOYSA-N					
2,2,4,6,6-pentamethyl-3-heptene	3.6×10^{-6}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_{24}$	5.2×10^{-7}		Zhang et al. (2010)	Q	288, 290
[123-48-8]	1.8×10^{-5}		Zhang et al. (2010)	Q	288, 291
NBUMCEJRJRRLCA-UHFFFAOYSA-N	1.5×10^{-5}		Zhang et al. (2010)	Q	288, 292
1-tridecene	5.8×10^{-6}		Yaws (2003)	X	259
$C_{13}H_{26}$	5.8×10^{-6}		Yaws (2003)	X	238
[2437-56-1]	9.4×10^{-6}		Dupeux et al. (2022)	Q	260
VQOXUMQBYILCKR-UHFFFAOYSA-N	3.8×10^{-6}		HSDB (2015)	Q	100
	3.9×10^{-5}		Gharagheizi et al. (2012)	Q	
	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	247
	9.2×10^{-6}		Yao et al. (2002)	Q	230
	5.9×10^{-6}		Yaws (1999)	?	21
2-methyl-1-dodecene	4.1×10^{-6}		Yaws (2003)	X	238
$C_{13}H_{26}$	2.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[16435-49-7]	4.9×10^{-6}		Gharagheizi et al. (2010)	Q	247
PWRBDKMPAZFCSV-UHFFFAOYSA-N					

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-tetradecene	3.0×10^{-6}		Brockbank (2013)	L	
$C_{14}H_{28}$	1.4×10^{-5}		Yaws (2003)	X	238
[1120-36-1]	1.2×10^{-6}		HSDB (2015)	Q	100
HFDVRLIODXPAHB-UHFFFAOYSA-N	4.3×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
	1.5×10^{-5}		Yaws (1999)	?	21
2-tetradecene	7.5×10^{-6}		Yaws (2003)	X	238
$C_{14}H_{28}$	4.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[638-60-8]	4.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
OBDUMNZXAIUUTH-UHFFFAOYSA-N					
2-methyl-1-tridecene	8.9×10^{-6}		Yaws (2003)	X	238
$C_{14}H_{28}$	3.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[18094-01-4]	6.9×10^{-6}		Gharagheizi et al. (2010)	Q	247
VNBHQOHLCULRDN-UHFFFAOYSA-N					
1-pentadecene	2.2×10^{-6}		Brockbank (2013)	L	
$C_{15}H_{30}$	3.5×10^{-5}		Yaws (2003)	X	238
[13360-61-7]	4.7×10^{-5}		Gharagheizi et al. (2012)	Q	
PJLHTVIBELQURV-UHFFFAOYSA-N	2.6×10^{-5}		Gharagheizi et al. (2010)	Q	247
	8.7×10^{-5}		Yao et al. (2002)	Q	230, 268
	3.6×10^{-5}		Yaws (1999)	?	21
2-methyl-1-tetradecene	1.1×10^{-5}		Yaws (2003)	X	238
$C_{15}H_{30}$	2.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[52254-38-3]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
WSNMNSLVXDWAFZ-UHFFFAOYSA-N					
1-hexadecene	5.7×10^{-5}		Yaws (2003)	X	238
$C_{16}H_{32}$	4.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[629-73-2]	6.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
GQEZCXVZFLOKMC-UHFFFAOYSA-N	5.8×10^{-5}		Yaws (1999)	?	21
2-methyl-1-pentadecene	2.5×10^{-5}		Yaws (2003)	X	238
$C_{16}H_{32}$	3.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[29833-69-0]	2.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
FWQJRKLMXMTXDY-UHFFFAOYSA-N					
2,4-dimethylpentadecane	1.1×10^{-5}		Yaws (2003)	X	238
$C_{17}H_{36}$	4.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-07-3]	2.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
TXGHMPJBDYZJLF-UHFFFAOYSA-N					

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-butadiene	1.2×10^{-4}		Yaws (2003)	X	238
C_4H_6	1.0×10^{-4}		HSDB (2015)	Q	100
[590-19-2]	1.5×10^{-4}		Gharagheizi et al. (2012)	Q	
QNRMTGGDHLBXQZ-UHFFFAOYSA-N	1.2×10^{-4}		Gharagheizi et al. (2010)	Q	247
	1.1×10^{-4}		Hilal et al. (2008)	Q	
	1.2×10^{-4}		Yaws (1999)	?	21
1,3-butadiene	1.4×10^{-4}	3200	Plyasunov and Shock (2000)	L	
C_4H_6	1.3×10^{-4}		Mackay and Shiu (1981)	L	
[106-99-0]	1.4×10^{-4}	4500	Wilhelm et al. (1977)	L	
KAKZBPTYRLMSJV-UHFFFAOYSA-N	1.4×10^{-4}		Ross and Hudson (1957)	M	
	1.3×10^{-4}		Duchowicz et al. (2020)	V	187
	1.3×10^{-4}		HSDB (2015)	V	
	1.3×10^{-4}		Mackay et al. (2006a)	V	
	3.9×10^{-6}		Lide and Frederikse (1995)	V	
	4.8×10^{-5}		Mackay et al. (1993)	V	
	5.0×10^{-5}		Hwang et al. (1992)	V	
	1.6×10^{-4}		Hine and Mookerjee (1975)	V	
	1.2×10^{-4}		Irmann (1965)	V	
	1.4×10^{-4}		Yaws (2003)	X	238
	1.5×10^{-4}		Irmann (1965)	C	
	1.5×10^{-4}		Hayer et al. (2022)	Q	20
	5.6×10^{-3}		Duchowicz et al. (2020)	Q	
	6.3×10^{-4}		Wang et al. (2017)	Q	81, 239
	1.4×10^{-4}		Wang et al. (2017)	Q	81, 240
	2.0×10^{-4}		Wang et al. (2017)	Q	81, 241
	2.7×10^{-4}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.4×10^{-4}		Gharagheizi et al. (2010)	Q	247
	1.8×10^{-4}		Hilal et al. (2008)	Q	
	1.8×10^{-4}		Modarresi et al. (2007)	Q	68
		3600	Kühne et al. (2005)	Q	
	1.3×10^{-5}		Modarresi et al. (2005)	Q	248
	1.3×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	2.5×10^{-4}		Yao et al. (2002)	Q	230
	1.3×10^{-4}		English and Carroll (2001)	Q	231, 275
	1.8×10^{-4}		Suzuki et al. (1992)	Q	233
	9.2×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
		4100	Kühne et al. (2005)	?	
	1.4×10^{-4}		Yaws (1999)	?	21
	1.4×10^{-4}		Yaws and Yang (1992)	?	21

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-1,2-butadiene	1.1×10^{-4}		Yaws (2003)	X	238
C_5H_8	7.2×10^{-5}		Gharagheizi et al. (2012)	Q	
(2-methyl-2,3-butadiene)	9.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
[598-25-4]	1.0×10^{-5}		Modarresi et al. (2005)	Q	248
PAKGDPSCXSUALC-UHFFFAOYSA-N	1.1×10^{-4}		Yaws (1999)	?	21
2-methyl-1,3-butadiene	1.3×10^{-4}	2700	Plyasunov and Shock (2000)	L	
C_5H_8	1.3×10^{-4}		Mackay and Shiu (1981)	L	
(isoprene)	3.0×10^{-4}		Schuhfried et al. (2015)	M	
[78-79-5]	3.4×10^{-4}	4400	Leng et al. (2013)	M	
RRHGJUQNOFWUDK-UHFFFAOYSA-N	1.2×10^{-4}	4400	Ooki and Yokouchi (2011)	M	71
	2.9×10^{-4}		Karl et al. (2003)	M	28
	1.3×10^{-4}		Duchowicz et al. (2020)	V	187
	1.3×10^{-4}		Martins et al. (2017)	V	316
	1.3×10^{-4}		HSDB (2015)	V	
	1.3×10^{-4}		Mackay et al. (2006a)	V	
	1.3×10^{-4}		Copolovici and Niinemets (2005)	V	
	1.3×10^{-4}		Mackay et al. (1993)	V	
	1.3×10^{-4}		Hine and Mookerjee (1975)	V	
	1.3×10^{-4}		Yaws (2003)	X	238
	1.8×10^{-3}		Duchowicz et al. (2020)	Q	
	4.1×10^{-4}		Wang et al. (2017)	Q	81, 239
	1.6×10^{-4}		Wang et al. (2017)	Q	81, 240
	1.9×10^{-4}		Wang et al. (2017)	Q	81, 241
	1.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	1.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
	2.7×10^{-4}		Hilal et al. (2008)	Q	
	1.1×10^{-5}		Modarresi et al. (2005)	Q	248
	1.3×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	1.0×10^{-4}		Yao et al. (2002)	Q	230
	1.1×10^{-4}		Yao et al. (2002)	Q	230
	1.0×10^{-4}		English and Carroll (2001)	Q	231, 232
	1.4×10^{-4}		Suzuki et al. (1992)	Q	233
	6.7×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	1.1×10^{-4}		Yaws (1999)	?	21
	1.3×10^{-4}		Yaws (1999)	?	21
	1.3×10^{-4}		Yaws and Yang (1992)	?	21
1,2-pentadiene	1.1×10^{-4}		Yaws (2003)	X	238
C_5H_8	1.2×10^{-4}		Gharagheizi et al. (2012)	Q	
[591-95-7]	1.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
LVMTVPFRTKXRPH-UHFFFAOYSA-N	9.7×10^{-5}		Hilal et al. (2008)	Q	
	1.1×10^{-4}		Yaws (1999)	?	21

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3-pentadiene C_5H_8 [504-60-9] PMJHHCWVYXUKFD-UHFFFAOYSA-N	1.4×10^{-4}		HSDB (2015)	Q	100
trans-1,3-pentadiene	1.0×10^{-4}		Yaws (2003)	X	238
C_5H_8	8.2×10^{-5}		HSDB (2015)	Q	100
[2004-70-8]	2.2×10^{-4}		Gharagheizi et al. (2012)	Q	
PMJHHCWVYXUKFD-SNAWJCMRSA-N	1.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
	1.1×10^{-4}		Yaws (1999)	?	21
cis-1,3-pentadiene	1.1×10^{-4}		Yaws (2003)	X	238
C_5H_8	2.4×10^{-4}		Gharagheizi et al. (2012)	Q	
[1574-41-0]	1.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
PMJHHCWVYXUKFD-PLNGDYQASA-N	1.1×10^{-4}		Yaws (1999)	?	21
1,4-pentadiene	8.0×10^{-5}		Plyasunov and Shock (2000)	L	
C_5H_8	8.3×10^{-5}		Mackay and Shiu (1981)	L	
[591-93-5]	8.2×10^{-5}		Duchowicz et al. (2020)	V	187
QYZLKGVUSQXAMU-UHFFFAOYSA-N	8.4×10^{-5}		Mackay et al. (2006a)	V	
	8.4×10^{-5}		Mackay et al. (1993)	V	
	8.2×10^{-5}		Hine and Mookerjee (1975)	V	
	8.3×10^{-5}		Yaws (2003)	X	238
	5.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.1×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	8.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
	9.9×10^{-5}		Hilal et al. (2008)	Q	
	8.2×10^{-5}		Modarresi et al. (2007)	Q	68
	1.2×10^{-5}		Modarresi et al. (2005)	Q	248
	8.4×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	1.1×10^{-4}		Yao et al. (2002)	Q	230, 268
	9.9×10^{-5}		English and Carroll (2001)	Q	231, 261
	1.5×10^{-4}		Russell et al. (1992)	Q	280
	1.6×10^{-4}		Suzuki et al. (1992)	Q	233
	7.3×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	8.4×10^{-5}		Yaws (1999)	?	21
	8.3×10^{-5}		Yaws and Yang (1992)	?	21
2,3-pentadiene	1.1×10^{-4}		Yaws (2003)	X	238
C_5H_8	8.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[591-96-8]	9.6×10^{-5}		Gharagheizi et al. (2010)	Q	247
PODAMDNJNMAKAZ-UHFFFAOYSA-N	1.1×10^{-4}		Hilal et al. (2008)	Q	
	1.1×10^{-4}		Yaws (1999)	?	21

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-hexadiene	7.5×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	1.2×10^{-4}		Gharagheizi et al. (2012)	Q	
[592-44-9]	9.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
XIAJQOBRHVKGSP-UHFFFAOYSA-N					
cis-1,3-hexadiene	7.7×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	2.1×10^{-4}		Gharagheizi et al. (2012)	Q	
[14596-92-0]	8.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
AHAREKHAZNPPMI-WAYWQWQTSA-N					
trans-1,3-hexadiene	7.7×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	2.1×10^{-4}		Gharagheizi et al. (2012)	Q	
[20237-34-7]	8.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
AHAREKHAZNPPMI-AATRIKPKSA-N					
1,4-hexadiene	8.4×10^{-5}		HSDB (2015)	Q	100
C_6H_{10}					
[592-45-0]					
PRBHEGAFLDMLAL-UHFFFAOYSA-N					
cis-1,4-hexadiene	8.3×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	1.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[7318-67-4]	8.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
PRBHEGAFLDMLAL-XQRVVYSFSA-N					
trans-1,4-hexadiene	8.3×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	1.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[7319-00-8]	8.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
PRBHEGAFLDMLAL-GQCTYLIASA-N					
1,5-hexadiene	6.8×10^{-5}		Plyasunov and Shock (2000)	L	
C_6H_{10}	7.0×10^{-5}		Duchowicz et al. (2020)	V	187
[592-42-7]	6.9×10^{-5}		Mackay et al. (2006a)	V	
PYGSKMBEVAICCR-UHFFFAOYSA-N	6.7×10^{-5}		Hwang et al. (1992)	V	
	7.3×10^{-5}		Hine and Mookerjee (1975)	V	
	8.1×10^{-5}		Yaws (2003)	X	238
	5.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.0×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
	5.8×10^{-5}		Hilal et al. (2008)	Q	
	1.0×10^{-4}		Modarresi et al. (2007)	Q	68
	9.4×10^{-6}		Modarresi et al. (2005)	Q	248
	5.8×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	3.5×10^{-5}		Yao et al. (2002)	Q	230
	7.5×10^{-5}		English and Carroll (2001)	Q	231, 232
	1.2×10^{-4}		Suzuki et al. (1992)	Q	233
	5.8×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	8.4×10^{-5}		Yaws (1999)	?	21

Table A2.3: Aliphatic alkenes and cycloalkenes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-hexadiene	8.1×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	6.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[592-49-4]	8.0×10^{-5}		Gharagheizi et al. (2010)	Q	247
DPUXQWOMYBMHRN-UHFFFAOYSA-N					
cis-2,*cis*-4-hexadiene	7.1×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	1.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[6108-61-8]	7.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
APPOKADJQUIAHP-GLIMQPGKSA-N					
cis-2,*trans*-4-hexadiene	6.8×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	1.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[5194-50-3]	7.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
APPOKADJQUIAHP-CIIODKQPSA-N	7.0×10^{-5}		Yaws (1999)	?	21
trans-2,*trans*-4-hexadiene	7.0×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	1.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[5194-51-4]	7.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
APPOKADJQUIAHP-GGWOSOGESA-N	7.2×10^{-5}		Yaws (1999)	?	21
2-methyl-1,4-pentadiene	8.8×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	1.1×10^{-4}		Gharagheizi et al. (2012)	Q	
[763-30-4]	9.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
DRWYRROCDFQZQF-UHFFFAOYSA-N					
2-methyl-1,*cis*-3-pentadiene	7.3×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[1501-60-6]	7.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
RCJMVGJKROQDCB-PLNGDYQASA-N					
2-methyl-1,*trans*-3-pentadiene	7.3×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[926-54-5]	7.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
RCJMVGJKROQDCB-SNAWJCMRSA-N					
2-methyl-2,3-pentadiene	7.6×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	5.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[3043-33-2]	8.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
JWMDOGMKTRMFDS-UHFFFAOYSA-N					
3-methyl-1,2-pentadiene	7.8×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	7.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[7417-48-3]	7.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
INFFCVIZNSUFGK-UHFFFAOYSA-N					
3-methyl-1,*cis*-3-pentadiene	7.2×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[2787-45-3]	7.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
BOGRNZQRTNVZCZ-WAYWQWQTSA-N					

Table A2.3: Aliphatic alkenes and cycloalkenes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-1,*trans*-3-pentadiene	7.2×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[2787-43-1]	7.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
BOGRNZQRTNVZCZ-AATRIKPKSA-N					
3-methyl-1,4-pentadiene	8.6×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	1.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[1115-08-8]	9.6×10^{-5}		Gharagheizi et al. (2010)	Q	247
IKQUUYYDRTYXAP-UHFFFAOYSA-N					
4-methyl-1,2-pentadiene	7.8×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	9.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[13643-05-5]	9.2×10^{-5}		Gharagheizi et al. (2010)	Q	247
CAAAXQFHDYHTTC-UHFFFAOYSA-N					
4-methyl-1,3-pentadiene	7.3×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[926-56-7]	7.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
CJSBUWDGPXGFGA-UHFFFAOYSA-N					
2-ethyl-1,3-butadiene	7.4×10^{-5}		Yaws (2003)	X	238
C_6H_{10}	2.2×10^{-4}		Gharagheizi et al. (2012)	Q	
[3404-63-5]	8.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
IGLWCQMNTGCUBB-UHFFFAOYSA-N					
2,3-dimethyl-1,3-butadiene	2.0×10^{-4}		Duchowicz et al. (2020)	V	187
C_6H_{10}	2.0×10^{-4}		Mackay et al. (2006a)	V	
[513-81-5]	2.0×10^{-4}		Mackay et al. (1993)	V	
SDJHPPZKZZWAKF-UHFFFAOYSA-N	2.0×10^{-4}		Meylan and Howard (1991)	V	
	2.1×10^{-4}		Hine and Mookerjee (1975)	V	
	7.7×10^{-5}		Yaws (2003)	X	238
	6.0×10^{-4}		Duchowicz et al. (2020)	Q	
	1.3×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
	1.9×10^{-4}		Hilal et al. (2008)	Q	
	8.1×10^{-6}		Modarresi et al. (2005)	Q	248
	4.7×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	3.8×10^{-5}		Yao et al. (2002)	Q	230
	9.9×10^{-5}		Suzuki et al. (1992)	Q	233
	5.2×10^{-5}		Meylan and Howard (1991)	Q	
	4.7×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	8.0×10^{-5}		Yaws (1999)	?	21
1,6-heptadiene	5.6×10^{-5}		Plyasunov and Shock (2000)	L	
C_7H_{12}	4.6×10^{-5}		Hilal et al. (2008)	Q	
[3070-53-9]	1.5×10^{-4}		Yaffe et al. (2003)	Q	249, 250
GEAWFZNTIFJMHR-UHFFFAOYSA-N					

Table A2.3: Aliphatic alkenes and cycloalkenes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,5-dimethyl-2,4-hexadiene C_8H_{14} [764-13-6] DZPCYXCBXGQBRN-UHFFFAOYSA-N	2.1×10^{-4}		Ebert et al. (2023)	?	317
1-methylcyclopropene C_4H_6 [3100-04-7] SHDPRTQPPWIEJG-UHFFFAOYSA-N	2.5×10^{-4}		HSDB (2015)	Q	100
cyclopentene	2.0×10^{-4}	3300	Brockbank (2013)	L	
C_5H_8	1.6×10^{-4}		Plyasunov and Shock (2000)	L	
[142-29-0]	2.3×10^{-4}	2200	Bakierowska and Trzeszczyński (2003)	M	
LPIQUOYDBNQMRZ-UHFFFAOYSA-N	1.5×10^{-4}		Duchowicz et al. (2020)	V	187
	1.5×10^{-4}		Mackay et al. (2006a)	V	
	1.5×10^{-4}		Mackay et al. (1993)	V	
	1.6×10^{-4}		Hwang et al. (1992)	V	
	1.6×10^{-4}		Hine and Mookerjee (1975)	V	
	1.5×10^{-4}		Yaws (2003)	X	238
	4.3×10^{-3}		Duchowicz et al. (2020)	Q	
	1.5×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
	3.1×10^{-4}		Hilal et al. (2008)	Q	
		3400	Kühne et al. (2005)	Q	
	1.5×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	2.8×10^{-4}		Yao et al. (2002)	Q	230
	4.5×10^{-4}		English and Carroll (2001)	Q	231, 232
	1.4×10^{-4}		Katritzky et al. (1998)	Q	
	1.7×10^{-4}		Suzuki et al. (1992)	Q	233
	1.6×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
		2200	Kühne et al. (2005)	?	
	1.6×10^{-4}		Yaws (1999)	?	21
	1.5×10^{-4}		Yaws and Yang (1992)	?	21
cyclohexene	2.9×10^{-4}	3600	Brockbank (2013)	L	
C_6H_{10}	2.2×10^{-4}		Plyasunov and Shock (2000)	L	
[110-83-8]	3.3×10^{-4}	2000	Bakierowska and Trzeszczyński (2003)	M	
HGCIXCUEYOPUTN-UHFFFAOYSA-N	2.5×10^{-4}		Nielsen et al. (1994)	M	
	2.2×10^{-4}		Mackay et al. (2006a)	V	
	2.2×10^{-4}		Mackay et al. (1993)	V	
	2.2×10^{-4}		Hwang et al. (1992)	V	
	2.2×10^{-4}		Hine and Mookerjee (1975)	V	
	2.2×10^{-4}		Yaws (2003)	X	259

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{-4}		Yaws (2003)	X	238
	3.3×10^{-4}		Dupeux et al. (2022)	Q	260
	6.6×10^{-5}		Keshavarz et al. (2022)	Q	
	4.3×10^{-3}		Duchowicz et al. (2020)	Q	185
	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	9.9×10^{-5}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
	2.5×10^{-4}		Hilal et al. (2008)	Q	
	1.4×10^{-4}		Modarresi et al. (2007)	Q	68
		3700	Kühne et al. (2005)	Q	
	2.2×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	2.5×10^{-4}		Yao et al. (2002)	Q	230
	3.3×10^{-4}		English and Carroll (2001)	Q	231, 232
	1.5×10^{-4}		Katritzky et al. (1998)	Q	
	2.0×10^{-4}		Russell et al. (1992)	Q	280
	1.3×10^{-4}		Suzuki et al. (1992)	Q	233
	1.3×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	2.2×10^{-4}		Duchowicz et al. (2020)	?	186, 21
		3600	Kühne et al. (2005)	?	
	2.2×10^{-4}		Yaws (1999)	?	21
	2.2×10^{-4}		Yaws and Yang (1992)	?	21
1-methylcyclopentene C_6H_{10} [693-89-0] ATQUFXWBVZUTKO-UHFFFAOYSA-N	2.4×10^{-4}		Hilal et al. (2008)	Q	
cycloheptene C_7H_{12} [628-92-2] ZXIJMRYMVAMXQP-UHFFFAOYSA-N	2.0×10^{-4}		Brockbank (2013)	L	
	2.0×10^{-4}		Plyasunov and Shock (2000)	L	
	2.6×10^{-4}		Mackay et al. (2006a)	V	
	2.0×10^{-4}		Mackay et al. (1993)	V	
	1.3×10^{-4}		Hilal et al. (2008)	Q	
1-methylcyclohexene $C_6H_9CH_3$ [591-49-1] CTMHWPIWNRWQEG-UHFFFAOYSA-N	1.4×10^{-4}		Plyasunov and Shock (2000)	L	
	1.3×10^{-4}		Duchowicz et al. (2020)	V	187
	1.2×10^{-4}		Mackay et al. (2006a)	V	
	1.3×10^{-4}		Hine and Mookerjee (1975)	V	
	1.4×10^{-3}		Duchowicz et al. (2020)	Q	
	1.9×10^{-4}		Hilal et al. (2008)	Q	
	1.2×10^{-4}		Modarresi et al. (2007)	Q	68
	1.3×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	2.4×10^{-4}		English and Carroll (2001)	Q	231, 232
	1.6×10^{-4}		Katritzky et al. (1998)	Q	
	9.2×10^{-5}		Suzuki et al. (1992)	Q	233

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyclooctene	2.1×10^{-4}	4300	Brockbank (2013)	L	1
C_8H_{14}	2.1×10^{-4}	4300	Dohányosová et al. (2004)	M	318
[931-88-4]	2.1×10^{-4}		Mackay et al. (2006a)	V	
URYYVOIYTNXXBN-UPHRSURJSA-N		4400	Kühne et al. (2005)	Q	
		4400	Kühne et al. (2005)	?	
1,1,2,3,3-pentamethyl-2,3,4,5,6,7-hexahydro-1H-indene	2.5×10^{-5}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_{24}$	2.5×10^{-6}		Zhang et al. (2010)	Q	288, 290
[33704-59-5]	1.1×10^{-3}		Zhang et al. (2010)	Q	288, 291
CDEGOUYLXTUDAU-UHFFFAOYSA-N	7.3×10^{-5}		Zhang et al. (2010)	Q	288, 292
1,3-cyclopentadiene	1.8×10^{-4}		Plyasunov and Shock (2000)	L	
C_5H_6	4.7×10^{-4}		Duchowicz et al. (2020)	V	187
[542-92-7]	4.7×10^{-4}		HSDB (2015)	V	
ZSWFCLXCOIISFI-UHFFFAOYSA-N	5.1×10^{-3}		Duchowicz et al. (2020)	Q	
	1.2×10^{-3}		Hilal et al. (2008)	Q	
1,3-cyclohexadiene	6.7×10^{-4}		Yaws (2003)	X	238
C_6H_8	8.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[592-57-4]	4.4×10^{-4}		Gharagheizi et al. (2010)	Q	247
MGNZXYYWBUKAII-UHFFFAOYSA-N	1.1×10^{-3}		Hilal et al. (2008)	Q	
	6.7×10^{-4}		Yaws (1999)	?	21
1,4-cyclohexadiene	1.3×10^{-3}	4000	Brockbank (2013)	L	
C_6H_8	1.0×10^{-3}	3800	Plyasunov and Shock (2000)	L	
(1,4-dihydrobenzene)	1.1×10^{-3}		Mackay et al. (2006a)	V	
[628-41-1]	9.7×10^{-4}		Mackay et al. (1993)	V	
UVJHQYIOXKWHFD-UHFFFAOYSA-N	1.0×10^{-3}		Hilal et al. (2008)	C	
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	8.0×10^{-4}		Hilal et al. (2008)	Q	
	5.4×10^{-4}		Modarresi et al. (2007)	Q	68
1,3-cycloheptadiene C_7H_{10} [4054-38-0] GWYPDXLJACEENP-UHFFFAOYSA-N	6.2×10^{-4}		Hilal et al. (2008)	Q	
1,3,5-cycloheptatriene	2.2×10^{-3}	3900	Plyasunov and Shock (2000)	L	
C_7H_8	2.1×10^{-3}		Duchowicz et al. (2020)	V	187
[544-25-2]			Mackay et al. (2006a)	V	293
CHVJITGCYZJHLR-UHFFFAOYSA-N	2.1×10^{-3}		Mackay et al. (1993)	V	
	2.1×10^{-3}		Cabani et al. (1981)	V	
	2.2×10^{-3}		Yaws (2003)	X	238
	6.0×10^{-3}		Duchowicz et al. (2020)	Q	
	4.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.3×10^{-3}		Gharagheizi et al. (2010)	Q	247

Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.8×10^{-3}		Hilal et al. (2008)	Q	
	3.4×10^{-4}		Modarresi et al. (2007)	Q	68
	3.0×10^{-3}		English and Carroll (2001)	Q	231, 232
	8.4×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	2.1×10^{-3}		Yaws (1999)	?	21
	2.1×10^{-3}		Yaws and Yang (1992)	?	21
1,5-cyclooctadiene C_8H_{12} [111-78-4] VYXHVRARDIDEHS-QGTKBVGQSA-N	3.8×10^{-4}		Hilal et al. (2008)	Q	
1-ethenylcyclohexene C_8H_{12} [2622-21-1] SDRZFSPCVYEJTP-UHFFFAOYSA-N	7.7×10^{-4}		Hilal et al. (2008)	Q	
4-ethenylcyclohexene C_8H_{12} (4-vinylcyclohexene) [100-40-3] BBDKZWKEPDTENS-UHFFFAOYSA-N	2.2×10^{-4}		Plyasunov and Shock (2000)	L	
	2.2×10^{-4}		Duchowicz et al. (2020)	V	187
	2.2×10^{-4}		HSDB (2015)	V	
	5.9×10^{-3}		Duchowicz et al. (2020)	Q	
	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	1.8×10^{-4}		Hilal et al. (2008)	Q	
	2.7×10^{-4}		Modarresi et al. (2007)	Q	68
	2.2×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	2.7×10^{-4}		Katritzky et al. (1998)	Q	
	2.2×10^{-4}		Yaws (1999)	?	21
1,3,5,7-cyclooctatetraene C_8H_8 [629-20-9] KDUIUFJBNGTBMD-DLMDZQPMSA-N	3.6×10^{-2}		Hilal et al. (2008)	Q	
3a,4,7,7a-tetrahydro-4,7-methano-1H-indene $C_{10}H_{12}$ (dicyclopentadiene) [77-73-6] HECLRDQVFMWTQS-UHFFFAOYSA-N	1.6×10^{-4}		HSDB (2015)	Q	100
	2.8×10^{-5}		Hilal et al. (2008)	Q	
1,5,9-cyclododecatriene $C_{12}H_{18}$ [4904-61-4] ZOLLIQAKMYWTBR-UHFFFAOYSA-N	3.3×10^{-4}		HSDB (2015)	Q	100

Table A2.3: Aliphatic alkenes and cycloalkenes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(E,E,Z)-1,5,9-cyclododecatriene $C_{12}H_{18}$ [706-31-0] ZOLLIQAKMYWTBR-RYMQXAEESA-N	1.8×10^{-4}		Ebert et al. (2023)	?	319

A2.4 Aliphatic alkynes

Table A2.4: Aliphatic alkynes

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethyne	4.1×10^{-4}	1800	Burkholder et al. (2019)	L	1
C_2H_2	4.1×10^{-4}	1800	Burkholder et al. (2015)	L	1
(acetylene)	4.1×10^{-4}	1700	Sander et al. (2011)	L	1
[74-86-2]	4.1×10^{-4}	1800	Sander et al. (2006)	L	1
HSFWRNGVRCDJHI-UHFFFAOYSA-N	4.1×10^{-4}	1700	Fogg et al. (2002)	L	
	4.1×10^{-4}	1800	Plyasunov and Shock (2000)	L	
	4.1×10^{-4}	1800	Wilhelm et al. (1977)	L	
	4.0×10^{-4}	2500	Jadkar and Chaudhari (1980)	M	
	2.5×10^{-4}		Maillard and Rosenthal (1952)	M	320
	3.3×10^{-4}		Grollman (1929)	M	59
	4.2×10^{-4}	1900	Gatterer (1926)	M	
	3.7×10^{-4}		Kremann and Hönel (1913)	M	
	4.1×10^{-4}	2000	Winkler (1906)	M	
	5.1×10^{-4}		Billitzer (1902)	M	81, 321
	4.5×10^{-4}		Duchowicz et al. (2020)	V	187
	4.5×10^{-4}		HSDB (2015)	V	
	3.9×10^{-4}		Hwang et al. (1992)	V	
	4.1×10^{-4}		Hine and Mookerjee (1975)	V	
	1.8×10^{-5}		Pierotti (1965)	T	
	3.9×10^{-4}		Yaws (2003)	X	238
	4.1×10^{-4}	1800	Schoen (1923)	X	322
	4.4×10^{-4}		Vítovec (1968)	X	322, 12
	4.1×10^{-4}		Deno and Berkheimer (1960)	C	
	4.2×10^{-4}		Hayer et al. (2022)	Q	20
	8.9×10^{-3}		Duchowicz et al. (2020)	Q	
	3.5×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.8×10^{-3}		Wang et al. (2017)	Q	81, 240
	2.9×10^{-3}		Wang et al. (2017)	Q	81, 241
	8.4×10^{-5}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
	1.4×10^{-3}		Hilal et al. (2008)	Q	
		1800	Kühne et al. (2005)	Q	
	3.8×10^{-4}		Suzuki et al. (1992)	Q	233
	5.8×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	5.0×10^{-4}		Irmann (1965)	Q	
		1800	Kühne et al. (2005)	?	
	3.9×10^{-4}		Yaws (1999)	?	21
	4.1×10^{-4}	1800	Yaws et al. (1999)	?	21
	4.1×10^{-4}	1800	Dean and Lange (1999)	?	323, 23
	3.9×10^{-4}		Yaws and Yang (1992)	?	21
	4.1×10^{-4}		Abraham et al. (1990)	?	

Table A2.4: Aliphatic alkynes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
propyne	7.5×10^{-4}	2400	Plyasunov and Shock (2000)	L	
CH_3CCH	9.0×10^{-4}		Mackay and Shiu (1981)	L	
[74-99-7]	9.2×10^{-4}		McAuliffe (1966)	M	
MWWATHDPGQKSAR-UHFFFAOYSA-N	7.7×10^{-4}	2500	Simpson and Lovell (1962)	M	
	6.2×10^{-4}	2000	Inga and McKetta (1961)	M	
	9.0×10^{-4}		Duchowicz et al. (2020)	V	187
	9.0×10^{-4}		HSDB (2015)	V	
	9.0×10^{-4}		Hine and Mookerjee (1975)	V	
	6.6×10^{-4}		Irmann (1965)	V	
	9.2×10^{-4}		Yaws (2003)	X	238
	7.6×10^{-4}		Hayer et al. (2022)	Q	20
	3.2×10^{-3}		Duchowicz et al. (2020)	Q	
	1.1×10^{-4}		Gharagheizi et al. (2012)	Q	
	9.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
	6.0×10^{-4}		Hilal et al. (2008)	Q	
	4.0×10^{-4}		Modarresi et al. (2007)	Q	68
		2100	Kühne et al. (2005)	Q	
	9.2×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	2.7×10^{-4}		Suzuki et al. (1992)	Q	233
	4.4×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	8.4×10^{-4}		Irmann (1965)	Q	
		2400	Kühne et al. (2005)	?	
	9.3×10^{-4}		Yaws (1999)	?	21
	9.2×10^{-4}		Yaws and Yang (1992)	?	21
	9.0×10^{-4}		Abraham et al. (1990)	?	
			Wilhelm et al. (1977)	W	87
1-butyne	5.6×10^{-4}		Brockbank (2013)	L	
C_2H_5CCH	6.2×10^{-4}	1900	Plyasunov and Shock (2000)	L	
(ethylacetylene)	5.2×10^{-4}		Mackay and Shiu (1981)	L	
[107-00-6]	7.5×10^{-4}	1900	Wilhelm et al. (1977)	L	
KDKYADYSIPSCCQ-UHFFFAOYSA-N	5.4×10^{-4}		McAuliffe (1966)	M	
	7.2×10^{-4}	1900	Simpson and Lovell (1962)	M	
	5.2×10^{-4}		Mackay et al. (2006a)	V	
	2.9×10^{-4}		Hwang et al. (1992)	V	
	5.3×10^{-4}		Hine and Mookerjee (1975)	V	
	5.4×10^{-4}		Yaws (2003)	X	238
	8.3×10^{-5}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Gharagheizi et al. (2010)	Q	247
	3.6×10^{-4}		Hilal et al. (2008)	Q	
	2.1×10^{-4}		Modarresi et al. (2007)	Q	68
		2500	Kühne et al. (2005)	Q	
	6.9×10^{-4}		English and Carroll (2001)	Q	231, 232
	2.1×10^{-4}		Suzuki et al. (1992)	Q	233
	3.7×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	6.4×10^{-4}		Irmann (1965)	Q	

Table A2.4: Aliphatic alkynes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		1900	Kühne et al. (2005)	?	
	5.4×10^{-4}		Yaws (1999)	?	21
	5.4×10^{-4}		Yaws and Yang (1992)	?	21
	5.3×10^{-4}		Abraham et al. (1990)	?	
			Burkholder et al. (2019)	W	324
2-butyne	4.6×10^{-4}		Yaws (2003)	X	238
C_4H_6	1.1×10^{-4}		Gharagheizi et al. (2012)	Q	
(dimethylacetylene)	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
[503-17-3]	1.9×10^{-3}		Hilal et al. (2008)	Q	
XNMQEEKYCVKGBD-UHFFFAOYSA-N	4.7×10^{-4}		Yaws (1999)	?	21
1-pentyne	3.9×10^{-4}		Brockbank (2013)	L	
C_3H_7CCH	3.2×10^{-4}		Plyasunov and Shock (2000)	L	
[627-19-0]	4.0×10^{-4}		Mackay and Shiu (1981)	L	
IBXNCJKFFQIKKY-UHFFFAOYSA-N	4.0×10^{-4}		Duchowicz et al. (2020)	V	187
	4.0×10^{-4}		Mackay et al. (2006a)	V	
	4.0×10^{-4}		Mackay et al. (1993)	V	
	2.5×10^{-4}		Amoore and Buttery (1978)	V	
	3.9×10^{-4}		Hine and Mookerjee (1975)	V	
	4.0×10^{-4}		Yaws (2003)	X	238
	3.2×10^{-3}		Duchowicz et al. (2020)	Q	
	6.0×10^{-5}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
	2.4×10^{-4}		Hilal et al. (2008)	Q	
	1.5×10^{-4}		Modarresi et al. (2007)	Q	68
	1.3×10^{-5}		Modarresi et al. (2005)	Q	248
	4.6×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	7.5×10^{-5}		Yao et al. (2002)	Q	230
	2.3×10^{-4}		English and Carroll (2001)	Q	231, 261
	6.1×10^{-5}		Russell et al. (1992)	Q	280
	1.6×10^{-4}		Suzuki et al. (1992)	Q	233
	2.9×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	4.0×10^{-4}		Yaws (1999)	?	21
	2.0×10^{-4}		Yaws and Yang (1992)	?	21
	3.9×10^{-4}		Abraham et al. (1990)	?	
2-pentyne	5.6×10^{-4}		Yaws (2003)	X	238
C_5H_8	6.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[627-21-4]	7.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
NKTDTMONXHODTI-UHFFFAOYSA-N	1.1×10^{-3}		Hilal et al. (2008)	Q	
	1.1×10^{-5}		Modarresi et al. (2005)	Q	248
	7.9×10^{-5}		Yao et al. (2002)	Q	230
	4.0×10^{-4}		Yaws (1999)	?	21

Table A2.4: Aliphatic alkynes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-1-butyne	5.3×10^{-4}		Yaws (2003)	X	238
C_5H_8	4.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[598-23-2]	6.3×10^{-4}		Gharagheizi et al. (2010)	Q	247
USCSRAJGJYMJFZ-UHFFFAOYSA-N	3.7×10^{-4}		Yaws (1999)	?	21
1-hexyne	2.6×10^{-4}		Brockbank (2013)	L	
C_4H_9CCH	3.0×10^{-4}		Plyasunov and Shock (2000)	L	
[693-02-7]	2.5×10^{-4}		Duchowicz et al. (2020)	V	187
CGHIBGNXEGJPQZ-UHFFFAOYSA-N	2.5×10^{-4}		Duchowicz et al. (2020)	V	187
	2.4×10^{-4}		Mackay et al. (2006a)	V	
	2.4×10^{-4}		Mackay et al. (1993)	V	
	2.5×10^{-4}		Hine and Mookerjee (1975)	V	
	2.5×10^{-4}		Yaws (2003)	X	238
	3.2×10^{-3}		Duchowicz et al. (2020)	Q	
	3.2×10^{-3}		Duchowicz et al. (2020)	Q	
	4.8×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
	1.7×10^{-4}		Hilal et al. (2008)	Q	
	1.5×10^{-4}		Modarresi et al. (2007)	Q	68
	1.1×10^{-5}		Modarresi et al. (2005)	Q	248
	2.4×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	2.7×10^{-5}		Yao et al. (2002)	Q	230
	1.8×10^{-4}		English and Carroll (2001)	Q	231, 275
	1.2×10^{-4}		Suzuki et al. (1992)	Q	233
	2.3×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	2.5×10^{-4}		Yaws (1999)	?	21
	4.6×10^{-4}		Yaws and Yang (1992)	?	21
	2.5×10^{-4}		Abraham et al. (1990)	?	
2-hexyne	3.5×10^{-4}		Yaws (2003)	X	238
C_6H_{10}	4.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[764-35-2]	3.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
MELUCTCJOARQQG-UHFFFAOYSA-N	5.8×10^{-4}		Hilal et al. (2008)	Q	
	1.0×10^{-5}		Modarresi et al. (2005)	Q	248
	3.1×10^{-5}		Yao et al. (2002)	Q	230
	2.5×10^{-4}		Yaws (1999)	?	21
3-hexyne	5.5×10^{-4}		Plyasunov and Shock (2000)	L	
C_6H_{10}	5.6×10^{-4}		Yaws (2003)	X	238
[928-49-4]	4.1×10^{-5}		Gharagheizi et al. (2012)	Q	
DQQNMIPXXNPGCV-UHFFFAOYSA-N	3.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
	6.0×10^{-4}		Hilal et al. (2008)	Q	
	1.0×10^{-5}		Modarresi et al. (2005)	Q	248
	3.2×10^{-5}		Yao et al. (2002)	Q	230, 268
	2.6×10^{-4}		Yaws (1999)	?	21

Table A2.4: Aliphatic alkynes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-1-pentyne	4.6×10^{-4}		Yaws (2003)	X	238
C_6H_{10}	3.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[922-59-8]	3.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
PLHJCCHSCFNKCC-UHFFFAOYSA-N					
4-methyl-1-pentyne	4.5×10^{-4}		Yaws (2003)	X	238
C_6H_{10}	3.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[7154-75-8]	3.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
OXRWICUICBZVAE-UHFFFAOYSA-N					
4-methyl-2-pentyne	4.1×10^{-4}		Yaws (2003)	X	238
C_6H_{10}	3.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[21020-27-9]	4.6×10^{-4}		Gharagheizi et al. (2010)	Q	247
SLMFWJQZLPEDDU-UHFFFAOYSA-N					
3,3-dimethyl-1-butyne	4.6×10^{-4}		Yaws (2003)	X	238
C_6H_{10}	2.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[917-92-0]	4.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
PPWNCLVNXGCGAF-UHFFFAOYSA-N					
1-heptyne	1.8×10^{-4}		Brockbank (2013)	L	
$C_5H_{11}CCH$	1.8×10^{-4}		Plyasunov and Shock (2000)	L	
[628-71-7]	1.4×10^{-4}		Duchowicz et al. (2020)	V	187
YVXHZKKCZYLQOP-UHFFFAOYSA-N	1.3×10^{-4}		Mackay et al. (2006a)	V	
	2.2×10^{-4}		Mackay et al. (1993)	V	
	1.5×10^{-4}		Hine and Mookerjee (1975)	V	
	1.4×10^{-4}		Yaws (2003)	X	238
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	4.1×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-4}		Gharagheizi et al. (2010)	Q	247
	1.1×10^{-4}		Hilal et al. (2008)	Q	
	1.1×10^{-4}		Modarresi et al. (2007)	Q	68
	9.6×10^{-6}		Modarresi et al. (2005)	Q	248
	1.5×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	2.4×10^{-5}		Yao et al. (2002)	Q	230
	1.3×10^{-4}		English and Carroll (2001)	Q	231, 232
	9.5×10^{-5}		Suzuki et al. (1992)	Q	233
	1.8×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	1.4×10^{-4}		Yaws (1999)	?	21
	1.4×10^{-4}		Yaws and Yang (1992)	?	21
	1.5×10^{-4}		Abraham et al. (1990)	?	
2-heptyne	4.9×10^{-4}		Plyasunov and Shock (2000)	L	
C_7H_{12}	5.0×10^{-4}		Yaws (2003)	X	238
[1119-65-9]	4.1×10^{-5}		Gharagheizi et al. (2012)	Q	
AMSFEMSYKQQCHL-UHFFFAOYSA-N	2.1×10^{-4}		Gharagheizi et al. (2010)	Q	247

Table A2.4: Aliphatic alkynes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-heptyne	2.2×10^{-4}		Yaws (2003)	X	238
C_7H_{12}	3.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[2586-89-2]	2.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
KLYHSJRCIZOUHE-UHFFFAOYSA-N					
2-methyl-3-hexyne	2.2×10^{-4}		Plyasunov and Shock (2000)	L	
C_7H_{12}	2.6×10^{-4}		Yaws (2003)	X	238
[36566-80-0]	2.6×10^{-5}		Gharagheizi et al. (2012)	Q	
POBOUPFSQKXZFZ-UHFFFAOYSA-N	2.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
3-methyl-1-hexyne	3.1×10^{-4}		Yaws (2003)	X	238
C_7H_{12}	2.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[40276-93-5]	2.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
OPZULQHRFNTFFZ-UHFFFAOYSA-N					
4-methyl-1-hexyne	2.9×10^{-4}		Yaws (2003)	X	238
C_7H_{12}	3.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[52713-81-2]	2.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
YFZSGTDENCTWGW-UHFFFAOYSA-N					
4-methyl-2-hexyne	2.5×10^{-4}		Yaws (2003)	X	238
C_7H_{12}	2.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
[20198-49-6]					
ABEXZFRJQJSEBW-UHFFFAOYSA-N					
5-methyl-1-hexyne	2.8×10^{-4}		Yaws (2003)	X	238
C_7H_{12}	3.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[2203-80-7]	2.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
HKNANEMUCJGPMS-UHFFFAOYSA-N					
5-methyl-2-hexyne	2.4×10^{-4}		Yaws (2003)	X	238
C_7H_{12}	3.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[53566-37-3]	2.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
SVGAHRUSRQTQES-UHFFFAOYSA-N					
3,3-dimethyl-1-pentyne	3.6×10^{-4}		Yaws (2003)	X	238
C_7H_{12}	1.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[918-82-1]	3.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
KQIIKSQUHGGYCU-UHFFFAOYSA-N					
3,4-dimethyl-1-pentyne	3.3×10^{-4}		Yaws (2003)	X	238
C_7H_{12}	2.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[61064-08-2]	3.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
JDQKSTIAVKXRSK-UHFFFAOYSA-N					
4,4-dimethyl-1-pentyne	3.3×10^{-4}		Yaws (2003)	X	238
C_7H_{12}	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[13361-63-2]	3.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
KHBYKPSFBHWBJQ-UHFFFAOYSA-N					

Table A2.4: Aliphatic alkynes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,4-dimethyl-2-pentyne C_7H_{12} [999-78-0] FOALCTWKQSWRST-UHFFFAOYSA-N	3.0×10^{-4} 1.9×10^{-5} 2.7×10^{-4}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
3-ethyl-1-pentyne C_7H_{12} [21020-26-8] WGWGXWSBPXLXTA-UHFFFAOYSA-N	3.2×10^{-4} 2.7×10^{-5} 2.5×10^{-4}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
1-octyne $C_6H_{13}CCH$ [629-05-0] UMIPWJGWASORKV-UHFFFAOYSA-N	1.2×10^{-4} 1.2×10^{-4} 1.2×10^{-4} 1.3×10^{-4} 1.3×10^{-4} 1.2×10^{-4} 1.3×10^{-4} 3.1×10^{-3} 3.1×10^{-5} 1.1×10^{-4} 6.4×10^{-5} 1.0×10^{-4} 1.2×10^{-4} 1.0×10^{-4} 7.2×10^{-5} 1.5×10^{-4} 1.2×10^{-4} 1.2×10^{-4}		Brockbank (2013) Plyasunov and Shock (2000) Duchowicz et al. (2020) Mackay et al. (2006a) Mackay et al. (1993) Hine and Mookerjee (1975) Yaws (2003) Duchowicz et al. (2020) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Yaffe et al. (2003) English and Carroll (2001) Suzuki et al. (1992) Nirmalakhandan and Speece (1988) Yaws and Yang (1992) Abraham et al. (1990)	L L V V V V X Q Q Q Q Q Q Q Q Q ? ?	 187 238 247 68 249, 250 231, 232 233 21
2-octyne C_8H_{14} [2809-67-8] QCQALVMFTWRCFI-UHFFFAOYSA-N	1.3×10^{-4} 3.2×10^{-5} 1.3×10^{-4} 2.2×10^{-4}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Hilal et al. (2008)	X Q Q Q	238 247
3-octyne C_8H_{14} [15232-76-5] UDEISTCPVNLKRJ-UHFFFAOYSA-N	1.5×10^{-4} 2.8×10^{-5} 1.3×10^{-4}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
2,2-dimethyl-3-hexyne C_8H_{14} [4911-60-8] XYBFBXTUWDPXLK-UHFFFAOYSA-N	1.4×10^{-4}		Plyasunov and Shock (2000)	L	

Table A2.4: Aliphatic alkynes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-nonyne	8.5×10^{-5}		Brockbank (2013)	L	
$C_7H_{15}CCH$	9.7×10^{-5}		Plyasunov and Shock (2000)	L	
[3452-09-3]	6.9×10^{-5}		Duchowicz et al. (2020)	V	187
OSSQSXOTMIGBCF-UHFFFAOYSA-N	6.9×10^{-5}		Meylan and Howard (1991)	V	
	6.9×10^{-5}		Hine and Mookerjee (1975)	V	
	7.2×10^{-5}		Yaws (2003)	X	238
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	2.6×10^{-5}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
	4.4×10^{-5}		Hilal et al. (2008)	Q	
	8.2×10^{-5}		Modarresi et al. (2007)	Q	68
	6.9×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	7.9×10^{-5}		English and Carroll (2001)	Q	231, 232
	5.6×10^{-5}		Suzuki et al. (1992)	Q	233
	1.1×10^{-4}		Meylan and Howard (1991)	Q	
	1.2×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	6.9×10^{-5}		Yaws and Yang (1992)	?	21
	6.9×10^{-5}		Abraham et al. (1990)	?	
2-nonyne	7.3×10^{-5}		Yaws (2003)	X	238
C_9H_{16}	2.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[19447-29-1]	8.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
LXKRETAGISZJAD-UHFFFAOYSA-N					
3-nonyne	7.8×10^{-5}		Yaws (2003)	X	238
C_9H_{16}	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[20184-89-8]	8.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
SRRDSRCWRHKEKU-UHFFFAOYSA-N					
2,2,5-trimethyl-3-hexyne	5.5×10^{-5}		Plyasunov and Shock (2000)	L	
C_9H_{16}					
[17530-23-3]					
DKFPMSNUJIRAMR-UHFFFAOYSA-N					
2,2,5,5-tetramethyl-3-hexyne	3.4×10^{-5}		Plyasunov and Shock (2000)	L	
$C_{10}H_{18}$					
[17530-24-4]					
FXVDWKZNFZMSOU-UHFFFAOYSA-N					
1-decyne	6.6×10^{-5}		Yaws (2003)	X	238
$C_{10}H_{18}$	3.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[764-93-2]	6.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
ILLHQJIJCRNRCJ-UHFFFAOYSA-N					
2-decyne	5.2×10^{-5}		Yaws (2003)	X	238
$C_{10}H_{18}$	2.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[2384-70-5]	5.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
RWDDSTHSVISBEA-UHFFFAOYSA-N					

Table A2.4: Aliphatic alkynes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-decyne	5.5×10^{-5}		Yaws (2003)	X	238
$C_{10}H_{18}$	2.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[2384-85-2]	5.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
JUWXVJKQNKKRLD-UHFFFAOYSA-N					
1-undecyne	5.9×10^{-5}		Yaws (2003)	X	238
$C_{11}H_{20}$	5.3×10^{-5}		Gharagheizi et al. (2010)	Q	247
[2243-98-3]					
YVSFLVNWJIEJRV-UHFFFAOYSA-N					
2-undecyne	4.5×10^{-5}		Yaws (2003)	X	238
$C_{11}H_{20}$	3.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[60212-29-5]	4.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
XZSXEDPHMIFYOS-UHFFFAOYSA-N					
3-undecyne	4.6×10^{-5}		Yaws (2003)	X	238
$C_{11}H_{20}$	2.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[60212-30-8]	4.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
DPWGJNPCPLQVKQ-UHFFFAOYSA-N					
1-dodecyne	5.8×10^{-5}		Yaws (2003)	X	238
$C_{12}H_{22}$	3.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[765-03-7]	5.4×10^{-5}		Gharagheizi et al. (2010)	Q	247
ZVDBUOGYYYNMQI-UHFFFAOYSA-N					
2-dodecyne	4.9×10^{-5}		Yaws (2003)	X	238
$C_{12}H_{22}$	3.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[629-49-2]	4.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
NDIJGAGRSOPRNJ-UHFFFAOYSA-N					
3-dodecyne	4.5×10^{-5}		Yaws (2003)	X	238
$C_{12}H_{22}$	3.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[6790-27-8]	4.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
ZFAGQZXKTQFQLE-UHFFFAOYSA-N					
1-tridecyne	7.4×10^{-5}		Yaws (2003)	X	238
$C_{13}H_{24}$	4.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[26186-02-7]	6.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
GZEDKDBFUBPZNG-UHFFFAOYSA-N					
2-tridecyne	6.7×10^{-5}		Yaws (2003)	X	238
$C_{13}H_{24}$	3.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[28467-75-6]	5.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
ZGKKGWBQPYIOBH-UHFFFAOYSA-N					
3-tridecyne	5.8×10^{-5}		Yaws (2003)	X	238
$C_{13}H_{24}$	3.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[60186-78-9]	5.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
HDLJOUCNTFYRPD-UHFFFAOYSA-N					

Table A2.4: Aliphatic alkynes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-tetradecyne	7.4×10^{-5}		Yaws (2003)	X	238
$C_{14}H_{26}$	4.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[765-10-6]	9.9×10^{-5}		Gharagheizi et al. (2010)	Q	247
DZEFNRWGWQDGTR-UHFFFAOYSA-N					
3-tetradecyne	8.6×10^{-5}		Yaws (2003)	X	238
$C_{14}H_{26}$	3.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[60212-32-0]	8.0×10^{-5}		Gharagheizi et al. (2010)	Q	247
DWWMJIDVLGUCDE-UHFFFAOYSA-N					
1-pentadecyne	2.2×10^{-4}		Yaws (2003)	X	238
$C_{15}H_{28}$	4.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[765-13-9]	1.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
DONJGKADZJEXRJ-UHFFFAOYSA-N					
2-pentadecyne	2.3×10^{-4}		Yaws (2003)	X	238
$C_{15}H_{28}$	4.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[52112-25-1]	1.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
VWWAVTXUUYIIEE-UHFFFAOYSA-N					
3-pentadecyne	1.5×10^{-4}		Yaws (2003)	X	238
$C_{15}H_{28}$	3.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[61886-61-1]	1.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
RUHQUJVXUGQUNY-UHFFFAOYSA-N					
1-hexadecyne	8.3×10^{-4}		Yaws (2003)	X	238
$C_{16}H_{30}$	5.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
[629-74-3]					
UCIDYSLOTJMRAM-UHFFFAOYSA-N					
3-hexadecyne	3.3×10^{-4}		Yaws (2003)	X	238
$C_{16}H_{30}$	3.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[61886-62-2]	3.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
HRFPRVYNMNOAQO-UHFFFAOYSA-N					
3-buten-1-yne	4.1×10^{-4}	1700	Plyasunov and Shock (2000)	L	
CH_2CHCCH	3.7×10^{-4}	1700	Wilhelm et al. (1977)	L	
(vinylacetylene)	3.8×10^{-4}	1800	Simpson and Lovell (1962)	M	325
[689-97-4]	3.4×10^{-4}		Duchowicz et al. (2020)	V	187
WFYPICNXBKQZGB-UHFFFAOYSA-N	3.4×10^{-4}		HSDB (2015)	V	
	1.1×10^{-2}		Duchowicz et al. (2020)	Q	
	1.1×10^{-3}		Hilal et al. (2008)	Q	
		2600	Kühne et al. (2005)	Q	
		2100	Kühne et al. (2005)	?	
	3.5×10^{-4}		Yaws (1999)	?	21, 38

Table A2.4: Aliphatic alkynes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
butadiyne	2.0×10^{-3}		Irmann (1965)	C	
C_4H_2	2.7×10^{-1}		Hayer et al. (2022)	Q	20
(biacetylene)	8.6×10^{-3}		Hilal et al. (2008)	Q	
[460-12-8]	1.9×10^{-3}		Yaws (1999)	?	21
LLCSWKVOHICRDD-UHFFFAOYSA-N	1.9×10^{-3}		Yaws and Yang (1992)	?	21
1,6-heptadiyne C_7H_8 [2396-63-6] RSPZSDWVQWRAEF-UHFFFAOYSA-N	4.6×10^{-3}		Plyasunov and Shock (2000)	L	
1,8-nonadiyne C_9H_{12} [2396-65-8] DMOVPHYFYSASTC-UHFFFAOYSA-N	3.0×10^{-3}		Plyasunov and Shock (2000)	L	

A2.5 Mononuclear aromatics

Table A2.5: Mononuclear aromatics

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benzene	1.8×10^{-3}	3800	Schwardt et al. (2021)	L	1
C_6H_6	1.8×10^{-3}	3700	Brockbank (2013)	L	1
[71-43-2]	1.7×10^{-3}	4200	Staudinger and Roberts (2001)	L	
UHOVQNZJYSORNB-UHFFFAOYSA-N	1.8×10^{-3}	3800	Plyasunov and Shock (2000)	L	
	1.6×10^{-3}	4100	Staudinger and Roberts (1996)	L	
	1.8×10^{-3}		Mackay and Shiu (1981)	L	
	1.7×10^{-3}		Kim and Kim (2014)	M	
	1.8×10^{-3}	3800	Hiatt (2013)	M	
	2.7×10^{-3}	1400	Zhang et al. (2013)	M	326
	3.5×10^{-3}		Zhang et al. (2013)	M	327
	1.4×10^{-3}	2400	Lau et al. (2010)	M	11
	1.7×10^{-3}	4200	Sieg et al. (2009)	M	328
	1.8×10^{-3}		Li et al. (2008)	M	
	2.5×10^{-3}		Lodge and Danso (2007)	M	
	1.4×10^{-3}	2200	Lei et al. (2004)	M	329
			Cheng et al. (2003)	M	330
	1.8×10^{-3}		Karl et al. (2003)	M	88
	1.8×10^{-3}	4200	Bakierowska and Trzeszczyński (2003)	M	
	1.7×10^{-3}	3800	Görgényi et al. (2002)	M	331
	1.9×10^{-3}	3200	Bierwagen and Keller (2001)	M	
	2.1×10^{-3}		Kochetkov et al. (2001)	M	298, 332
	1.7×10^{-3}		Kochetkov et al. (2001)	M	298, 333
	1.8×10^{-3}		Miller and Stuart (2000)	M	73
	3.7×10^{-3}		Altschuh et al. (1999)	M	
	1.7×10^{-3}		Ryu and Park (1999)	M	
	1.8×10^{-3}		Dohnal and Hovorka (1999)	M	
	1.8×10^{-3}		Allen et al. (1998)	M	
	2.2×10^{-3}		Peng and Wan (1998)	M	
	1.4×10^{-3}	3300	Peng and Wan (1998)	M	71
	2.2×10^{-3}		de Wolf and Lieder (1998)	M	88
	1.6×10^{-3}		Welke et al. (1998)	M	
	1.9×10^{-3}	3200	Peng and Wan (1997)	M	
	1.8×10^{-3}	2700	Kondoh and Nakajima (1997)	M	
	1.4×10^{-3}	3300	Park et al. (1997)	M	
	1.8×10^{-3}	4200	Alaee et al. (1996)	M	
	1.6×10^{-3}	4300	Turner et al. (1996)	M	
	2.1×10^{-3}	3900	Dewulf et al. (1995)	M	
	2.0×10^{-3}		Nielsen et al. (1994)	M	
	1.7×10^{-3}	4100	Khalfaoui and Newsham (1994b)	M	334
	1.8×10^{-3}	3400	Robbins et al. (1993)	M	335
	1.7×10^{-3}		Hoff et al. (1993)	M	
	1.8×10^{-3}	2300	Ettre et al. (1993)	M	11
	1.5×10^{-3}		Hansen et al. (1993)	M	336

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.7×10^{-3}	4000	Perlinger et al. (1993)	M	
	1.7×10^{-3}		Li and Carr (1993)	M	
	1.8×10^{-3}		Li et al. (1993)	M	
	1.5×10^{-3}		Zhang and Pawliszyn (1993)	M	
	1.7×10^{-3}	4300	Cooling et al. (1992)	M	337
	1.8×10^{-3}		Anderson (1992)	M	73
	1.9×10^{-3}		Yu (1992)	M	12
	1.6×10^{-3}	4300	Bissonette et al. (1990)	M	
	2.0×10^{-3}		Guitart et al. (1989)	M	14
	1.8×10^{-3}	3200	Ashworth et al. (1988)	M	279
	1.7×10^{-3}		Keeley et al. (1988)	M	
	2.0×10^{-3}		Hellmann (1987)	M	88
	1.3×10^{-3}		Yurteri et al. (1987)	M	12
	1.8×10^{-3}	3600	Tsonopoulos and Wilson (1983)	M	1
	1.7×10^{-3}	3900	Sanemasa et al. (1982)	M	
	1.8×10^{-3}	4000	Leighton and Calo (1981)	M	
	1.7×10^{-3}	3500	Sanemasa et al. (1981)	M	
	1.2×10^{-3}	5300	Ervin et al. (1980)	M	
	1.8×10^{-3}		Warner et al. (1980)	M	
	1.8×10^{-3}		Mackay et al. (1979)	M	
	1.1×10^{-3}		Sato and Nakajima (1979a)	M	14
	1.6×10^{-3}	3800	Tsibul'skii et al. (1979)	M	
	1.8×10^{-3}	4200	Green and Frank (1979)	M	
	1.8×10^{-3}		Vitenberg et al. (1975)	M	
	1.2×10^{-3}		Vitenberg et al. (1974)	M	12
	1.7×10^{-3}	4400	Brown and Wasik (1974)	M	
	2.1×10^{-3}	4500	Hartkopf and Karger (1973)	M	
	1.6×10^{-3}	4500	Wasik and Tsang (1970)	M	
	1.5×10^{-3}		Saylor et al. (1938)	M	38
	3.5×10^{-4}		Abraham and Acree (2007)	V	
	1.8×10^{-3}		Mackay et al. (2006a)	V	
	1.8×10^{-3}		Kochetkov et al. (2001)	V	
	1.8×10^{-3}		Shiu and Ma (2000)	V	
	1.8×10^{-3}		Shiu and Mackay (1997)	V	
	1.8×10^{-3}		Park et al. (1997)	V	
	1.8×10^{-3}		Mackay et al. (1992a)	V	
	1.8×10^{-3}		Hwang et al. (1992)	V	
	1.8×10^{-3}		Eastcott et al. (1988)	V	
	1.8×10^{-3}	3800	Abraham (1984)	V	
	1.8×10^{-3}	3600	Ben-Naim and Wilf (1980)	V	1
	1.8×10^{-3}		Warner et al. (1980)	V	
	1.8×10^{-3}		Hine and Mookerjee (1975)	V	
	1.8×10^{-3}	4100	Mackay and Leinonen (1975)	V	
	1.7×10^{-3}	3800	Wauchope and Haque (1972)	V	
	1.7×10^{-3}	3800	Wauchope and Haque (1972)	V	
	2.0×10^{-3}		McAuliffe (1966)	V	24

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.8×10^{-3}	3800	Andon et al. (1954)	V	338
	1.8×10^{-3}		Bohon and Claussen (1951)	V	
	1.8×10^{-3}	3800	Plyasunov et al. (2001)	T	
	1.8×10^{-3}		Mackay et al. (1979)	T	
		3800	Gill et al. (1976)	T	
	2.7×10^{-3}		Pierotti (1965)	T	
	1.8×10^{-3}		Yaws (2003)	X	259
	1.8×10^{-3}		Yaws (2003)	X	238
	1.8×10^{-3}	2200	Goldstein (1982)	X	299
	1.8×10^{-3}		Sieg et al. (2008)	C	
	1.8×10^{-3}		Schüürmann (2000)	C	21
	1.8×10^{-3}		Smith et al. (1993)	C	12
	1.8×10^{-3}		Ryan et al. (1988)	C	
	1.8×10^{-3}		Shen (1982)	C	
	1.8×10^{-3}		Dupeux et al. (2022)	Q	260
	1.4×10^{-3}		Hayer et al. (2022)	Q	20
	7.2×10^{-4}		Keshavarz et al. (2022)	Q	
	6.0×10^{-3}		Duchowicz et al. (2020)	Q	300
	6.5×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.3×10^{-3}		Wang et al. (2017)	Q	81, 240
	3.2×10^{-3}		Wang et al. (2017)	Q	81, 241
	1.8×10^{-3}		Li et al. (2014)	Q	242
	4.4×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.7×10^{-3}		Hilal et al. (2008)	Q	
	2.2×10^{-3}		Modarresi et al. (2007)	Q	68
		4000	Kühne et al. (2005)	Q	
	1.8×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	7.4×10^{-4}		Yao et al. (2002)	Q	230
	2.2×10^{-3}		English and Carroll (2001)	Q	231, 232
	7.7×10^{-5}		Katritzky et al. (1998)	Q	
	2.1×10^{-3}		Suzuki et al. (1992)	Q	233
	2.2×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.8×10^{-3}		Arbuckle (1983)	Q	
	1.8×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		3700	Kühne et al. (2005)	?	
	1.8×10^{-3}		Yaws (1999)	?	21
	1.1×10^{-3}		Abraham and Weathersby (1994)	?	21
	1.8×10^{-3}		Yaws and Yang (1992)	?	21
	1.8×10^{-3}		Abraham et al. (1990)	?	
	2.2×10^{-3}		Mackay and Yeun (1983)	?	

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benzene-d6	1.8×10^{-3}	4000	Hiatt (2013)	M	
C_6D_6	1.6×10^{-3}	4500	Wasik and Tsang (1970)	M	
[1076-43-3]		3800	Gill et al. (1976)	T	
UHOVQNZJYSORNB-MZWXYZOWSA-N					
methylbenzene	1.6×10^{-3}	4100	Schwardt et al. (2021)	L	1
$C_6H_5CH_3$	1.9×10^{-3}	4000	Brockbank (2013)	L	1, 339
(toluene)	1.5×10^{-3}	4300	Staudinger and Roberts (2001)	L	
[108-88-3]	1.6×10^{-3}	4400	Plyasunov and Shock (2000)	L	
YXFVVABEGXRONW-UHFFFAOYSA-N	1.5×10^{-3}	4000	Staudinger and Roberts (1996)	L	
	1.5×10^{-3}		Mackay and Shiu (1981)	L	
	1.5×10^{-3}	4600	Kutsuna and Kaneyasu (2021)	M	
	1.5×10^{-3}		Kim and Kim (2014)	M	
	2.1×10^{-3}	4400	Hiatt (2013)	M	
	2.8×10^{-3}		Zhang et al. (2013)	M	327
	1.7×10^{-3}	4200	Lee et al. (2013)	M	
	1.5×10^{-3}		Kish et al. (2013)	M	
	1.3×10^{-3}	2700	Lau et al. (2010)	M	11
	1.5×10^{-3}	4300	Sieg et al. (2009)	M	328
	1.4×10^{-3}		Helburn et al. (2008)	M	
	1.5×10^{-3}		Li et al. (2008)	M	
	1.3×10^{-3}	2100	Falabella and Teja (2008)	M	11, 340
	1.4×10^{-3}		Lodge and Danso (2007)	M	
	1.5×10^{-3}	3900	Lin and Chou (2006)	M	
			Cheng et al. (2004)	M	330
	1.4×10^{-3}	2200	Lei et al. (2004)	M	329
			Cheng et al. (2003)	M	330
	1.4×10^{-3}		Karl et al. (2003)	M	88
	2.1×10^{-3}		Bobadilla et al. (2003)	M	
	1.7×10^{-3}	4300	Bakierowska and Trzeszczyński (2003)	M	
	2.0×10^{-3}		Destaillats and Charles (2002)	M	
	1.5×10^{-3}	4200	Görgényi et al. (2002)	M	341
	1.7×10^{-3}	3600	Bierwagen and Keller (2001)	M	
	1.0×10^{-3}		Ayuttaya et al. (2001)	M	342
	1.7×10^{-4}		Ayuttaya et al. (2001)	M	343
	7.8×10^{-4}		Ayuttaya et al. (2001)	M	344
	2.3×10^{-3}		Ayuttaya et al. (2001)	M	345
	1.5×10^{-3}		David et al. (2000)	M	73
	1.6×10^{-3}		Miller and Stuart (2000)	M	73
	1.9×10^{-3}	4000	Vane and Giroux (2000)	M	
	8.5×10^{-4}		McIntosh and Heffron (2000)	M	14
	1.5×10^{-3}	4700	Dewulf et al. (1999)	M	
	1.7×10^{-3}		Altschuh et al. (1999)	M	
	1.5×10^{-3}		Ryu and Park (1999)	M	
	1.6×10^{-3}		Dohnal and Hovorka (1999)	M	

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.5×10^{-3}		Allen et al. (1998)	M	
	2.1×10^{-3}		Peng and Wan (1998)	M	
	1.2×10^{-3}	3600	Peng and Wan (1998)	M	71
	2.0×10^{-3}		de Wolf and Lieder (1998)	M	88
	1.4×10^{-3}		Welke et al. (1998)	M	
	1.7×10^{-3}	3700	Peng and Wan (1997)	M	
	1.7×10^{-3}	2800	Kondoh and Nakajima (1997)	M	
	1.3×10^{-3}	3900	Park et al. (1997)	M	
	1.4×10^{-3}	4100	Turner et al. (1996)	M	
	1.5×10^{-3}		Ramachandran et al. (1996)	M	
	1.8×10^{-3}	4400	Dewulf et al. (1995)	M	
	1.6×10^{-3}		Nielsen et al. (1994)	M	
	1.5×10^{-3}	4400	Robbins et al. (1993)	M	346
	1.3×10^{-3}		Hoff et al. (1993)	M	
	1.5×10^{-3}	2500	Ettre et al. (1993)	M	11
	1.4×10^{-3}		Hansen et al. (1993)	M	336
	1.5×10^{-3}	4500	Perlinger et al. (1993)	M	
	1.6×10^{-3}		Li and Carr (1993)	M	
	1.6×10^{-3}		Li et al. (1993)	M	
	1.5×10^{-3}		Zhang and Pawliszyn (1993)	M	
	1.6×10^{-3}	2500	Kolb et al. (1992)	M	278
	1.5×10^{-3}		Anderson (1992)	M	73
	3.7×10^{-3}		Yu (1992)	M	12
	1.4×10^{-3}	5000	Bissonette et al. (1990)	M	
	1.5×10^{-3}	6500	Lamarche and Droste (1989)	M	347
	1.5×10^{-3}	3000	Ashworth et al. (1988)	M	279
	1.6×10^{-3}		Keeley et al. (1988)	M	
	1.7×10^{-3}		Yurteri et al. (1987)	M	12
	1.2×10^{-3}	5400	Schoene and Steinhanses (1985)	M	
	1.5×10^{-3}		Garbarini and Lion (1985)	M	
	1.5×10^{-3}	4200	Sanemasa et al. (1982)	M	
	1.5×10^{-3}	3800	Leighton and Calo (1981)	M	
	1.6×10^{-3}	4100	Sanemasa et al. (1981)	M	
	1.5×10^{-3}	4900	Ervin et al. (1980)	M	
	1.7×10^{-3}		Warner et al. (1980)	M	
	1.5×10^{-3}		Mackay et al. (1979)	M	
	8.6×10^{-4}		Sato and Nakajima (1979a)	M	14
	1.5×10^{-3}	4700	Tsibul'skii et al. (1979)	M	
	1.9×10^{-3}		Vitenberg et al. (1975)	M	
	1.6×10^{-3}	5000	Brown and Wasik (1974)	M	
	2.0×10^{-3}	4900	Hartkopf and Karger (1973)	M	
	1.7×10^{-3}	5900	Wasik and Tsang (1970)	M	
	1.6×10^{-3}		Martins et al. (2017)	V	316
	1.5×10^{-3}		Mackay et al. (2006a)	V	
	1.9×10^{-3}	4300	Fogg and Sangster (2003)	V	348
	1.5×10^{-3}		Shiu and Ma (2000)	V	

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.5×10^{-3}		Park et al. (1997)	V	
	1.5×10^{-3}		Mackay et al. (1992a)	V	
	1.3×10^{-3}		Hwang et al. (1992)	V	
	1.7×10^{-3}		Eastcott et al. (1988)	V	
	1.5×10^{-3}	4400	Abraham (1984)	V	
	1.9×10^{-3}	4200	Ben-Naim and Wilf (1980)	V	1
	1.5×10^{-3}		Warner et al. (1980)	V	
	1.5×10^{-3}		Hine and Mookerjee (1975)	V	
	1.5×10^{-3}		Mackay and Leinonen (1975)	V	
	1.8×10^{-3}	4400	Wauchope and Haque (1972)	V	
	1.7×10^{-3}		McAuliffe (1966)	V	24
	1.8×10^{-3}	4300	Andon et al. (1954)	V	338
	1.8×10^{-3}		Bohon and Claussen (1951)	V	
	1.6×10^{-3}	4400	Plyasunov et al. (2001)	T	
	1.5×10^{-3}		Mackay et al. (1979)	T	
		4400	Gill et al. (1976)	T	
	1.6×10^{-3}		Yaws (2003)	X	259
	1.5×10^{-3}		Yaws (2003)	X	238
	1.5×10^{-3}	1900	Goldstein (1982)	X	299
	1.5×10^{-3}		McAuliffe (1971)	X	349
	1.5×10^{-3}		Sieg et al. (2008)	C	
	1.5×10^{-3}		Schüürmann (2000)	C	21
	1.7×10^{-3}		Smith et al. (1993)	C	12
	1.4×10^{-3}		Ryan et al. (1988)	C	
	1.7×10^{-3}		Shen (1982)	C	
	1.5×10^{-3}		Dupeux et al. (2022)	Q	260
	1.2×10^{-3}		Hayer et al. (2022)	Q	20
	9.7×10^{-4}		Keshavarz et al. (2022)	Q	
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	300
	3.8×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.1×10^{-3}		Wang et al. (2017)	Q	81, 240
	3.0×10^{-3}		Wang et al. (2017)	Q	81, 241
	1.5×10^{-3}		Li et al. (2014)	Q	242
	2.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.5×10^{-3}		Hilal et al. (2008)	Q	
	1.2×10^{-3}		Modarresi et al. (2007)	Q	68
		4300	Kühne et al. (2005)	Q	
	1.6×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	7.2×10^{-4}		Yao et al. (2002)	Q	230
	1.6×10^{-3}		English and Carroll (2001)	Q	231, 232
	2.7×10^{-4}		Katritzky et al. (1998)	Q	
	1.5×10^{-3}		Suzuki et al. (1992)	Q	233

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.2×10^{-3}		Arbuckle (1983)	Q	
	1.5×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4200	Kühne et al. (2005)	?	
	1.6×10^{-3}		Yaws (1999)	?	21
	9.0×10^{-4}		Abraham and Weathersby (1994)	?	21
	1.5×10^{-3}		Yaws and Yang (1992)	?	21
	1.5×10^{-3}		Abraham et al. (1990)	?	
	1.9×10^{-3}		Mackay and Yeun (1983)	?	
methylbenzene-d8 $C_6D_5CD_3$ (toluene-d8) [2037-26-5] YXFVVABEGXRONW-JGUCLWPXSA-N	2.0×10^{-3}	4300	Hiatt (2013)	M	
1,2-dimethylbenzene	2.0×10^{-3}	4600	Schwardt et al. (2021)	L	1
$C_6H_4(CH_3)_2$	2.0×10^{-3}	4700	Brockbank (2013)	L	1
(*o*-xylene)	2.4×10^{-3}	4200	Fogg and Sangster (2003)	L	
[95-47-6]	2.0×10^{-3}	4300	Staudinger and Roberts (2001)	L	
CTQNGGLPUBDAKN-UHFFFAOYSA-N	2.0×10^{-3}	4400	Plyasunov and Shock (2000)	L	
	1.9×10^{-3}	4000	Staudinger and Roberts (1996)	L	
	2.0×10^{-3}		Mackay and Shiu (1981)	L	
	1.9×10^{-3}		Kim and Kim (2014)	M	
	3.2×10^{-3}	4500	Hiatt (2013)	M	
	2.7×10^{-3}	8500	Zhang et al. (2013)	M	326
	2.2×10^{-3}		Zhang et al. (2013)	M	327
	2.0×10^{-3}	4300	Sieg et al. (2009)	M	328
	2.3×10^{-3}		Li et al. (2008)	M	
	1.7×10^{-3}	2500	Falabella and Teja (2008)	M	11, 340
	9.6×10^{-4}		McIntosh and Heffron (2000)	M	14
	2.1×10^{-3}		Dohnal and Hovorka (1999)	M	
	2.2×10^{-3}		Welke et al. (1998)	M	
	1.9×10^{-3}	3400	Kondoh and Nakajima (1997)	M	
	1.4×10^{-3}		Turner et al. (1996)	M	
	2.4×10^{-3}	4500	Dewulf et al. (1995)	M	
	2.0×10^{-3}	5800	Robbins et al. (1993)	M	350
	1.9×10^{-3}		Li and Carr (1993)	M	
	2.1×10^{-3}		Li et al. (1993)	M	
	2.7×10^{-3}		Zhang and Pawliszyn (1993)	M	
	1.4×10^{-3}	3000	Kolb et al. (1992)	M	278
	1.7×10^{-3}		Anderson (1992)	M	73
	2.1×10^{-3}	5600	Bissonette et al. (1990)	M	
	1.9×10^{-3}	3200	Ashworth et al. (1988)	M	279
	2.3×10^{-3}		Yurteri et al. (1987)	M	12
	1.9×10^{-3}	4500	Sanemasa et al. (1982)	M	
	1.0×10^{-3}		Sato and Nakajima (1979a)	M	14

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.9×10^{-3}	5400	Wasik and Tsang (1970)	M	
	1.8×10^{-3}		Mackay et al. (2006a)	V	
	1.8×10^{-3}		Shiu and Ma (2000)	V	
	1.8×10^{-3}		Mackay et al. (1992a)	V	
	2.3×10^{-3}		Eastcott et al. (1988)	V	
	1.8×10^{-3}		Hine and Mookerjee (1975)	V	
	1.9×10^{-3}		Mackay and Leinonen (1975)	V	
	1.9×10^{-3}		McAuliffe (1966)	V	24
	2.3×10^{-3}		Yaws (2003)	X	238
	1.9×10^{-3}		Sieg et al. (2008)	C	
	1.3×10^{-3}		Keshavarz et al. (2022)	Q	
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.3×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.6×10^{-3}		Wang et al. (2017)	Q	81, 240
	3.2×10^{-3}		Wang et al. (2017)	Q	81, 241
	1.3×10^{-3}		Gharagheizi et al. (2012)	Q	
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.0×10^{-3}		Hilal et al. (2008)	Q	
	1.1×10^{-3}		Modarresi et al. (2007)	Q	68
		4100	Kühne et al. (2005)	Q	
	1.9×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.7×10^{-3}		English and Carroll (2001)	Q	231, 275
	3.8×10^{-4}		Katritzky et al. (1998)	Q	
	1.0×10^{-3}		Suzuki et al. (1992)	Q	233
	1.1×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.9×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4100	Kühne et al. (2005)	?	
	2.4×10^{-3}		Yaws (1999)	?	21
	1.1×10^{-3}		Abraham and Weathersby (1994)	?	21
	2.3×10^{-3}		Yaws and Yang (1992)	?	21
	1.9×10^{-3}		Abraham et al. (1990)	?	
1,2-dimethylbenzene-d10 $C_6D_4(CD_3)_2$ (*o*-xylene-d10) [56004-61-6] CTQNGGLPUBDAKN-ZGYYUIRESA-N	3.0×10^{-3}	4700	Hiatt (2013)	M	

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3-dimethylbenzene	1.4×10^{-3}	4100	Schwardt et al. (2021)	L	1
$C_6H_4(CH_3)_2$	1.5×10^{-3}	4300	Brockbank (2013)	L	1
(*m*-xylene)	1.4×10^{-3}	4200	Staudinger and Roberts (2001)	L	
[108-38-3]	1.4×10^{-3}	4600	Plyasunov and Shock (2000)	L	
IVSZLXZYQVIEFR-UHFFFAOYSA-N	1.3×10^{-3}	4200	Staudinger and Roberts (1996)	L	
	1.4×10^{-3}		Mackay and Shiu (1981)	L	
	1.3×10^{-3}		Kim and Kim (2014)	M	
	1.4×10^{-3}		Li et al. (2008)	M	
	1.3×10^{-3}		Karl et al. (2003)	M	88
	6.6×10^{-4}		McIntosh and Heffron (2000)	M	14
	1.5×10^{-3}		Dohnal and Hovorka (1999)	M	
	1.5×10^{-3}	2900	Kondoh and Nakajima (1997)	M	
	1.6×10^{-3}	4300	Dewulf et al. (1995)	M	
	1.3×10^{-3}		Li and Carr (1993)	M	
	1.5×10^{-3}		Li et al. (1993)	M	
	1.4×10^{-3}	6000	Bissonette et al. (1990)	M	
	1.3×10^{-3}	3300	Ashworth et al. (1988)	M	279
	1.4×10^{-3}	4700	Sanemasa et al. (1982)	M	
	6.4×10^{-4}		Sato and Nakajima (1979a)	M	14
	1.8×10^{-3}	4500	Tsibul'skii et al. (1979)	M	
	1.4×10^{-3}		Mackay et al. (2006a)	V	
	1.7×10^{-3}	4300	Fogg and Sangster (2003)	V	
	1.4×10^{-3}		Shiu and Ma (2000)	V	
	1.4×10^{-3}		Mackay et al. (1992a)	V	
	1.4×10^{-3}		Eastcott et al. (1988)	V	
	1.6×10^{-3}		Hine and Mookerjee (1975)	V	
	1.6×10^{-3}	4800	Wauchope and Haque (1972)	V	
	1.7×10^{-3}	5000	Andon et al. (1954)	V	338
	1.7×10^{-3}		Bohon and Claussen (1951)	V	
	1.5×10^{-3}		Yaws (2003)	X	238
	1.4×10^{-3}		Sieg et al. (2008)	C	
	1.3×10^{-3}		Keshavarz et al. (2022)	Q	
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.3×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.2×10^{-3}		Wang et al. (2017)	Q	81, 240
	2.8×10^{-3}		Wang et al. (2017)	Q	81, 241
	1.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.5×10^{-3}		Hilal et al. (2008)	Q	
	7.5×10^{-4}		Modarresi et al. (2007)	Q	68
		4700	Kühne et al. (2005)	Q	
	1.4×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	4.4×10^{-4}		Yao et al. (2002)	Q	230

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.7×10^{-3}		English and Carroll (2001)	Q	231, 232
	3.8×10^{-4}		Katritzky et al. (1998)	Q	
	1.4×10^{-3}		Russell et al. (1992)	Q	280
	1.0×10^{-3}		Suzuki et al. (1992)	Q	233
	1.1×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.4×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4900	Kühne et al. (2005)	?	
	1.5×10^{-3}		Yaws (1999)	?	21
	6.7×10^{-4}		Abraham and Weathersby (1994)	?	21
	1.5×10^{-3}		Yaws and Yang (1992)	?	21
	1.3×10^{-3}		Abraham et al. (1990)	?	
1,4-dimethylbenzene	1.5×10^{-3}	5000	Schwardt et al. (2021)	L	1
$C_6H_4(CH_3)_2$	1.4×10^{-3}	5000	Brockbank (2013)	L	1
(p-xylene)	1.9×10^{-3}	4200	Fogg and Sangster (2003)	L	
[106-42-3]	1.3×10^{-3}	4000	Staudinger and Roberts (2001)	L	
URLKBWYHVLBVBO-UHFFFAOYSA-N	1.4×10^{-3}	4600	Plyasunov and Shock (2000)	L	
	1.3×10^{-3}	3800	Staudinger and Roberts (1996)	L	
	1.4×10^{-3}		Mackay and Shiu (1981)	L	
	1.0×10^{-3}	2600	Schwardt et al. (2021)	M	351, 11
	1.3×10^{-3}		Kim and Kim (2014)	M	
	1.4×10^{-3}		Li et al. (2008)	M	
	1.6×10^{-3}	4800	Lin and Chou (2006)	M	
	2.0×10^{-3}		Bobadilla et al. (2003)	M	
	6.7×10^{-4}		McIntosh and Heffron (2000)	M	14
	1.4×10^{-3}		Ryu and Park (1999)	M	
	1.5×10^{-3}		Dohnal and Hovorka (1999)	M	
	1.5×10^{-3}	2900	Kondoh and Nakajima (1997)	M	
	9.8×10^{-4}	3200	Park et al. (1997)	M	
	1.7×10^{-3}	4800	Dewulf et al. (1995)	M	
	1.2×10^{-3}	3100	Hansen et al. (1993)	M	282
	1.3×10^{-3}		Li and Carr (1993)	M	
	1.4×10^{-3}		Li et al. (1993)	M	
	1.7×10^{-3}		Zhang and Pawliszyn (1993)	M	
	1.2×10^{-3}	5300	Bissonette et al. (1990)	M	
	1.3×10^{-3}	3500	Ashworth et al. (1988)	M	279
	1.3×10^{-3}	4800	Sanemasa et al. (1982)	M	
	6.1×10^{-4}		Sato and Nakajima (1979a)	M	14
	2.3×10^{-3}	5400	Wasik and Tsang (1970)	M	
	1.2×10^{-3}		Martins et al. (2017)	V	316
	1.8×10^{-4}		Abraham and Acree (2007)	V	
	1.7×10^{-3}		Mackay et al. (2006a)	V	
	1.4×10^{-3}		Shiu and Ma (2000)	V	
	1.5×10^{-3}		Park et al. (1997)	V	
	1.7×10^{-3}		Mackay et al. (1992a)	V	
	1.5×10^{-3}		Hwang et al. (1992)	V	

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.8×10^{-3}		Eastcott et al. (1988)	V	
	1.6×10^{-3}		Hine and Mookerjee (1975)	V	
	1.6×10^{-3}	4800	Wauchope and Haque (1972)	V	
	1.6×10^{-3}	4900	Andon et al. (1954)	V	338
	1.6×10^{-3}		Bohon and Claussen (1951)	V	
	1.4×10^{-3}		Foster et al. (1994)	X	352
	1.6×10^{-3}		Yaws (2003)	X	238
	1.4×10^{-3}		Sieg et al. (2008)	C	
	1.3×10^{-3}		Schüürmann (2000)	C	21
	1.3×10^{-3}		Keshavarz et al. (2022)	Q	
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	185
	2.3×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.4×10^{-3}		Wang et al. (2017)	Q	81, 240
	2.6×10^{-3}		Wang et al. (2017)	Q	81, 241
	9.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.5×10^{-3}		Hilal et al. (2008)	Q	
	1.1×10^{-3}		Modarresi et al. (2007)	Q	68
		4700	Kühne et al. (2005)	Q	
	1.5×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	8.1×10^{-4}		Yao et al. (2002)	Q	230
	1.7×10^{-3}		English and Carroll (2001)	Q	231, 232
	3.9×10^{-4}		Katritzky et al. (1998)	Q	
	1.0×10^{-3}		Suzuki et al. (1992)	Q	233
	1.1×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.4×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4500	Kühne et al. (2005)	?	
	1.6×10^{-3}		Yaws (1999)	?	21
	6.4×10^{-4}		Abraham and Weathersby (1994)	?	21
	1.6×10^{-3}		Yaws and Yang (1992)	?	21
	1.4×10^{-3}		Abraham et al. (1990)	?	
1,2,3-trimethylbenzene	2.4×10^{-3}	4600	Brockbank (2013)	L	
$C_6H_3(CH_3)_3$	2.7×10^{-3}	4800	Fogg and Sangster (2003)	L	
[526-73-8]	2.6×10^{-3}	4500	Plyasunov and Shock (2000)	L	
FYGHSUNMUKGBRK-UHFFFAOYSA-N	3.1×10^{-3}		Mackay and Shiu (1981)	L	
	1.1×10^{-3}		Järnberg and Johanson (1995)	M	14
	2.4×10^{-3}	4500	Sanemasa et al. (1982)	M	
	2.9×10^{-3}		Mackay et al. (2006a)	V	
	2.9×10^{-3}		Shiu and Ma (2000)	V	
	3.1×10^{-3}		Abraham et al. (1994a)	V	
	2.9×10^{-3}		Mackay et al. (1992a)	V	
	2.7×10^{-3}		Eastcott et al. (1988)	V	

Table A2.5: Mononuclear aromatics (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.3×10^{-3}		Yaws (2003)	X	238
	1.8×10^{-3}		Keshavarz et al. (2022)	Q	
	7.9×10^{-4}		Duchowicz et al. (2020)	Q	300
	1.4×10^{-3}		Wang et al. (2017)	Q	81, 239
	2.2×10^{-3}		Wang et al. (2017)	Q	81, 240
	3.5×10^{-3}		Wang et al. (2017)	Q	81, 241
	8.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.6×10^{-3}		Gharagheizi et al. (2010)	Q	247
	3.1×10^{-3}		Hilal et al. (2008)	Q	
	8.2×10^{-4}		Modarresi et al. (2007)	Q	68
		3900	Kühne et al. (2005)	Q	
	3.1×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	2.0×10^{-3}		English and Carroll (2001)	Q	231, 275
	4.6×10^{-4}		Katritzky et al. (1998)	Q	
	8.2×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	2.3×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4400	Kühne et al. (2005)	?	
	1.3×10^{-3}		Yaws (1999)	?	21
	2.7×10^{-3}		Yaws and Yang (1992)	?	21
	2.1×10^{-3}		Abraham et al. (1990)	?	
1,2,4-trimethylbenzene	1.6×10^{-3}	4700	Brockbank (2013)	L	
$C_6H_3(CH_3)_3$	1.7×10^{-3}	3100	Fogg and Sangster (2003)	L	
[95-63-6]	1.6×10^{-3}	4800	Plyasunov and Shock (2000)	L	
GWHJZXXIDMPWGX-UHFFFAOYSA-N	1.7×10^{-3}		Mackay and Shiu (1981)	L	
	3.2×10^{-3}	5200	Hiatt (2013)	M	
	1.7×10^{-3}		Li et al. (2008)	M	
	2.3×10^{-3}	3600	Kondoh and Nakajima (1997)	M	
	6.2×10^{-4}		Järnberg and Johanson (1995)	M	14
	1.5×10^{-3}	4300	Hansen et al. (1993)	M	282
	2.1×10^{-3}		Yurteri et al. (1987)	M	12
	1.6×10^{-3}	4800	Sanemasa et al. (1982)	M	
	1.8×10^{-3}		Mackay et al. (2006a)	V	
	1.8×10^{-3}		Shiu and Ma (2000)	V	
	1.7×10^{-3}		Abraham et al. (1994a)	V	
	1.8×10^{-3}		Mackay et al. (1992a)	V	
	1.6×10^{-3}		Eastcott et al. (1988)	V	
	1.7×10^{-3}		Hine and Mookerjee (1975)	V	
	1.4×10^{-3}		Yaws (2003)	X	238
	1.8×10^{-3}		Keshavarz et al. (2022)	Q	
	7.9×10^{-4}		Duchowicz et al. (2020)	Q	300
	1.4×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.9×10^{-3}		Wang et al. (2017)	Q	81, 240

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.8×10^{-3}		Wang et al. (2017)	Q	81, 241
	6.3×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.6×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.1×10^{-3}		Hilal et al. (2008)	Q	
	7.5×10^{-4}		Modarresi et al. (2007)	Q	68
		4500	Kühne et al. (2005)	Q	
	1.8×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	2.0×10^{-3}		English and Carroll (2001)	Q	231, 232
	4.7×10^{-4}		Katritzky et al. (1998)	Q	
	7.3×10^{-4}		Suzuki et al. (1992)	Q	233
	8.0×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	8.2×10^{-4}		Arbuckle (1983)	Q	
	1.6×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4700	Kühne et al. (2005)	?	
	1.5×10^{-3}		Yaws (1999)	?	21
	1.7×10^{-3}		Yaws and Yang (1992)	?	21
	1.6×10^{-3}		Abraham et al. (1990)	?	
1,3,5-trimethylbenzene	1.2×10^{-3}	4400	Brockbank (2013)	L	1
$C_6H_3(CH_3)_3$	1.3×10^{-3}	4900	Plyasunov and Shock (2000)	L	
(mesitylene)	1.7×10^{-3}		Mackay and Shiu (1981)	L	
[108-67-8]	2.3×10^{-3}	5100	Hiatt (2013)	M	
AUHZEENZYGFFBQ-UHFFFAOYSA-N	2.0×10^{-3}		Karl et al. (2003)	M	88
	1.5×10^{-3}	3000	Kondoh and Nakajima (1997)	M	
	4.8×10^{-4}		Järnberg and Johanson (1995)	M	14
	1.3×10^{-3}		Li and Carr (1993)	M	
	1.4×10^{-3}		Li et al. (1993)	M	
	1.4×10^{-3}	3600	Ashworth et al. (1988)	M	279
	1.1×10^{-3}	4700	Sanemasa et al. (1982)	M	
	1.1×10^{-3}	4600	Sanemasa et al. (1981)	M	
	1.4×10^{-4}		Abraham and Acree (2007)	V	
	1.3×10^{-3}		Mackay et al. (2006a)	V	
	1.3×10^{-3}		Shiu and Ma (2000)	V	
	1.8×10^{-3}		Abraham et al. (1994a)	V	
	1.3×10^{-3}		Mackay et al. (1992a)	V	
	1.2×10^{-3}		Eastcott et al. (1988)	V	
	1.2×10^{-3}		Yaws (2003)	X	238
	9.1×10^{-4}		Hayer et al. (2022)	Q	20
	1.8×10^{-3}		Keshavarz et al. (2022)	Q	
	7.9×10^{-4}		Duchowicz et al. (2020)	Q	300
	1.4×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.1×10^{-3}		Wang et al. (2017)	Q	81, 240
	2.5×10^{-3}		Wang et al. (2017)	Q	81, 241

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.4×10^{-3}		Hilal et al. (2008)	Q	
	9.0×10^{-4}		Modarresi et al. (2007)	Q	68
		5000	Kühne et al. (2005)	Q	
	1.8×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	4.6×10^{-4}		Katritzky et al. (1998)	Q	
	8.0×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	1.1×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4400	Kühne et al. (2005)	?	
	1.2×10^{-3}		Yaws (1999)	?	21
	1.2×10^{-3}		Yaws and Yang (1992)	?	21
	1.3×10^{-3}		Abraham et al. (1990)	?	
1,2,3,4-tetramethylbenzene $C_{10}H_{14}$ [488-23-3] UOHMMEJUHBCKEE-UHFFFAOYSA-N	2.9×10^{-3}	5900	Brockbank (2013)	L	
1,2,3,5-tetramethylbenzene $C_{10}H_{14}$ [527-53-7] BFIMMTCNYPIMRN-UHFFFAOYSA-N	1.2×10^{-3}		Zhang et al. (2010)	Q	288, 289
	2.2×10^{-3}		Zhang et al. (2010)	Q	288, 290
	2.2×10^{-3}		Zhang et al. (2010)	Q	288, 291
	4.1×10^{-4}		Zhang et al. (2010)	Q	288, 292
	1.2×10^{-3}		Yaws (1999)	?	21
1,2,4,5-tetramethylbenzene $C_{10}H_{14}$ [95-93-2] SQNZJJAZBFDUTD-UHFFFAOYSA-N	1.4×10^{-3}		Brockbank (2013)	L	
	1.3×10^{-3}		Plyasunov and Shock (2000)	L	
	3.9×10^{-4}		Mackay and Shiu (1981)	L	
	3.9×10^{-4}		Mackay et al. (2006a)	V	
	3.9×10^{-4}		Mackay et al. (1992a)	V	
	3.9×10^{-4}		Eastcott et al. (1988)	V	
	3.5×10^{-4}		Yaws (2003)	X	238
	1.4×10^{-3}		Abraham et al. (2019)	Q	
	3.7×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-3}		Zhang et al. (2010)	Q	288, 289
	2.5×10^{-3}		Zhang et al. (2010)	Q	288, 290
	1.9×10^{-3}		Zhang et al. (2010)	Q	288, 291
	4.1×10^{-4}		Zhang et al. (2010)	Q	288, 292
	3.7×10^{-4}		Gharagheizi et al. (2010)	Q	247
	2.9×10^{-3}		Hilal et al. (2008)	Q	
	8.2×10^{-4}		Modarresi et al. (2007)	Q	68
	3.9×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	3.9×10^{-4}		Yaws and Yang (1992)	?	21

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethylbenzene	1.4×10^{-3}	4500	Schwardt et al. (2021)	L	1, 353
$C_6H_5C_2H_5$	1.3×10^{-3}	5000	Brockbank (2013)	L	1
[100-41-4]	1.4×10^{-3}	4800	Fogg and Sangster (2003)	L	
YNQLUTRBYVCPMQ-UHFFFAOYSA-N	1.3×10^{-3}	5100	Staudinger and Roberts (2001)	L	
	1.3×10^{-3}	4800	Plyasunov and Shock (2000)	L	
	1.2×10^{-3}	5100	Staudinger and Roberts (1996)	L	
	1.3×10^{-3}		Mackay and Shiu (1981)	L	
	1.3×10^{-3}	4400	Schwardt et al. (2021)	M	354
	2.0×10^{-3}	4100	Hiatt (2013)	M	
	1.9×10^{-3}	4200	Zhang et al. (2013)	M	326
	1.4×10^{-3}		Zhang et al. (2013)	M	327
	1.3×10^{-3}	5100	Sieg et al. (2009)	M	328
	1.4×10^{-3}		Li et al. (2008)	M	
	1.2×10^{-3}	2700	Falabella and Teja (2008)	M	11, 340
	1.1×10^{-3}		Lodge and Danso (2007)	M	
			Cheng et al. (2003)	M	330
	1.6×10^{-3}		Miller and Stuart (2000)	M	73
	1.1×10^{-3}		Ryu and Park (1999)	M	355
	1.3×10^{-3}		Allen et al. (1998)	M	
	1.4×10^{-3}	2800	Kondoh and Nakajima (1997)	M	
	1.1×10^{-3}		Turner et al. (1996)	M	
	1.5×10^{-3}	4900	Dewulf et al. (1995)	M	
	1.3×10^{-3}	5000	Robbins et al. (1993)	M	356
	1.3×10^{-3}	5300	Perlinger et al. (1993)	M	
	1.3×10^{-3}		Li and Carr (1993)	M	
	1.3×10^{-3}		Li et al. (1993)	M	
	2.5×10^{-3}		Zhang and Pawliszyn (1993)	M	
	1.1×10^{-3}	5500	Bissonette et al. (1990)	M	
	1.2×10^{-3}	5000	Ashworth et al. (1988)	M	279
	1.3×10^{-3}	4400	Heidman et al. (1985)	M	1
	1.3×10^{-3}	4600	Sanemasa et al. (1982)	M	
	1.4×10^{-3}	4500	Sanemasa et al. (1981)	M	
	1.4×10^{-3}	5500	Ervin et al. (1980)	M	
	1.5×10^{-3}		Warner et al. (1980)	M	
	1.2×10^{-3}		Mackay et al. (1979)	M	
	6.6×10^{-4}		Sato and Nakajima (1979a)	M	14
	1.3×10^{-3}	5600	Brown and Wasik (1974)	M	
	1.6×10^{-3}	6400	Hartkopf and Karger (1973)	M	
	1.6×10^{-4}		Abraham and Acree (2007)	V	
	1.1×10^{-3}		Mackay et al. (2006a)	V	
	1.2×10^{-3}		Shiu and Ma (2000)	V	
	1.2×10^{-3}		Lide and Frederikse (1995)	V	
	1.1×10^{-3}		Mackay et al. (1992a)	V	
	1.2×10^{-3}		Hwang et al. (1992)	V	
	1.0×10^{-3}		Eastcott et al. (1988)	V	
	1.2×10^{-3}	4800	Abraham (1984)	V	

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{-3}	4900	Ben-Naim and Wilf (1980)	V	1
	1.5×10^{-3}		Warner et al. (1980)	V	
	1.1×10^{-3}		Hine and Mookerjee (1975)	V	
	1.5×10^{-3}	4800	Wauchope and Haque (1972)	V	
	1.3×10^{-3}		McAuliffe (1966)	V	24
	1.5×10^{-3}	4900	Andon et al. (1954)	V	338
	1.5×10^{-3}		Bohon and Claussen (1951)	V	
	1.4×10^{-3}	4900	Owens et al. (1986)	T	
	1.1×10^{-3}		Mackay et al. (1979)	T	
		4800	Gill et al. (1976)	T	
	1.2×10^{-3}		Yaws (2003)	X	238
	1.6×10^{-3}	1700	Goldstein (1982)	X	299
	1.3×10^{-3}		Sieg et al. (2008)	C	
	1.6×10^{-3}		Ryan et al. (1988)	C	
	1.5×10^{-3}		Shen (1982)	C	
	9.7×10^{-4}		Hayer et al. (2022)	Q	20
	1.3×10^{-3}		Keshavarz et al. (2022)	Q	
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	3.1×10^{-3}		Wang et al. (2017)	Q	81, 239
	9.3×10^{-4}		Wang et al. (2017)	Q	81, 240
	2.8×10^{-3}		Wang et al. (2017)	Q	81, 241
	1.4×10^{-3}		Gharagheizi et al. (2012)	Q	
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.4×10^{-3}		Hilal et al. (2008)	Q	
	9.6×10^{-4}		Modarresi et al. (2007)	Q	68
		4700	Kühne et al. (2005)	Q	
	1.2×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	5.8×10^{-4}		Yao et al. (2002)	Q	230
	1.4×10^{-3}		English and Carroll (2001)	Q	231, 261
	4.1×10^{-4}		Katritzky et al. (1998)	Q	
	1.6×10^{-3}		Russell et al. (1992)	Q	280
	1.1×10^{-3}		Suzuki et al. (1992)	Q	233
	1.3×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.3×10^{-3}		Arbuckle (1983)	Q	
	1.3×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		5000	Kühne et al. (2005)	?	
	1.2×10^{-3}		Yaws (1999)	?	21
	6.9×10^{-4}		Abraham and Weathersby (1994)	?	21
	1.1×10^{-3}		Hoff et al. (1993)	?	21
	1.2×10^{-3}		Yaws and Yang (1992)	?	21
	1.2×10^{-3}		Abraham et al. (1990)	?	

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethylbenzene-d10 $C_6D_5C_2D_5$ [25837-05-2] YNQLUTRBYVCPMQ-CFTAVCBPSA-N	2.0×10^{-3}	4200	Hiatt (2013)	M	
1,2-diethylbenzene	3.8×10^{-3}		Duchowicz et al. (2020)	V	187
$C_{10}H_{14}$	3.8×10^{-3}		HSDB (2015)	V	
(*o*-diethylbenzene)	1.3×10^{-3}		Yaws (2003)	X	238
[135-01-3]	1.2×10^{-3}		Hilal et al. (2008)	C	
KVNYFPKFSJIPBJ-UHFFFAOYSA-N	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	5.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.3×10^{-3}		Hilal et al. (2008)	Q	
	1.2×10^{-3}		Modarresi et al. (2007)	Q	68
		4800	Kühne et al. (2005)	Q	
	3.8×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	5.6×10^{-4}		Katritzky et al. (1998)	Q	
		5100	Kühne et al. (2005)	?	
	1.3×10^{-3}		Yaws (1999)	?	21
1,3-diethylbenzene	1.2×10^{-3}		Duchowicz et al. (2020)	V	187
$C_{10}H_{14}$	1.1×10^{-3}		HSDB (2015)	V	
(*m*-diethylbenzene)	1.3×10^{-3}		Yaws (2003)	X	238
[141-93-5]	3.8×10^{-3}		Hilal et al. (2008)	C	
AFZZYIJIWUTJFO-UHFFFAOYSA-N	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	4.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
	9.7×10^{-4}		Hilal et al. (2008)	Q	
	4.7×10^{-4}		Modarresi et al. (2007)	Q	68
		5300	Kühne et al. (2005)	Q	
	5.6×10^{-4}		Katritzky et al. (1998)	Q	
		5300	Kühne et al. (2005)	?	
	1.3×10^{-3}		Yaws (1999)	?	21
1,4-diethylbenzene	1.3×10^{-3}		Duchowicz et al. (2020)	V	187
$C_{10}H_{14}$	1.4×10^{-3}		HSDB (2015)	V	
(*p*-diethylbenzene)	1.2×10^{-3}		Yaws (2003)	X	238
[105-05-5]	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
DSNHSQKRULAAEI-UHFFFAOYSA-N	5.0×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.1×10^{-3}		Hilal et al. (2008)	Q	
	7.6×10^{-4}		Modarresi et al. (2007)	Q	68
		5300	Kühne et al. (2005)	Q	
	1.4×10^{-3}		Yaffe et al. (2003)	Q	249, 250

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.7×10^{-4}		Katritzky et al. (1998)	Q	
	7.9×10^{-4}		Nirmalakhandan et al. (1997)	Q	
		5900	Kühne et al. (2005)	?	
	1.2×10^{-3}		Yaws (1999)	?	21
			Brockbank (2013)	W	357
propylbenzene	9.0×10^{-4}	3800	Schwardt et al. (2021)	L	1
$C_6H_5C_3H_7$	9.1×10^{-4}	4700	Brockbank (2013)	L	1
[103-65-1]	9.1×10^{-4}	5300	Plyasunov and Shock (2000)	L	
ODLMAHJVESYWTB-UHFFFAOYSA-N	1.4×10^{-3}		Mackay and Shiu (1981)	L	
	1.9×10^{-3}	4500	Hiatt (2013)	M	
	1.5×10^{-3}		Karl et al. (2003)	M	88
	1.1×10^{-3}	2600	Kondoh and Nakajima (1997)	M	
	8.6×10^{-4}	5400	Perlinger et al. (1993)	M	
	9.3×10^{-4}		Li and Carr (1993)	M	
	9.1×10^{-4}		Li et al. (1993)	M	
	9.0×10^{-4}	3700	Ashworth et al. (1988)	M	279
	9.5×10^{-4}	4700	Sanemasa et al. (1982)	M	
	5.0×10^{-4}		Sato and Nakajima (1979a)	M	14
	9.6×10^{-4}		Mackay et al. (2006a)	V	
	9.6×10^{-4}		Shiu and Ma (2000)	V	
	9.6×10^{-4}		Mackay et al. (1992a)	V	
	9.7×10^{-4}		Eastcott et al. (1988)	V	
	9.7×10^{-4}	5300	Abraham (1984)	V	
	1.5×10^{-3}	5500	Ben-Naim and Wilf (1980)	V	1
	9.9×10^{-4}		Hine and Mookerjee (1975)	V	
	9.6×10^{-4}	5100	Owens et al. (1986)	T	
		5300	Gill et al. (1976)	T	
	7.4×10^{-4}		Yaws (2003)	X	238
	1.8×10^{-3}		Keshavarz et al. (2022)	Q	
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	2.5×10^{-3}		Wang et al. (2017)	Q	81, 239
	6.6×10^{-4}		Wang et al. (2017)	Q	81, 240
	2.6×10^{-3}		Wang et al. (2017)	Q	81, 241
	9.9×10^{-4}		Li et al. (2014)	Q	242
	1.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	8.6×10^{-4}		Gharagheizi et al. (2010)	Q	247
	9.9×10^{-4}		Hilal et al. (2008)	Q	
	8.6×10^{-4}		Modarresi et al. (2007)	Q	68
		5000	Kühne et al. (2005)	Q	
	1.0×10^{-3}		Yaffe et al. (2003)	Q	249, 273
	1.1×10^{-3}		English and Carroll (2001)	Q	231, 232
	5.1×10^{-4}		Katritzky et al. (1998)	Q	

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.3×10^{-3}		Russell et al. (1992)	Q	280
	8.8×10^{-4}		Suzuki et al. (1992)	Q	233
	1.1×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	9.4×10^{-4}		Duchowicz et al. (2020)	?	186, 21
		4700	Kühne et al. (2005)	?	
	1.7×10^{-3}		Yaws (1999)	?	21
	5.2×10^{-4}		Abraham and Weathersby (1994)	?	21
	9.6×10^{-4}		Yaws and Yang (1992)	?	21
	9.7×10^{-4}		Abraham et al. (1990)	?	
(2-propyl)-benzene	9.0×10^{-4}	4800	Brockbank (2013)	L	
$C_6H_5C_3H_7$	1.2×10^{-3}	3200	Staudinger and Roberts (2001)	L	
(isopropylbenzene; cumene)	8.4×10^{-4}	4800	Plyasunov and Shock (2000)	L	
[98-82-8]	7.7×10^{-3}		Mackay and Shiu (1981)	L	
RWGFKTVRMDUZSP-UHFFFAOYSA-N	1.4×10^{-3}	4900	Hiatt (2013)	M	
	1.0×10^{-3}	2500	Kondoh and Nakajima (1997)	M	
	8.7×10^{-4}	3300	Hansen et al. (1993)	M	282
	9.1×10^{-4}		Li and Carr (1993)	M	
	8.9×10^{-4}		Li et al. (1993)	M	
	1.6×10^{-3}	3200	Ashworth et al. (1988)	M	279
	8.9×10^{-4}	4700	Sanemasa et al. (1982)	M	
	5.6×10^{-4}		Sato and Nakajima (1979a)	M	14
	6.8×10^{-4}		Mackay et al. (2006a)	V	
	6.8×10^{-4}		Shiu and Ma (2000)	V	
	6.8×10^{-4}		Mackay et al. (1992a)	V	
	6.8×10^{-4}		Hwang et al. (1992)	V	
	6.6×10^{-4}		Eastcott et al. (1988)	V	
	6.7×10^{-4}		Hine and Mookerjee (1975)	V	
	6.8×10^{-4}		Mackay and Leinonen (1975)	V	
	1.1×10^{-3}	5000	Wauchope and Haque (1972)	V	
	1.1×10^{-3}		McAuliffe (1966)	V	24
	6.8×10^{-4}		Yaws (2003)	X	238
	1.8×10^{-3}		Keshavarz et al. (2022)	Q	
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	300
	2.9×10^{-3}		Wang et al. (2017)	Q	81, 239
	5.3×10^{-4}		Wang et al. (2017)	Q	81, 240
	2.8×10^{-3}		Wang et al. (2017)	Q	81, 241
	9.4×10^{-4}		Savary et al. (2014)	Q	
	8.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	8.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
	8.6×10^{-4}		Hilal et al. (2008)	Q	
	7.7×10^{-4}		Modarresi et al. (2007)	Q	68
		5000	Kühne et al. (2005)	Q	

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
			Yaffe et al. (2003)	Q	358
	3.6×10^{-4}		Yao et al. (2002)	Q	230
	1.2×10^{-3}		English and Carroll (2001)	Q	231, 232
	4.7×10^{-4}		Katritzky et al. (1998)	Q	
	9.2×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	8.0×10^{-4}		Suzuki et al. (1992)	Q	233
	9.2×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	8.6×10^{-4}		Duchowicz et al. (2020)	?	186, 21
		4400	Kühne et al. (2005)	?	
	6.9×10^{-4}		Yaws (1999)	?	21
	5.8×10^{-4}		Abraham and Weathersby (1994)	?	21
	6.8×10^{-4}		Hoff et al. (1993)	?	21
	6.8×10^{-4}		Yaws and Yang (1992)	?	21
	8.8×10^{-4}		Abraham et al. (1990)	?	
			Fogg and Sangster (2003)	W	359
1-ethyl-2-methylbenzene	1.8×10^{-3}		Plyasunov and Shock (2000)	L	
$C_6H_4CH_3C_2H_5$	2.3×10^{-3}		Mackay and Shiu (1981)	L	
(*o*-ethyltoluene)	1.8×10^{-3}		Duchowicz et al. (2020)	V	187
[611-14-3]	1.9×10^{-3}		Mackay et al. (2006a)	V	
HYFLWBNQFMXCPA-UHFFFAOYSA-N	1.9×10^{-3}		Mackay et al. (1992a)	V	
	1.9×10^{-3}		Eastcott et al. (1988)	V	
	2.2×10^{-3}		Yaws (2003)	X	238
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.8×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.2×10^{-3}		Wang et al. (2017)	Q	81, 240
	3.0×10^{-3}		Wang et al. (2017)	Q	81, 241
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.8×10^{-3}		Hilal et al. (2008)	Q	
	8.9×10^{-4}		Modarresi et al. (2007)	Q	68
		4500	Kühne et al. (2005)	Q	
	2.4×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	5.1×10^{-4}		Katritzky et al. (1998)	Q	
	9.5×10^{-4}		Nirmalakhandan et al. (1997)	Q	
		3200	Kühne et al. (2005)	?	
	2.2×10^{-3}		Yaws (1999)	?	21
	2.3×10^{-3}		Yaws and Yang (1992)	?	21

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-ethyl-3-methylbenzene	1.7×10^{-3}		Yaws (2003)	X	238
$C_6H_4CH_3C_2H_5$	1.8×10^{-3}		Wang et al. (2017)	Q	81, 239
(*m*-ethyltoluene)	9.8×10^{-4}		Wang et al. (2017)	Q	81, 240
[620-14-4]	2.6×10^{-3}		Wang et al. (2017)	Q	81, 241
ZLCSFXXPPANWQY-UHFFFAOYSA-N	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.3×10^{-3}		Hilal et al. (2008)	Q	
	1.7×10^{-3}		Yaws (1999)	?	21
1-ethyl-4-methylbenzene	2.0×10^{-3}		Mackay and Shiu (1981)	L	
$C_6H_4CH_3C_2H_5$	2.0×10^{-3}		Duchowicz et al. (2020)	V	187
(*p*-ethyltoluene)	1.6×10^{-3}		Duchowicz et al. (2020)	V	187
[622-96-8]	2.0×10^{-3}		Mackay et al. (2006a)	V	
JRLPEMVDPFPYPJ-UHFFFAOYSA-N	2.0×10^{-3}		Mackay et al. (1992a)	V	
	2.0×10^{-3}		Eastcott et al. (1988)	V	
	2.0×10^{-3}		Yaws (2003)	X	238
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.8×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.1×10^{-3}		Wang et al. (2017)	Q	81, 240
	2.5×10^{-3}		Wang et al. (2017)	Q	81, 241
	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.4×10^{-3}		Hilal et al. (2008)	Q	
	7.1×10^{-4}		Modarresi et al. (2007)	Q	68
	2.1×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.7×10^{-3}		English and Carroll (2001)	Q	231, 261
	5.1×10^{-4}		Katritzky et al. (1998)	Q	
	9.5×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	2.0×10^{-3}		Yaws (1999)	?	21
	2.0×10^{-3}		Yaws and Yang (1992)	?	21
butylbenzene	7.1×10^{-4}	5100	Brockbank (2013)	L	1
$C_6H_5C_4H_9$	7.1×10^{-4}	5500	Plyasunov and Shock (2000)	L	
[104-51-8]	7.7×10^{-4}		Mackay and Shiu (1981)	L	
OCKPCBLVNKHBMX-UHFFFAOYSA-N	2.0×10^{-3}	4500	Hiatt (2013)	M	
	7.4×10^{-4}		Ryu and Park (1999)	M	
	9.1×10^{-4}	2700	Kondoh and Nakajima (1997)	M	
	6.2×10^{-4}	6000	Perlinger et al. (1993)	M	
	7.1×10^{-4}		Li and Carr (1993)	M	
	6.7×10^{-4}		Li et al. (1993)	M	
	6.2×10^{-4}		Duchowicz et al. (2020)	V	187
	6.2×10^{-4}		HSDB (2015)	V	
	9.9×10^{-5}		Abraham and Acree (2007)	V	
	7.5×10^{-4}		Mackay et al. (2006a)	V	
	7.5×10^{-4}		Shiu and Ma (2000)	V	
	7.5×10^{-4}		Mackay et al. (1992a)	V	
	7.6×10^{-4}		Meylan and Howard (1991)	V	
	7.5×10^{-4}		Eastcott et al. (1988)	V	

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.4×10^{-4}		Abraham (1984)	V	
	1.7×10^{-3}	6500	Ben-Naim and Wilf (1980)	V	1
	7.9×10^{-4}		Hine and Mookerjee (1975)	V	
	7.2×10^{-4}	5300	Owens et al. (1986)	T	
	7.5×10^{-4}		Yaws (2003)	X	238
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	7.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	7.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
	7.7×10^{-4}		Hilal et al. (2008)	Q	
	4.9×10^{-4}		Modarresi et al. (2007)	Q	68
		5300	Kühne et al. (2005)	Q	
	7.2×10^{-4}		Yaffe et al. (2003)	Q	249, 273
	6.4×10^{-4}		Yao et al. (2002)	Q	230
	7.9×10^{-4}		English and Carroll (2001)	Q	231, 232
	5.7×10^{-4}		Katritzky et al. (1998)	Q	
	6.9×10^{-4}		Russell et al. (1992)	Q	360
	6.9×10^{-4}		Suzuki et al. (1992)	Q	233
	7.1×10^{-4}		Meylan and Howard (1991)	Q	
	8.4×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
		4900	Kühne et al. (2005)	?	
	7.6×10^{-4}		Yaws (1999)	?	21
	7.5×10^{-4}		Yaws and Yang (1992)	?	21
	7.5×10^{-4}		Abraham et al. (1990)	?	
(1-methylpropyl)-benzene	5.3×10^{-4}		Plyasunov and Shock (2000)	L	
$C_6H_5C_4H_9$	7.1×10^{-4}		Mackay and Shiu (1981)	L	
(*sec*-butylbenzene)	1.3×10^{-3}	4600	Hiatt (2013)	M	
[135-98-8]	7.5×10^{-4}	2300	Kondoh and Nakajima (1997)	M	
ZJMWRROPUADPEA-UHFFFAOYSA-N	5.6×10^{-4}		Duchowicz et al. (2020)	V	187
	5.5×10^{-4}		HSDB (2015)	V	
	5.3×10^{-4}		Mackay et al. (2006a)	V	
	5.3×10^{-4}		Mackay et al. (1992a)	V	
	5.4×10^{-4}		Eastcott et al. (1988)	V	
	8.6×10^{-4}		Hine and Mookerjee (1975)	V	
	5.9×10^{-4}		Yaws (2003)	X	238
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	5.9×10^{-4}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	6.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
	8.6×10^{-4}		Hilal et al. (2008)	Q	
	6.9×10^{-4}		Modarresi et al. (2007)	Q	68

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.2×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	9.0×10^{-4}		English and Carroll (2001)	Q	231, 232
	9.9×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	6.1×10^{-4}		Suzuki et al. (1992)	Q	233
	7.2×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	1.3×10^{-3}		Yaws (1999)	?	21
(2-methylpropyl)-benzene	2.9×10^{-4}		Plyasunov and Shock (2000)	L	
$C_6H_5C_4H_9$	3.0×10^{-4}		Mackay and Shiu (1981)	L	
(isobutylbenzene)	2.9×10^{-4}		Duchowicz et al. (2020)	V	187
[538-93-2]	3.0×10^{-4}		Mackay et al. (2006a)	V	
KXUHSQYYJYAXGZ-UHFFFAOYSA-N	3.0×10^{-4}		Mackay et al. (1992a)	V	
	3.0×10^{-4}		Eastcott et al. (1988)	V	
	5.5×10^{-4}		Yaws (2003)	X	238
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	6.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	6.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
	7.0×10^{-4}		Hilal et al. (2008)	Q	
	5.2×10^{-4}		Modarresi et al. (2007)	Q	68
	3.1×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	4.3×10^{-4}		Yao et al. (2002)	Q	230
	7.7×10^{-4}		English and Carroll (2001)	Q	231, 232
	5.4×10^{-4}		Katritzky et al. (1998)	Q	
	7.0×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	1.3×10^{-3}		Yaws (1999)	?	21
(1,1-dimethylethyl)-benzene	7.9×10^{-4}		Plyasunov and Shock (2000)	L	
$C_6H_5C_4H_9$	8.3×10^{-4}		Mackay and Shiu (1981)	L	
(*tert*-butylbenzene)	1.6×10^{-3}	4700	Hiatt (2013)	M	
[98-06-6]	9.4×10^{-4}	2400	Kondoh and Nakajima (1997)	M	
YTZKOQUCBOVLHL-UHFFFAOYSA-N	7.5×10^{-4}		Duchowicz et al. (2020)	V	187
	7.5×10^{-4}		HSDB (2015)	V	
	7.8×10^{-4}		Mackay et al. (2006a)	V	
	7.8×10^{-4}		Mackay et al. (1992a)	V	
	7.7×10^{-4}		Eastcott et al. (1988)	V	
	8.4×10^{-4}		Hine and Mookerjee (1975)	V	
	6.1×10^{-4}		Yaws (2003)	X	238
	5.3×10^{-4}		Duchowicz et al. (2020)	Q	
	5.3×10^{-4}		Gharagheizi et al. (2012)	Q	
	5.6×10^{-4}		Gharagheizi et al. (2010)	Q	247
	7.7×10^{-4}		Hilal et al. (2008)	Q	
	6.6×10^{-4}		Modarresi et al. (2007)	Q	68
	8.6×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	9.0×10^{-4}		English and Carroll (2001)	Q	231, 232
	4.8×10^{-4}		Katritzky et al. (1998)	Q	
	5.3×10^{-4}		Suzuki et al. (1992)	Q	233
	6.0×10^{-4}		Nirmalakhandan and Speece (1988)	Q	

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.4×10^{-3}		Yaws (1999)	?	21
1-methyl-2-propylbenzene	7.2×10^{-4}		Yaws (2003)	X	238
$C_{10}H_{14}$	5.3×10^{-4}		Gharagheizi et al. (2012)	Q	
[1074-17-5]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
YQZBFMJOASEONC-UHFFFAOYSA-N					
1-methyl-3-propylbenzene	7.7×10^{-4}		Yaws (2003)	X	238
$C_{10}H_{14}$	4.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[1074-43-7]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
QUEBYVKXYIKVSO-UHFFFAOYSA-N					
1-methyl-4-propylbenzene	9.6×10^{-4}		Yaws (2003)	X	238
$C_{10}H_{14}$	4.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[1074-55-1]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
JXFVMNFKABWTHD-UHFFFAOYSA-N					
2-ethyl-*m*-xylene	1.3×10^{-3}		Yaws (2003)	X	238
$C_{10}H_{14}$	4.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[2870-04-4]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
CHIKRULMSSADAF-UHFFFAOYSA-N	1.3×10^{-3}		Yaws (1999)	?	21
2-ethyl-*p*-xylene	1.2×10^{-3}		Yaws (2003)	X	238
$C_{10}H_{14}$	3.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[1758-88-9]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
AXIUBBVSOWPLDA-UHFFFAOYSA-N	1.2×10^{-3}		Yaws (1999)	?	21
3-ethyl-*o*-xylene	1.2×10^{-3}		Yaws (2003)	X	238
$C_{10}H_{14}$	4.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[933-98-2]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
QUBBAXISAHIDNM-UHFFFAOYSA-N	1.2×10^{-3}		Yaws (1999)	?	21
4-ethyl-*o*-xylene	1.3×10^{-3}		Yaws (2003)	X	238
$C_{10}H_{14}$	4.2×10^{-4}		Gharagheizi et al. (2012)	Q	
[934-80-5]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
SBUYFICWQNHBCM-UHFFFAOYSA-N	4.5×10^{-4}		Yao et al. (2002)	Q	230
	1.3×10^{-3}		Yaws (1999)	?	21
4-ethyl-*m*-xylene	1.1×10^{-3}		Yaws (2003)	X	238
$C_{10}H_{14}$	4.0×10^{-4}		Gharagheizi et al. (2012)	Q	
[874-41-9]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
MEMBJMDZWKVOTB-UHFFFAOYSA-N	3.0×10^{-4}		Yao et al. (2002)	Q	230
	1.1×10^{-3}		Yaws (1999)	?	21

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5-ethyl-*m*-xylene	1.3×10^{-3}		Yaws (2003)	X	238
$C_{10}H_{14}$	1.1×10^{-3}		Wang et al. (2017)	Q	81, 239
(1-ethyl-3,5-dimethylbenzene)	9.3×10^{-4}		Wang et al. (2017)	Q	81, 240
[934-74-7]	2.2×10^{-3}		Wang et al. (2017)	Q	81, 241
LMAUULKNZLEMGN-UHFFFAOYSA-N	3.3×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.3×10^{-3}		Yaws (1999)	?	21
1-methyl-2-(1-methylethyl)-benzene	1.6×10^{-3}		Plyasunov and Shock (2000)	L	
$C_{10}H_{14}$	8.7×10^{-4}		Duchowicz et al. (2020)	V	187
(*o*-cymene)	9.0×10^{-4}		HSDB (2015)	V	
[527-84-4]	1.2×10^{-3}		Yaws (2003)	X	259
WWRCMNKATXZARA-UHFFFAOYSA-N	1.2×10^{-3}		Yaws (2003)	X	238
	1.3×10^{-3}		Dupeux et al. (2022)	Q	260
	6.1×10^{-4}		Duchowicz et al. (2020)	Q	
	4.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.2×10^{-3}		Hilal et al. (2008)	Q	
	6.6×10^{-4}		Modarresi et al. (2007)	Q	68
	5.3×10^{-4}		Katritzky et al. (1998)	Q	
	1.2×10^{-3}		Yaws (1999)	?	21
1-methyl-3-(1-methylethyl)-benzene	1.4×10^{-3}		Plyasunov and Shock (2000)	L	
$C_{10}H_{14}$	1.4×10^{-3}		Duchowicz et al. (2020)	V	187
(*m*-cymene)	1.4×10^{-3}		HSDB (2015)	V	
[535-77-3]	9.0×10^{-4}		Copolovici and Niinemets (2005)	V	
XCYJPXQACVEIOS-UHFFFAOYSA-N	1.2×10^{-3}		Yaws (2003)	X	259
	1.2×10^{-3}		Yaws (2003)	X	238
	8.2×10^{-4}		Dupeux et al. (2022)	Q	260
	6.1×10^{-4}		Duchowicz et al. (2020)	Q	
	4.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-3}		Gharagheizi et al. (2010)	Q	247
	8.6×10^{-4}		Hilal et al. (2008)	Q	
	4.5×10^{-4}		Modarresi et al. (2007)	Q	68
	1.2×10^{-3}		Yaws (1999)	?	21

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methyl-4-(1-methylethyl)-benzene	9.6×10^{-4}		Plyasunov and Shock (2000)	L	
$C_{10}H_{14}$	1.3×10^{-3}		Mackay and Shiu (1981)	L	
(*p*-cymene; *p*-isopropyltoluene)	1.8×10^{-3}	4900	Hiatt (2013)	M	
[99-87-6]	1.0×10^{-3}	2600	Kondoh and Nakajima (1997)	M	
HFPZCAJZSCWRBC-UHFFFAOYSA-N	9.0×10^{-4}		Duchowicz et al. (2020)	V	187
	8.0×10^{-4}		Duchowicz et al. (2020)	V	187
	1.1×10^{-3}		Martins et al. (2017)	V	316
	9.0×10^{-4}		HSDB (2015)	V	
	1.2×10^{-3}		Mackay et al. (2006a)	V	
	1.1×10^{-3}		Copolovici and Niinemets (2005)	V	
	9.1×10^{-4}		Niinemets and Reichstein (2002)	V	
	1.3×10^{-3}		Abraham et al. (1994a)	V	
	1.2×10^{-3}		Mackay et al. (1992a)	V	
	1.2×10^{-3}		Eastcott et al. (1988)	V	
	1.3×10^{-3}		Yaws (2003)	X	259
	1.3×10^{-3}		Yaws (2003)	X	238
	7.6×10^{-4}		Dupeux et al. (2022)	Q	260
	6.1×10^{-4}		Duchowicz et al. (2020)	Q	
	6.1×10^{-4}		Duchowicz et al. (2020)	Q	
	4.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-3}		Gharagheizi et al. (2010)	Q	247
	8.8×10^{-4}		Hilal et al. (2008)	Q	
	5.4×10^{-4}		Modarresi et al. (2007)	Q	68
	5.5×10^{-4}		Modarresi et al. (2007)	Q	68
		5300	Kühne et al. (2005)	Q	
	8.0×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	1.4×10^{-3}		English and Carroll (2001)	Q	231, 275
	5.4×10^{-4}		Katritzky et al. (1998)	Q	
	6.5×10^{-4}		Nirmalakhandan et al. (1997)	Q	
		4500	Kühne et al. (2005)	?	
	1.3×10^{-3}		Yaws (1999)	?	21
4-*tert*-butyltoluene	7.8×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	6.4×10^{-4}		HSDB (2015)	Q	100
[98-51-1]	2.7×10^{-4}		Gharagheizi et al. (2012)	Q	
QCWXDVFBZVHKLV-UHFFFAOYSA-N	6.4×10^{-4}		Zhang et al. (2010)	Q	288, 289
	5.2×10^{-4}		Zhang et al. (2010)	Q	288, 290
	1.3×10^{-3}		Zhang et al. (2010)	Q	288, 291
	4.7×10^{-4}		Zhang et al. (2010)	Q	288, 292
	8.2×10^{-4}		Gharagheizi et al. (2010)	Q	247

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pentylbenzene	6.0×10^{-4}	6000	Brockbank (2013)	L	1, 361
$C_6H_5C_5H_{11}$	5.1×10^{-4}	5900	Plyasunov and Shock (2000)	L	
[538-68-1]	1.7×10^{-3}		Mackay and Shiu (1981)	L	
PWATWSYOIIXYMA-UHFFFAOYSA-N	6.1×10^{-4}		Ryu and Park (1999)	M	
	3.9×10^{-4}		Duchowicz et al. (2020)	V	187
	5.9×10^{-4}		Mackay et al. (2006a)	V	
	5.9×10^{-4}		Mackay et al. (1992a)	V	
	1.6×10^{-3}		Eastcott et al. (1988)	V	
	6.0×10^{-4}		Abraham (1984)	V	
	3.0×10^{-3}	7800	Ben-Naim and Wilf (1980)	V	1
	5.3×10^{-4}	5900	Owens et al. (1986)	T	
	4.4×10^{-4}		Yaws (2003)	X	238
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	5.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	6.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
	6.1×10^{-4}		Hilal et al. (2008)	Q	
	4.3×10^{-4}		Modarresi et al. (2007)	Q	68
	6.1×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	4.4×10^{-4}		Yao et al. (2002)	Q	230
	5.8×10^{-4}		English and Carroll (2001)	Q	231, 261
	5.7×10^{-4}		Katritzky et al. (1998)	Q	
	6.4×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	4.4×10^{-4}		Yaws (1999)	?	21
	5.9×10^{-4}		Yaws and Yang (1992)	?	21
	6.0×10^{-4}		Abraham et al. (1990)	?	
pentamethylbenzene	7.7×10^{-3}		Hilal et al. (2008)	Q	
$C_{11}H_{16}$	7.0×10^{-4}		Modarresi et al. (2007)	Q	68
[700-12-9]					
BEZDDPMMPIDMGJ-UHFFFAOYSA-N					
1,2-dimethyl-3-propylbenzene	8.7×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[17059-44-8]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
IRUSTUOJENXLMN-UHFFFAOYSA-N					
1,2-dimethyl-4-propylbenzene	8.8×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[3982-66-9]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
FZJVYOOQGFZCSY-UHFFFAOYSA-N					

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3-dimethyl-2-propylbenzene	8.9×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[17059-45-9]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
POVRSTNZQPBWAS-UHFFFAOYSA-N					
1,3-dimethyl-4-propylbenzene	9.0×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[61827-85-8]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
HPAXKQMKDWCLGU-UHFFFAOYSA-N					
1,3-dimethyl-5-propylbenzene	9.3×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.3×10^{-4}		Gharagheizi et al. (2012)	Q	
[3982-64-7]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
NBICXWXPZRNMPF-UHFFFAOYSA-N					
1,4-dimethyl-2-propylbenzene	9.2×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.4×10^{-4}		Gharagheizi et al. (2012)	Q	
[3042-50-0]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
PWEDYOIWLPZSRP-UHFFFAOYSA-N					
1,2-dimethyl-3-isopropylbenzene	8.4×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.4×10^{-4}		Gharagheizi et al. (2012)	Q	
[22539-65-7]	9.4×10^{-4}		Gharagheizi et al. (2010)	Q	247
GDEQPEBFOWYWSA-UHFFFAOYSA-N					
1,2-dimethyl-4-isopropylbenzene	8.5×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.3×10^{-4}		Gharagheizi et al. (2012)	Q	
[4132-77-8]	9.4×10^{-4}		Gharagheizi et al. (2010)	Q	247
MGMSKQZIAGFMRU-UHFFFAOYSA-N					
1,3-dimethyl-2-isopropylbenzene	8.7×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.1×10^{-4}		Gharagheizi et al. (2012)	Q	
[14411-75-7]	9.4×10^{-4}		Gharagheizi et al. (2010)	Q	247
IVCIQLTVLDOHKA-UHFFFAOYSA-N					
1,3-dimethyl-4-isopropylbenzene	8.7×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.1×10^{-4}		Gharagheizi et al. (2012)	Q	
[4706-89-2]	9.4×10^{-4}		Gharagheizi et al. (2010)	Q	247
AADQFNAACHHRLT-UHFFFAOYSA-N					
1,3-dimethyl-5-isopropylbenzene	9.2×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	1.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[4706-90-5]	9.4×10^{-4}		Gharagheizi et al. (2010)	Q	247
RMKJTYPFCFNTGQ-UHFFFAOYSA-N					
1,4-dimethyl-2-isopropylbenzene	9.0×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	1.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[4132-72-3]	9.4×10^{-4}		Gharagheizi et al. (2010)	Q	247
CLSBTDGUHSQYTO-UHFFFAOYSA-N					

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-ethyl-2-propylbenzene	9.4×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	3.5×10^{-4}		Gharagheizi et al. (2012)	Q	
[16021-20-8]	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
DMUVQFCRCMDZPW-UHFFFAOYSA-N	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	8.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
1-ethyl-3-propylbenzene	9.6×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	3.3×10^{-4}		Gharagheizi et al. (2012)	Q	
[20024-91-3]	8.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
QCYGXOCMWHSXSU-UHFFFAOYSA-N					
1-ethyl-4-propylbenzene	9.2×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	3.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[20024-90-2]	8.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
ADQDTIAWIXUACV-UHFFFAOYSA-N					
1-ethyl-2-isopropylbenzene	9.8×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.5×10^{-4}		Gharagheizi et al. (2012)	Q	
[18970-44-0]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
ZAJYARZMPOEGLK-UHFFFAOYSA-N					
1-ethyl-3-isopropylbenzene	9.6×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[4920-99-4]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
GSLSBTNLESMZTN-UHFFFAOYSA-N					
1-ethyl-4-isopropylbenzene	9.1×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	3.0×10^{-4}		Gharagheizi et al. (2012)	Q	
[4218-48-8]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
GUUDUUDWUWUTPD-UHFFFAOYSA-N					
1-methyl-2,3-diethylbenzene	9.0×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[13632-93-4]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
LRJOXARIJKBUFE-UHFFFAOYSA-N					
1-methyl-2,4-diethylbenzene	9.1×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.5×10^{-4}		Gharagheizi et al. (2012)	Q	
[1758-85-6]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
PZMJNJDRDKPVLB-UHFFFAOYSA-N					
1-methyl-2,5-diethylbenzene	9.0×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[13632-94-5]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
ZEHGGUIGEDITMM-UHFFFAOYSA-N					

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methyl-2,6-diethylbenzene	8.8×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[13632-95-6]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
XZZNTLNFQVAKFD-UHFFFAOYSA-N					
1-methyl-3,5-diethylbenzene	9.5×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	8.7×10^{-4}		Wang et al. (2017)	Q	81, 239
[2050-24-0]	5.8×10^{-4}		Wang et al. (2017)	Q	81, 240
HILAULICMJUOLK-UHFFFAOYSA-N	2.0×10^{-3}		Wang et al. (2017)	Q	81, 241
	2.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
1-methyl-2-butylbenzene	9.0×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	4.1×10^{-4}		Gharagheizi et al. (2012)	Q	
[1595-11-5]	8.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
NUJILYKLNKQOOX-UHFFFAOYSA-N					
1-methyl-3-butylbenzene	9.2×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	3.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[1595-04-6]	8.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
OAPCPUDMDJIBOQ-UHFFFAOYSA-N					
1-methyl-4-butylbenzene	9.1×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	4.0×10^{-4}		Gharagheizi et al. (2012)	Q	
[1595-05-7]	8.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
SBBKUBSYOVDBBC-UHFFFAOYSA-N					
1-methyl-2-isobutylbenzene	9.1×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[36301-29-8]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
XNMPJDZAHSMAMN-UHFFFAOYSA-N					
1-methyl-3-isobutylbenzene	9.3×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[5160-99-6]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
SDHYGAUOCHFYSR-UHFFFAOYSA-N					
1-methyl-4-isobutylbenzene	9.1×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[5161-04-6]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
VCGBZXLLPCGFQM-UHFFFAOYSA-N					
1-methyl-2-*sec*-butylbenzene	9.1×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[1595-06-8]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
AMBAWAHKHZZAAY-UHFFFAOYSA-N					

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methyl-3-*sec*-butylbenzene	9.3×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[1772-10-7]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
RMNILBOMCXQZFC-UHFFFAOYSA-N					
1-methyl-4-*sec*-butylbenzene	9.0×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	3.0×10^{-4}		Gharagheizi et al. (2012)	Q	
[1595-16-0]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
LWCFXYMSEGQWNB-UHFFFAOYSA-N					
1-methyl-2-*tert*-butyl benzene	7.2×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	3.4×10^{-4}		Gharagheizi et al. (2012)	Q	
[1074-92-6]	8.2×10^{-4}		Gharagheizi et al. (2010)	Q	247
AXHVNJGQOJFMHT-UHFFFAOYSA-N					
1-methyl-3-*tert*-butylbenzene	8.2×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.5×10^{-4}		Gharagheizi et al. (2012)	Q	
[1075-38-3]	8.2×10^{-4}		Gharagheizi et al. (2010)	Q	247
JTIAYWZZZOZUTK-UHFFFAOYSA-N					
1-methyl-3,4-diethylbenzene	9.2×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	2.4×10^{-4}		Gharagheizi et al. (2012)	Q	
[13732-80-4]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
MJQJAQGFUBIGIK-UHFFFAOYSA-N					
1-phenyl-2,2-dimethylpropane	3.8×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	3.4×10^{-4}		Gharagheizi et al. (2012)	Q	
[1007-26-7]	4.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
CJGXJKVMUHXVHL-UHFFFAOYSA-N					
1-phenyl-2-methylbutane	4.0×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	4.5×10^{-4}		Gharagheizi et al. (2012)	Q	
[3968-85-2]	5.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
IFDLFCDWOFLKEB-UHFFFAOYSA-N					
1-phenyl-3-methylbutane	3.9×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	4.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[2049-94-7]	5.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
XNXIYYFOYIUJIW-UHFFFAOYSA-N					
2-phenyl-3-methylbutane	4.1×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	3.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[4481-30-5]	5.3×10^{-4}		Gharagheizi et al. (2010)	Q	247
NQRMTOKLHZNAQH-UHFFFAOYSA-N					
2-phenylpentane	4.3×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	3.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[2719-52-0]	5.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
LTHAIAJHDPJXLG-UHFFFAOYSA-N					

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-phenylpentane	4.3×10^{-4}		Yaws (2003)	X	238
$C_{11}H_{16}$	3.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[1196-58-3]	5.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
PBWHJRFXUPLZDS-UHFFFAOYSA-N					
(1,1-dimethylpropyl)-benzene	5.4×10^{-4}		Hine and Mookerjee (1975)	V	
$C_6H_5C_5H_{11}$	3.5×10^{-4}		Yaws (2003)	X	238
(*tert*-amylbenzene)	4.1×10^{-4}		Gharagheizi et al. (2012)	Q	
[2049-95-8]	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
QHTJSSMHBLGUHV-UHFFFAOYSA-N	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	4.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
	9.9×10^{-4}		Hilal et al. (2008)	Q	
	5.8×10^{-4}		English and Carroll (2001)	Q	231, 232
	4.2×10^{-4}		Suzuki et al. (1992)	Q	233
	5.1×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
hexylbenzene	4.0×10^{-4}	6500	Brockbank (2013)	L	1
$C_6H_5C_6H_{13}$	4.0×10^{-4}	6300	Plyasunov and Shock (2000)	L	
[1077-16-3]	3.5×10^{-4}		Duchowicz et al. (2020)	V	187
LTEQMZWBSYACLV-UHFFFAOYSA-N	4.6×10^{-4}		Mackay et al. (2006a)	V	
	4.6×10^{-4}		Mackay et al. (1992a)	V	
	4.5×10^{-4}		Meylan and Howard (1991)	V	
	5.1×10^{-4}		Eastcott et al. (1988)	V	
	4.5×10^{-4}		Abraham (1984)	V	
	7.7×10^{-3}	9000	Ben-Naim and Wilf (1980)	V	1
	4.1×10^{-4}	6300	Owens et al. (1986)	T	
	3.9×10^{-4}		Yaws (2003)	X	238
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	6.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	5.3×10^{-4}		Gharagheizi et al. (2010)	Q	247
	4.8×10^{-4}		Hilal et al. (2008)	Q	
	4.3×10^{-4}		Modarresi et al. (2007)	Q	68
	4.6×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	3.7×10^{-4}		Yao et al. (2002)	Q	230
	4.2×10^{-4}		English and Carroll (2001)	Q	231, 232
	5.0×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	4.0×10^{-4}		Meylan and Howard (1991)	Q	
	3.9×10^{-4}		Yaws (1999)	?	21
	4.6×10^{-4}		Yaws and Yang (1992)	?	21
	4.3×10^{-4}		Abraham et al. (1990)	?	
hexamethylbenzene	8.6×10^{-3}		Hilal et al. (2008)	Q	
$C_{12}H_{18}$	1.5×10^{-3}		Modarresi et al. (2007)	Q	68
[87-85-4]					
YUWFEBAXEOLKSG-UHFFFAOYSA-N					

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3-triethylbenzene	3.5×10^{-4}		Yaws (2003)	X	238
$C_{12}H_{18}$	1.4×10^{-4}		Gharagheizi et al. (2012)	Q	
[42205-08-3]	6.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
VIDOPANCAUPXNH-UHFFFAOYSA-N					
1,2,4-triethylbenzene	7.2×10^{-4}		Yaws (2003)	X	238
$C_{12}H_{18}$	1.4×10^{-4}		Gharagheizi et al. (2012)	Q	
[877-44-1]	6.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
WNLWIOJSURYFIB-UHFFFAOYSA-N	7.2×10^{-4}		Yaws (1999)	?	21
1,3,5-triethylbenzene	1.0×10^{-3}		Plyasunov and Shock (2000)	L	
$C_{12}H_{18}$	3.4×10^{-4}		Yaws (2003)	X	238
[102-25-0]	1.4×10^{-4}		Gharagheizi et al. (2012)	Q	
WJYMPXJVHNDZHD-UHFFFAOYSA-N	6.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
4-*tert*-butyl-*o*-xylene	5.8×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_{18}$	7.2×10^{-4}		Zhang et al. (2010)	Q	288, 290
[7397-06-0]	9.0×10^{-4}		Zhang et al. (2010)	Q	288, 291
QRPPSTNABSMSCS-UHFFFAOYSA-N	2.7×10^{-4}		Zhang et al. (2010)	Q	288, 292
1-(1,1-dimethylethyl)-3,5-dimethylbenzene	5.8×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_{18}$	4.5×10^{-4}		Zhang et al. (2010)	Q	288, 290
[98-19-1]	7.7×10^{-4}		Zhang et al. (2010)	Q	288, 291
FZSPYHREEHYLCB-UHFFFAOYSA-N	2.7×10^{-4}		Zhang et al. (2010)	Q	288, 292
o-diisopropylbenzene	4.8×10^{-4}		HSDB (2015)	Q	100
$C_{12}H_{18}$					
[25321-09-9]					
OKIRBHVFJGXOIS-UHFFFAOYSA-N					
m-diisopropylbenzene	9.5×10^{-4}		Yaws (2003)	X	238
$C_{12}H_{18}$	7.2×10^{-4}		Gharagheizi et al. (2010)	Q	247
[99-62-7]	9.6×10^{-4}		Yaws (1999)	?	21
UNEATYXSUBPPKP-UHFFFAOYSA-N					
p-diisopropylbenzene	1.0×10^{-3}		Yaws (2003)	X	238
$C_{12}H_{18}$	1.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[100-18-5]	7.2×10^{-4}		Gharagheizi et al. (2010)	Q	247
SPPWGCYEYAMHDT-UHFFFAOYSA-N	1.0×10^{-3}		Yaws (1999)	?	21
4-phenylcyclohexene	7.9×10^{-3}		Ebert et al. (2023)	?	319
$C_{12}H_{14}$					
[4994-16-5]					
XWCWNUSFQVJNDI-UHFFFAOYSA-N					

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
heptylbenzene	2.7×10^{-4}		Brockbank (2013)	L	
$C_6H_5C_7H_{15}$	6.5×10^{-4}		Duchowicz et al. (2020)	V	187
[1078-71-3]	2.2×10^{-2}	11000	Ben-Naim and Wilf (1980)	V	1
LBNXAWYDQUGHGX-UHFFFAOYSA-N	6.5×10^{-4}		Yaws (2003)	X	238
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	1.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	5.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
	3.9×10^{-4}		Hilal et al. (2008)	Q	
	3.5×10^{-4}		Yao et al. (2002)	Q	230
	1.5×10^{-3}		Yaws (1999)	?	21
5-*tert*-butyl-1,2,3-trimethylbenzene	5.3×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_{13}H_{20}$	9.2×10^{-4}		Zhang et al. (2010)	Q	288, 290
[98-23-7]	9.0×10^{-4}		Zhang et al. (2010)	Q	288, 291
ZQVJKYPEIPJEIP-UHFFFAOYSA-N	1.5×10^{-4}		Zhang et al. (2010)	Q	288, 292
octylbenzene	1.8×10^{-4}		Brockbank (2013)	L	
$C_6H_5C_8H_{17}$	2.3×10^{-4}		Duchowicz et al. (2020)	V	187
[2189-60-8]	5.4×10^{-2}	12000	Ben-Naim and Wilf (1980)	V	1
CDKDZKXSXLNROY-UHFFFAOYSA-N	8.7×10^{-4}		Yaws (2003)	X	238
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	1.7×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
	3.2×10^{-4}		Hilal et al. (2008)	Q	
	2.0×10^{-3}		Yaws (1999)	?	21
nonylbenzene	1.4×10^{-4}		Brockbank (2013)	L	
$C_{15}H_{24}$	1.8×10^{-3}		Gharagheizi et al. (2012)	Q	
[1081-77-2]	3.3×10^{-3}		Yaws (1999)	?	21
LIXVMPBOGDCSRM-UHFFFAOYSA-N					
3,5-di-*tert*-butyltoluene	3.7×10^{-3}	9100	Hiatt (2013)	M	
$C_{15}H_{24}$					
[15181-11-0]					
WIXDSJRJFDWTNY-UHFFFAOYSA-N					
1,3,5-tris(1-methylethyl)benzene	2.5×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_{15}H_{24}$	1.8×10^{-4}		Zhang et al. (2010)	Q	288, 290
[717-74-8]	5.2×10^{-4}		Zhang et al. (2010)	Q	288, 291
VUMCUSHVMYIRMB-UHFFFAOYSA-N	2.6×10^{-4}		Zhang et al. (2010)	Q	288, 292
ethyl(phenylethyl)-benzene	1.1×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_{18}$	1.2×10^{-2}		Zhang et al. (2010)	Q	288, 290
[64800-83-5]	6.4×10^{-2}		Zhang et al. (2010)	Q	288, 291
BDEIYMXBPHSOSG-UHFFFAOYSA-N	1.8×10^{-2}		Zhang et al. (2010)	Q	288, 292

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-(1-phenylethyl)-*m*-xylene	1.3×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_{18}$	1.6×10^{-2}		Zhang et al. (2010)	Q	288, 290
[6165-52-2]	5.2×10^{-2}		Zhang et al. (2010)	Q	288, 291
JOUBGGHXBLOLFY-UHFFFAOYSA-N	1.5×10^{-2}		Zhang et al. (2010)	Q	288, 292
decylbenzene	7.6×10^{-5}		Brockbank (2013)	L	
$C_{16}H_{26}$	8.6×10^{-5}		Plyasunov and Shock (2000)	L	
(1-phenyldecane)	6.5×10^{-5}		Duchowicz et al. (2020)	V	187
[104-72-3]	1.3×10^{-4}		HSDB (2015)	V	
UZILCZKGXMQEQR-UHFFFAOYSA-N	8.6×10^{-5}		Sherblom et al. (1992)	V	
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	1.3×10^{-4}		Zhang et al. (2010)	Q	288, 289
	1.4×10^{-4}		Zhang et al. (2010)	Q	288, 290
	3.4×10^{-4}		Zhang et al. (2010)	Q	288, 291
	2.8×10^{-4}		Zhang et al. (2010)	Q	288, 292
	7.9×10^{-3}		Yaws (1999)	?	21
2-phenyldecane	1.0×10^{-4}		Sherblom et al. (1992)	V	
$C_{16}H_{26}$					
[4537-13-7]					
DDTJIQUCOLHYDL-UHFFFAOYSA-N					
3-phenyldecane	1.1×10^{-4}		Sherblom et al. (1992)	V	
$C_{16}H_{26}$					
[4621-36-7]					
PYVIFMPVFLOTLN-UHFFFAOYSA-N					
4-phenyldecane	9.2×10^{-5}		Sherblom et al. (1992)	V	
$C_{16}H_{26}$					
[4537-12-6]					
QTDBKYLPIZUTFN-UHFFFAOYSA-N					
5-phenyldecane	8.4×10^{-5}		Sherblom et al. (1992)	V	
$C_{16}H_{26}$					
[4537-11-5]					
CDOBABYRHNVZQG-UHFFFAOYSA-N					
undecylbenzene	9.9×10^{-5}		HSDB (2015)	Q	100
$C_{17}H_{28}$					
(1-phenylundecane)					
[6742-54-7]					
XBEADGFTLHRJRB-UHFFFAOYSA-N					
2-phenylundecane	8.2×10^{-5}		Sherblom et al. (1992)	V	
$C_{17}H_{28}$					
[4536-88-3]					
YHJBCRBYDBNEIK-UHFFFAOYSA-N					

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-phenylundecane $C_{17}H_{28}$ [4536-87-2] NVHBFHMWJJMQTG-UHFFFAOYSA-N	9.0×10^{-5}		Sherblom et al. (1992)	V	
4-phenylundecane $C_{17}H_{28}$ [4536-86-1] NSQAXMRLBNXEHK-UHFFFAOYSA-N	5.9×10^{-5}		Sherblom et al. (1992)	V	
5-phenylundecane $C_{17}H_{28}$ [4537-15-9] RRPCXIBGXYGQNC-UHFFFAOYSA-N	6.1×10^{-5}		Sherblom et al. (1992)	V	
6-phenylundecane $C_{17}H_{28}$ [4537-14-8] WCABIRIFXVXGQH-UHFFFAOYSA-N	6.4×10^{-5}		Sherblom et al. (1992)	V	
dodecylbenzene $C_{18}H_{30}$ (1-phenyldodecane) [123-01-3] KWKXNDCHNDYVRT-UHFFFAOYSA-N	7.6×10^{-5}		HSDB (2015)	Q	100
2-phenyldodecane $C_{18}H_{30}$ [2719-61-1] VRPRIAVYSREHAN-UHFFFAOYSA-N	1.1×10^{-4}		Sherblom et al. (1992)	V	
3-phenyldodecane $C_{18}H_{30}$ [2400-00-2] PGVOXXHNGYYHHB-UHFFFAOYSA-N	1.3×10^{-4}		Sherblom et al. (1992)	V	
4-phenyldodecane $C_{18}H_{30}$ [2719-64-4] RHDHXBLZBVAPTL-UHFFFAOYSA-N	8.3×10^{-5}		Sherblom et al. (1992)	V	
5-phenyldodecane $C_{18}H_{30}$ [2719-63-3] NPAWGLOPXKCTCV-UHFFFAOYSA-N	7.8×10^{-5}		Sherblom et al. (1992)	V	
6-phenyldodecane $C_{18}H_{30}$ [2719-62-2] ZYHJQFMTTFCBKH-UHFFFAOYSA-N	6.0×10^{-5}		Sherblom et al. (1992)	V	

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tridecylbenzene $C_{19}H_{32}$ (1-phenyltridecane) [123-02-4] MCVUKOYZUCWLQQ-UHFFFAOYSA-N	1.1×10^{-4} 5.5×10^{-5}		Sherblom et al. (1992) HSDB (2015)	V Q	 100
2-phenyltridecane $C_{19}H_{32}$ [4534-53-6] FCXPVFLEDIQLLO-UHFFFAOYSA-N	2.7×10^{-4}		Sherblom et al. (1992)	V	
3-phenyltridecane $C_{19}H_{32}$ [4534-52-5] VZZMNLVGDGMQQV-UHFFFAOYSA-N	2.1×10^{-4}		Sherblom et al. (1992)	V	
4-phenyltridecane $C_{19}H_{32}$ [4534-51-4] RZGVZPAWCGDMCK-UHFFFAOYSA-N	2.0×10^{-4}		Sherblom et al. (1992)	V	
5-phenyltridecane $C_{19}H_{32}$ [4534-50-3] MZTIRLOLMGVVEK-UHFFFAOYSA-N	1.5×10^{-4}		Sherblom et al. (1992)	V	
6-phenyltridecane $C_{19}H_{32}$ [4534-49-0] OTSYFFDVDLHIKX-UHFFFAOYSA-N	1.5×10^{-4}		Sherblom et al. (1992)	V	
tetradecylbenzene $C_{20}H_{34}$ (1-phenyltetradecane) [1459-10-5] JZALLXAUNPOCEU-UHFFFAOYSA-N	4.2×10^{-5}		HSDB (2015)	Q	100
2-phenyltetradecane $C_{20}H_{34}$ [4534-59-2] GDFUGKICRHMMOT-UHFFFAOYSA-N	6.7×10^{-4}		Sherblom et al. (1992)	V	
3-phenyltetradecane $C_{20}H_{34}$ [4534-58-1] ILOABSZOHZMWLD-UHFFFAOYSA-N	6.2×10^{-4}		Sherblom et al. (1992)	V	
4-phenyltetradecane $C_{20}H_{34}$ [4534-57-0] YXLRHYCRTUAPMC-UHFFFAOYSA-N	4.0×10^{-4}		Sherblom et al. (1992)	V	

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5-phenyltetradecane $C_{20}H_{34}$ [4534-56-9] RAWFVRXBPRHWLJ-UHFFFAOYSA-N	5.0×10^{-4}		Sherblom et al. (1992)	V	
6-phenyltetradecane $C_{20}H_{34}$ [4534-55-8] MTDIFFBFSKQPIA-UHFFFAOYSA-N	3.6×10^{-4}		Sherblom et al. (1992)	V	
pentadecylbenzene $C_{21}H_{36}$ [2131-18-2] JIRNEODMTPGRGV-UHFFFAOYSA-N	1.2×10^{-5}		HSDB (2015)	Q	100
ethenylbenzene	3.6×10^{-3}	3700	Brockbank (2013)	L	
C_8H_8	2.9×10^{-3}	4200	Plyasunov and Shock (2000)	L	
(styrene)	2.7×10^{-3}		Kim and Kim (2014)	M	
[100-42-5]	4.4×10^{-3}	4600	Hiatt (2013)	M	
PPBRXRYQALVLMV-UHFFFAOYSA-N	3.4×10^{-3}		Dohnal and Hovorka (1999)	M	
	2.5×10^{-3}		Welke et al. (1998)	M	
	3.8×10^{-3}	4100	Kondoh and Nakajima (1997)	M	
	2.9×10^{-3}	4800	Bissonette et al. (1990)	M	
	1.8×10^{-3}		Sato and Nakajima (1979a)	M	14
	3.6×10^{-3}		Lide and Frederikse (1995)	V	
	3.3×10^{-3}		Abraham et al. (1994a)	V	
	3.3×10^{-3}		Mackay et al. (1993)	V	
	3.8×10^{-3}		Yaws (2003)	X	259
	3.8×10^{-3}		Yaws (2003)	X	238
	3.8×10^{-3}	4200	Goldstein (1982)	X	299
	3.8×10^{-3}	3800	Fogg and Sangster (2003)	C	
	3.3×10^{-3}		Dupeux et al. (2022)	Q	260
	1.3×10^{-3}		Keshavarz et al. (2022)	Q	
	1.1×10^{-2}		Duchowicz et al. (2020)	Q	300
	8.7×10^{-3}		Wang et al. (2017)	Q	81, 239
	2.6×10^{-3}		Wang et al. (2017)	Q	81, 240
	7.6×10^{-3}		Wang et al. (2017)	Q	81, 241
	1.6×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	2.6×10^{-3}		Gharagheizi et al. (2010)	Q	247
	3.2×10^{-3}		Hilal et al. (2008)	Q	
	4.4×10^{-3}		Modarresi et al. (2007)	Q	68
		4800	Kühne et al. (2005)	Q	
	3.8×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	3.3×10^{-3}		English and Carroll (2001)	Q	231, 232

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-4}		Katritzky et al. (1998)	Q	
	3.7×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	3.6×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		3700	Kühne et al. (2005)	?	
	3.8×10^{-3}		Yaws (1999)	?	21
	1.9×10^{-3}		Abraham and Weathersby (1994)	?	21
	3.7×10^{-3}		Yaws and Yang (1992)	?	21
			Shiu and Ma (2000)	W	362
(*E*)-1-propenylbenzene C_9H_{10} [873-66-5] QROGIFZRVHSFLM-QHHAFSJGSA-N	2.9×10^{-3}		Hilal et al. (2008)	Q	
1-propenylbenzene C_9H_{10} [637-50-3] QROGIFZRVHSFLM-UHFFFAOYSA-N	3.7×10^{-3}		HSDB (2015)	Q	100
2-propenylbenzene	1.4×10^{-3}		Sato and Nakajima (1979a)	M	14
C_9H_{10}	2.2×10^{-3}		Hilal et al. (2008)	Q	
(allylbenzene)	1.5×10^{-3}		Yaffe et al. (2003)	Q	249, 250
[300-57-2]	2.9×10^{-3}		Nirmalakhandan et al. (1997)	Q	
HJWLCRVIBGQPNF-UHFFFAOYSA-N	1.4×10^{-3}		Abraham and Weathersby (1994)	?	21
1-ethenyl-3-methylbenzene	3.0×10^{-3}		Yaws (2003)	X	238
C_9H_{10}	7.0×10^{-3}		Gharagheizi et al. (2012)	Q	
(*m*-methylstyrene)	3.8×10^{-3}		Gharagheizi et al. (2010)	Q	247
[100-80-1]	3.1×10^{-3}		Hilal et al. (2008)	Q	
JZHGRUMIRATHIU-UHFFFAOYSA-N	1.6×10^{-3}		Modarresi et al. (2007)	Q	68
	3.0×10^{-3}		Yaws (1999)	?	21
	2.6×10^{-3}		Yaws and Yang (1992)	?	21
1-ethenyl-4-methylbenzene	3.1×10^{-3}		Duchowicz et al. (2020)	V	187
C_9H_{10}	3.1×10^{-3}		HSDB (2015)	V	
(*p*-methylstyrene)	3.1×10^{-3}		Yaws (2003)	X	238
[622-97-9]	5.5×10^{-3}		Duchowicz et al. (2020)	Q	
JLBJTVDPSNHSKJ-UHFFFAOYSA-N	7.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	3.8×10^{-3}		Gharagheizi et al. (2010)	Q	247
	3.4×10^{-3}		Hilal et al. (2008)	Q	
	2.8×10^{-3}		Modarresi et al. (2007)	Q	68
	1.5×10^{-3}		Yao et al. (2002)	Q	230
	3.1×10^{-3}		Yaws (1999)	?	21
	3.5×10^{-3}		Yaws and Yang (1992)	?	21

Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(1-methylethenyl)-benzene	3.9×10^{-3}		Duchowicz et al. (2020)	V	187
C_9H_{10}	3.8×10^{-3}		HSDB (2015)	V	
(α-methyl styrene)	3.3×10^{-3}		Abraham et al. (1994a)	V	
[98-83-9]	3.6×10^{-3}		Duchowicz et al. (2020)	Q	
XYLMUPLGERFSHI-UHFFFAOYSA-N	2.4×10^{-3}		Hilal et al. (2008)	Q	
	3.9×10^{-3}		English and Carroll (2001)	Q	231, 232
phenylacetylene	1.6×10^{-2}		Duchowicz et al. (2020)	V	187
C_8H_6	5.7×10^{-3}		Yaws (2003)	X	238
[536-74-3]	2.2×10^{-2}		Duchowicz et al. (2020)	Q	
UEXCJVNBTNXOEH-UHFFFAOYSA-N	2.0×10^{-2}		Gharagheizi et al. (2012)	Q	
	5.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
	3.9×10^{-3}		Hilal et al. (2008)	Q	
	6.5×10^{-3}		Modarresi et al. (2007)	Q	68
	1.5×10^{-3}		Yaffe et al. (2003)	Q	249, 250
α-methylstyrene dimer	1.1×10^{-2}		HSDB (2015)	Q	100
$C_{18}H_{20}$	5.7×10^{-3}		Zhang et al. (2010)	Q	288, 289
[6144-04-3]	7.2×10^{-3}		Zhang et al. (2010)	Q	288, 290
ATSCZMXECPRPEA-BUHFOSPRSA-N	2.4×10^{-1}		Zhang et al. (2010)	Q	288, 291
	9.0×10^{-2}		Zhang et al. (2010)	Q	288, 292

A2.6 Terpenes and terpenoids

Table A2.6: Terpenes and terpenoids

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methyl-4-(1-methylethyl)-cyclohexane	5.6×10^{-6}		Duchowicz et al. (2020)	V	187
$C_{10}H_{20}$	5.6×10^{-6}		Copolovici and Niinemets (2005)	V	
(p-menthane)	2.1×10^{-4}		Duchowicz et al. (2020)	Q	
[99-82-1]					
CFJYNSNXFXLKNS-UHFFFAOYSA-N					
α-pinene	7.0×10^{-5}	4700	Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	2.9×10^{-4}	1800	Leng et al. (2013)	M	
[80-56-8]	7.4×10^{-5}	4400	Copolovici and Niinemets (2005)	M	
GRWFGVWFFZKLTI-UHFFFAOYSA-N	5.8×10^{-4}		Karl et al. (2003)	M	88
	1.4×10^{-2}		van Ruth et al. (2002)	M	14
	7.4×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 363
	2.1×10^{-3}		van Ruth et al. (2001)	M	14
	7.0×10^{-5}		Fichan et al. (1999)	M	
	4.7×10^{-5}		Falk et al. (1990)	M	14
	3.4×10^{-5}		Duchowicz et al. (2020)	V	187
	3.4×10^{-5}		HSDB (2015)	V	
	7.4×10^{-5}		Copolovici and Niinemets (2005)	V	
	7.4×10^{-5}		Niinemets and Reichstein (2002)	V	
	2.8×10^{-5}	10000	Li et al. (1998)	V	
	3.5×10^{-5}		Hilal et al. (2008)	C	
	2.2×10^{-4}		Dupeux et al. (2022)	Q	260
	3.0×10^{-4}		Duchowicz et al. (2020)	Q	
	7.6×10^{-4}		Wang et al. (2017)	Q	81, 239
	2.4×10^{-5}		Wang et al. (2017)	Q	81, 240
	5.6×10^{-4}		Wang et al. (2017)	Q	81, 241
	3.1×10^{-5}		Hilal et al. (2008)	Q	
β-pinene	2.1×10^{-4}		Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	1.6×10^{-4}		Helburn et al. (2008)	M	
[127-91-3]	1.5×10^{-4}	4500	Copolovici and Niinemets (2005)	M	
WTARULDDTDQWMU-UHFFFAOYSA-N	4.9×10^{-4}		Karl et al. (2003)	M	88
	4.7×10^{-5}		Falk et al. (1990)	M	14
	1.5×10^{-4}		Copolovici and Niinemets (2005)	V	
	1.5×10^{-4}		Niinemets and Reichstein (2002)	V	
	4.3×10^{-4}		Dupeux et al. (2022)	Q	260
	4.5×10^{-4}		Wang et al. (2017)	Q	81, 239
	3.2×10^{-5}		Wang et al. (2017)	Q	81, 240
	1.1×10^{-3}		Wang et al. (2017)	Q	81, 241
	6.2×10^{-5}		HSDB (2015)	Q	100

Table A2.6: Terpenes and terpenoids (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methyl-4-(1-methylethyl)-1,3-cyclohexadiene	5.1×10^{-4}		Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	3.8×10^{-4}		Schuhfried et al. (2015)	M	
(α-terpinene)	2.9×10^{-4}	4800	Copolovici and Niinemets (2005)	M	
[99-86-5]	4.5×10^{-4}		Karl et al. (2003)	M	88
YHQGMYUVUMAZJR-UHFFFAOYSA-N	2.8×10^{-4}		Copolovici and Niinemets (2005)	V	
	5.1×10^{-4}		Niinemets and Reichstein (2002)	V	
	5.4×10^{-4}		Dupeux et al. (2022)	Q	260
1-methyl-4-(1-methylethyl)-1,4-cyclohexadiene	5.7×10^{-4}	4300	Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	4.5×10^{-4}		Schuhfried et al. (2015)	M	
(γ-terpinene)	3.8×10^{-4}	4800	Copolovici and Niinemets (2005)	M	
[99-85-4]	4.4×10^{-4}		Duchowicz et al. (2020)	V	187
YKFLAYDHMOASIY-UHFFFAOYSA-N	3.8×10^{-4}		Copolovici and Niinemets (2005)	V	
	2.8×10^{-4}		Niinemets and Reichstein (2002)	V	
	5.4×10^{-4}	8000	Li et al. (1998)	V	
	6.2×10^{-4}		Dupeux et al. (2022)	Q	260
	2.1×10^{-4}		Duchowicz et al. (2020)	Q	
	3.4×10^{-4}		Katritzky et al. (1998)	Q	
1-methyl-4-(1-methylethenyl)-cyclohexene	4.7×10^{-4}	4700	Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	4.8×10^{-4}	4600	Leng et al. (2013)	M	
(limonene)	2.6×10^{-4}		Copolovici and Niinemets (2007)	M	
[138-86-3]	7.0×10^{-4}		Fichan et al. (1999)	M	
XMGQYMWWDOXHJM-UHFFFAOYSA-N	2.4×10^{-4}		Welke et al. (1998)	M	
	7.0×10^{-4}		Falk et al. (1990)	M	14
	3.1×10^{-4}		Duchowicz et al. (2020)	V	187
	3.1×10^{-4}		HSDB (2015)	V	
	3.5×10^{-4}		Copolovici and Niinemets (2005)	V	
	6.4×10^{-4}	3000	van Roon et al. (2005)	V	
	3.5×10^{-4}		Niinemets and Reichstein (2002)	V	
	1.7×10^{-4}	10000	Li et al. (1998)	V	
	7.3×10^{-4}		Dupeux et al. (2022)	Q	260
	6.4×10^{-4}		Duchowicz et al. (2020)	Q	
	5.9×10^{-4}		Wang et al. (2017)	Q	81, 239
	1.1×10^{-4}		Wang et al. (2017)	Q	81, 240
	1.5×10^{-3}		Wang et al. (2017)	Q	81, 241
	1.1×10^{-4}		Hilal et al. (2008)	Q	
	1.9×10^{-4}		Modarresi et al. (2007)	Q	68

Table A2.6: Terpenes and terpenoids (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(*R*)-1-methyl-4-(1-methylethenyl)-cyclohexene	3.8×10^{-4}		Schuhfried et al. (2015)	M	
$C_{10}H_{16}$	2.6×10^{-4}		Helburn et al. (2008)	M	
(*R*-(+)-limonene; *D*-limonene)	3.5×10^{-4}	4500	Copolovici and Niinemets (2005)	M	
[5989-27-5]	3.8×10^{-4}		Duchowicz et al. (2020)	V	187
XMGQYMWWDOXHJM-SNVBAGLBSA-N	3.9×10^{-4}		HSDB (2015)	V	
	3.8×10^{-4}		Mackay et al. (2006a)	V	
	3.8×10^{-4}		Yaws (2003)	X	259
	3.8×10^{-4}		Yaws (2003)	X	238
	7.3×10^{-4}		Dupeux et al. (2022)	Q	260
	6.4×10^{-4}		Duchowicz et al. (2020)	Q	
	1.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	3.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
	1.9×10^{-4}		Modarresi et al. (2007)	Q	68
	3.8×10^{-4}		Yaws (1999)	?	21
(*S*)-1-methyl-4-(1-methylethenyl)-cyclohexene	3.7×10^{-4}		Schuhfried et al. (2015)	M	
$C_{10}H_{16}$	3.5×10^{-4}	4400	Copolovici and Niinemets (2005)	M	
(*S*-(-)-limonene)					
[5989-54-8]					
XMGQYMWWDOXHJM-JTQLQIEISA-N					
3,7,7-trimethyl-bicyclo[4.1.0]hept-3-ene	1.6×10^{-4}		Falk et al. (1990)	M	14
$C_{10}H_{16}$	7.3×10^{-5}		Copolovici and Niinemets (2005)	V	
(3-carene)	7.3×10^{-5}		Niinemets and Reichstein (2002)	V	
[13466-78-9]					
BQOFWKZOCNGFEC-UHFFFAOYSA-N					
7-methyl-3-methylene-1,6-octadiene	4.0×10^{-4}		Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	3.6×10^{-4}		Schuhfried et al. (2015)	M	
(myrcene)	8.7×10^{-4}		Fichan et al. (1999)	M	
[123-35-3]	1.5×10^{-4}		Duchowicz et al. (2020)	V	187
UAHWPYUMFXYFJY-UHFFFAOYSA-N	1.1×10^{-4}		HSDB (2015)	V	
	1.6×10^{-4}		Copolovici and Niinemets (2005)	V	
	7.2×10^{-4}	2800	van Roon et al. (2005)	V	
	1.6×10^{-4}		Niinemets and Reichstein (2002)	V	
	1.3×10^{-4}		Dupeux et al. (2022)	Q	260
	7.1×10^{-4}		Duchowicz et al. (2020)	Q	
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	6.2×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	246

Table A2.6: Terpenes and terpenoids (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methyl-4-(1-methylethylidene)-cyclohexene	7.9×10^{-4}	5500	Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	3.8×10^{-4}	5300	Copolovici and Niinemets (2005)	M	
(α-terpinolene)	7.0×10^{-4}		HSDB (2015)	V	
[586-62-9]	3.7×10^{-4}		Copolovici and Niinemets (2005)	V	
MOYAFQVGZZPNRA-UHFFFAOYSA-N	3.8×10^{-4}		Niinemets and Reichstein (2002)	V	
	5.7×10^{-4}	12000	Li et al. (1998)	V	
α-phellandrene	1.8×10^{-4}		Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	1.8×10^{-4}	4500	Copolovici and Niinemets (2005)	M	
[99-83-2]	1.8×10^{-4}		Copolovici and Niinemets (2005)	V	
OGLDWXZKYODSOB-UHFFFAOYSA-N	1.4×10^{-4}		Niinemets and Reichstein (2002)	V	
	5.3×10^{-4}		Dupeux et al. (2022)	Q	260
(R)-(−)-α-phellandrene	3.4×10^{-4}		Schuhfried et al. (2015)	M	
$C_{10}H_{16}$					
[4221-98-1]					
OGLDWXZKYODSOB-SNVBAGLBSA-N					
β-phellandrene	1.8×10^{-4}	5100	Copolovici and Niinemets (2005)	M	
$C_{10}H_{16}$	1.8×10^{-4}		Copolovici and Niinemets (2005)	V	
[555-10-2]	1.8×10^{-4}		Niinemets and Reichstein (2002)	V	
LFJQCDVYDGGFCH-UHFFFAOYSA-N	6.1×10^{-4}		Dupeux et al. (2022)	Q	260
3,7-dimethyl-1,3,6-octatriene	4.0×10^{-4}		Copolovici and Niinemets (2005)	V	
$C_{10}H_{16}$					
(β-ocimene)					
[13877-91-3]					
IHPKGUQCSIINRJ-UHFFFAOYSA-N					
(Z)-3,7-dimethyl-1,3,6-octatriene	4.0×10^{-4}		Niinemets and Reichstein (2002)	V	
$C_{10}H_{16}$					
(*cis*-β-ocimene)					
[3338-55-4]					
IHPKGUQCSIINRJ-NTMALXAHSA-N					
(E)-3,7-dimethyl-1,3,6-octatriene	3.0×10^{-4}		Niinemets and Reichstein (2002)	V	
$C_{10}H_{16}$					
(*trans*-β-ocimene)					
[3779-61-1]					
IHPKGUQCSIINRJ-CSKARUKUSA-N					
2,2-dimethyl-3-methylene-bicyclo[2.2.1]heptane	2.3×10^{-4}		Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	1.0×10^{-4}		HSDB (2015)	V	
(camphene)	3.1×10^{-4}		Copolovici and Niinemets (2005)	V	
[79-92-5]	6.3×10^{-4}		Niinemets and Reichstein (2002)	V	
CRPUJAZIXJMDBK-UHFFFAOYSA-N					

Table A2.6: Terpenes and terpenoids (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methylene-1-(1-methylethyl)- bicyclo[3.1.0]hexane	1.5×10^{-4}		Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	1.6×10^{-4}		Copolovici and Niinemets (2005)	V	
(sabinene)	1.6×10^{-4}		Niinemets and Reichstein (2002)	V	
[3387-41-5]					
NDVASEGYNIMXJL-UHFFFAOYSA-N					
tricyclo[3.3.1.1(3,7)]decane	8.0×10^{-4}	3400	van Roon et al. (2005)	V	
$C_{10}H_{16}$	1.1×10^{-4}		Hilal et al. (2008)	Q	
(adamantane)					
[281-23-2]					
ORILYTVJVMAKLC-UHFFFAOYSA-N					
β-caryophyllene	3.7×10^{-4}	4500	Copolovici and Niinemets (2015)	M	
$C_{15}H_{24}$	2.6×10^{-3}		Dupeux et al. (2022)	Q	260
[87-44-5]	6.5×10^{-4}		Wang et al. (2017)	Q	81, 239
NPNUFJAVOOONJE-IOMPXFEGSA-N	3.4×10^{-5}		Wang et al. (2017)	Q	81, 240
	1.0×10^{-2}		Wang et al. (2017)	Q	81, 241
α-cedrene	2.8×10^{-4}	4900	Copolovici and Niinemets (2015)	M	
$C_{15}H_{24}$					
[469-61-4]					
IRAQOCYXUMOFCW-KYEXWDHISA-N					
α-farnesene	3.4×10^{-4}	4300	Copolovici and Niinemets (2015)	M	
$C_{15}H_{24}$	8.1×10^{-6}		Schuhfried et al. (2015)	M	
[502-61-4]					
CXENHBSYCFFKJS-VDQVFBMKSA-N					
α-humulene	2.9×10^{-4}	4700	Copolovici and Niinemets (2015)	M	
$C_{15}H_{24}$					
[6753-98-6]					
FAMPSKZZVDUYOS-HRGUGZIWSA-N					
γ-gurjunene	3.3×10^{-4}	3700	Copolovici and Niinemets (2015)	M	
$C_{15}H_{24}$					
[22567-17-5]					
DUYRYUZIBGFLDD-UHFFFAOYSA-N					
isosativene	3.9×10^{-4}	3600	Copolovici and Niinemets (2015)	M	
$C_{15}H_{24}$					
[24959-83-9]					
CGZBLYYTRIVVTD-UHFFFAOYSA-N					
α-longipinene	3.4×10^{-4}	4100	Copolovici and Niinemets (2015)	M	
$C_{15}H_{24}$					
[5989-08-2]					
HICYDYJTCDBHMZ-UHFFFAOYSA-N					

Table A2.6: Terpenes and terpenoids (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
α-neoclovene $C_{15}H_{24}$ [4545-68-0] ZCJQJJWNFDNQGZ-UHFFFAOYSA-N	2.9×10^{-4}	3100	Copolovici and Niinemets (2015)	M	
β-neoclovene $C_{15}H_{24}$ [56684-96-9] BUDWHMNUSAOQBI-UHFFFAOYSA-N	2.9×10^{-4}	4600	Copolovici and Niinemets (2015)	M	
γ-neoclovene $C_{15}H_{24}$ ZYKFQRCKKGFKQR-UHFFFAOYSA-N	2.9×10^{-4}	3200	Copolovici and Niinemets (2015)	M	
valencene $C_{15}H_{24}$ [4630-07-3] QEBNYNLSCGVZOH-UHFFFAOYSA-N	3.2×10^{-4}	4500	Copolovici and Niinemets (2015)	M	

A2.7 Polynuclear aromatics

Table A2.7: Polynuclear aromatics

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bis(1-methylethyl)-1,1'-biphenyl	4.5×10^{-3}		HSDB (2015)	Q	100
$C_{18}H_{22}$	6.4×10^{-3}		Zhang et al. (2010)	Q	288, 289
[36876-13-8]	5.0×10^{-3}		Zhang et al. (2010)	Q	288, 290
NUEUMFZLNOCRCQ-UHFFFAOYSA-N	3.2×10^{-2}		Zhang et al. (2010)	Q	288, 291
	2.0×10^{-2}		Zhang et al. (2010)	Q	288, 292
1,1-bis(3,4-dimethylphenyl)ethane	1.0×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{18}H_{22}$	1.8×10^{-2}		Zhang et al. (2010)	Q	288, 290
[1742-14-9]	6.5×10^{-2}		Zhang et al. (2010)	Q	288, 291
NCSVCMFDHINRJE-UHFFFAOYSA-N	4.8×10^{-3}		Zhang et al. (2010)	Q	288, 292
1-benzyl-2-(2-methylbenzyl)benzene	2.1×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{21}H_{20}$	2.5×10^{-1}		Zhang et al. (2010)	Q	288, 290
[100404-06-6]	1.4		Zhang et al. (2010)	Q	288, 291
SMOZJCPUZPHHKQ-UHFFFAOYSA-N	4.1×10^{-1}		Zhang et al. (2010)	Q	288, 292
2,5-dibenzyltoluene	2.1×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{21}H_{20}$	2.9×10^{-1}		Zhang et al. (2010)	Q	288, 290
[56310-11-3]	4.5		Zhang et al. (2010)	Q	288, 291
INLIRICAUXXHSB-UHFFFAOYSA-N	4.1×10^{-1}		Zhang et al. (2010)	Q	288, 292
biphenyl	3.6×10^{-2}	7000	Brockbank (2013)	L	1
$(C_6H_5)_2$	3.6×10^{-2}		Mackay and Shiu (1981)	L	
[92-52-4]	3.4×10^{-2}		Destaillats and Charles (2002)	M	
ZUOUZKKEUPVFJK-UHFFFAOYSA-N			Dewulf et al. (1999)	M	364
	3.2×10^{-2}		Shiu and Mackay (1997)	M	
	5.1×10^{-2}		Fendinger and Glotfelty (1990)	M	
	3.3×10^{-2}		Mackay and Shiu (1981)	M	
	2.4×10^{-2}		Mackay et al. (1979)	M	
	3.5×10^{-2}		Mackay et al. (2006a)	V	
	3.5×10^{-2}		Mackay et al. (2006b)	V	
	3.6×10^{-2}		Shiu and Ma (2000)	V	
	3.5×10^{-2}		Shiu and Mackay (1997)	V	
	3.6×10^{-2}		Abraham et al. (1994a)	V	
	1.9×10^{-2}		Mackay et al. (1992a)	V	
	1.2×10^{-2}		Eastcott et al. (1988)	V	
	1.9×10^{-2}		Shiu and Mackay (1986)	V	
	7.3×10^{-2}		Burkhard et al. (1985)	V	
	2.0×10^{1}	6200	Bopp (1983)	V	
	3.5×10^{-2}		Cabani et al. (1981)	V	
	6.4×10^{-3}		Mackay and Leinonen (1975)	V	
	1.2×10^{-2}		Bohon and Claussen (1951)	V	
	7.6×10^{-3}	2900	Paasivirta et al. (1999)	T	
	1.7×10^{-2}		Yaws (2003)	X	259
	3.9×10^{-2}		Dupeux et al. (2022)	Q	260

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	2.8×10^{-2}		Duchowicz et al. (2020)	Q	300
	4.5×10^{-2}		Schröder et al. (2010)	Q	365
	1.3×10^{-2}		Hilal et al. (2008)	Q	
	5.0×10^{-2}		Modarresi et al. (2007)	Q	68
		5100	Kühne et al. (2005)	Q	
	3.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.5×10^{-2}		English and Carroll (2001)	Q	231, 232
	4.4×10^{-4}		Katritzky et al. (1998)	Q	
	8.0×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	2.9×10^{-2}		Arbuckle (1983)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		6000	Kühne et al. (2005)	?	
	1.2×10^{-2}		Yaws and Yang (1992)	?	21
2-methyl-1,1'-biphenyl $C_{13}H_{12}$ [643-58-3] ALLIZEAXNXSFGD-UHFFFAOYSA-N	2.2×10^{-2}		HSDB (2015)	Q	100
	1.0×10^{-2}		Hilal et al. (2008)	Q	
3-methyl-1,1'-biphenyl $C_{13}H_{12}$ [643-93-6] NPDIDUXTRAITDE-UHFFFAOYSA-N	1.5×10^{-2}		Hilal et al. (2008)	Q	
4-methyl-1,1'-biphenyl $C_{13}H_{12}$ [644-08-6] ZZLCFHIKESPLTH-UHFFFAOYSA-N	1.6×10^{-2}		Hilal et al. (2008)	Q	
diphenylmethane $C_{13}H_{12}$ (1,1'-methylenebisbenzene) [101-81-5] CZZYITDELCSZES-UHFFFAOYSA-N	7.7×10^{-2}		Duchowicz et al. (2020)	V	187
	7.6×10^{-2}		HSDB (2015)	V	
	1.1		Mackay et al. (2006a)	V	
	1.1		Mackay et al. (1993)	V	
	4.5×10^{-2}		Meylan and Howard (1991)	V	
	4.7×10^{-2}		Cabani et al. (1981)	V	
	1.0		Mackay et al. (1992b)	X	366
	4.3×10^{-2}		Yaws (2003)	X	238
	2.1×10^{-2}		Duchowicz et al. (2020)	Q	
	5.7×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.2×10^{-2}		Hilal et al. (2008)	Q	
	1.6×10^{-2}		Modarresi et al. (2007)	Q	68
	2.1×10^{-2}		Meylan and Howard (1991)	Q	
	4.3×10^{-2}		Yaws (1999)	?	21

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-diphenylethane	5.9×10^{-2}		Mackay et al. (2006a)	V	
$C_{14}H_{14}$	5.9×10^{-2}		Mackay et al. (1993)	V	
(dibenzyl)	5.9×10^{-2}		Mackay et al. (1992b)	X	366
[103-29-7]					
QWUWMCYKGHVNAV-UHFFFAOYSA-N					
3-isopropyl-1,1'-biphenyl	5.8×10^{-3}		Ebert et al. (2023)	?	367
$C_{15}H_{16}$					
[20282-30-8]					
LIWRTHVZRZXVFX-UHFFFAOYSA-N					
4-isopropyl-1,1'-biphenyl	4.2×10^{-3}		Ebert et al. (2023)	?	367
$C_{15}H_{16}$					
[7116-95-2]					
KWSHGRJUSUJPQD-UHFFFAOYSA-N					
o-terphenyl	1.6×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{18}H_{14}$	1.6×10^{-1}		HSDB (2015)	V	
[84-15-1]	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
OIAQMFOKAXHPNH-UHFFFAOYSA-N	3.1×10^{-1}		Zhang et al. (2010)	Q	288, 289
	8.2×10^{-2}		Zhang et al. (2010)	Q	288, 290
	7.3×10^{-1}		Zhang et al. (2010)	Q	288, 291
	4.0		Zhang et al. (2010)	Q	288, 292
m-terphenyl	2.8		Duchowicz et al. (2020)	V	187
$C_{18}H_{14}$	2.8		HSDB (2015)	V	
[92-06-8]	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
YJTKZCDBKVTVBY-UHFFFAOYSA-N	1.2		Schröder et al. (2010)	Q	365
p-terphenyl	6.0		Duchowicz et al. (2020)	V	187
$C_{18}H_{14}$			Mackay et al. (2006a)	V	293
[92-94-4]	2.0×10^{-2}		Yaws (2003)	X	238
XJKSTNDFUHDPQJ-UHFFFAOYSA-N	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
	2.9×10^{-1}		HSDB (2015)	Q	100
	3.1×10^{-1}		Zhang et al. (2010)	Q	288, 289
	2.4×10^{-1}		Zhang et al. (2010)	Q	288, 290
	1.1		Zhang et al. (2010)	Q	288, 291
	4.0		Zhang et al. (2010)	Q	288, 292
	2.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
indene	6.2×10^{-3}		HSDB (2015)	Q	100
C_9H_8					
[95-13-6]					
YBYIRNPNPLQARY-UHFFFAOYSA-N					
5-ethylidene-2-norbornene	7.6×10^{-5}		HSDB (2015)	Q	100
C_9H_{12}					
[16219-75-3]					
OJOWICOBYCXEKR-KRXBUXKQSA-N					

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
indane	4.3×10^{-3}		Plyasunov and Shock (2000)	L	
C_9H_{10}	4.3×10^{-3}		Mackay et al. (2006a)	V	
[496-11-7]	4.7×10^{-3}		Abraham et al. (1994a)	V	
PQNFLJBBNBOBRQ-UHFFFAOYSA-N	4.5×10^{-3}		Yaws (2003)	X	259
	4.5×10^{-3}		Yaws (2003)	X	238
	2.4×10^{-3}		Dupeux et al. (2022)	Q	260
	9.6×10^{-2}		Keshavarz et al. (2022)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	Q	300
	4.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	5.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-3}		Modarresi et al. (2007)	Q	68
	4.8×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	7.2×10^{-3}		English and Carroll (2001)	Q	231, 232
	5.8×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	4.5×10^{-3}		Yaws (1999)	?	21
azulene	1.5×10^{-1}	7800	Hiatt (2013)	M	
$C_{10}H_8$					
[275-51-4]					
CUFNKYGDVFVPHO-UHFFFAOYSA-N					
naphthalene	2.1×10^{-2}	4400	Schwardt et al. (2021)	L	1
$C_{10}H_8$	2.1×10^{-2}	5400	Brockbank (2013)	L	1
[91-20-3]	2.1×10^{-2}		Ma et al. (2010b)	L	368
UFWIBTONFRDIAS-UHFFFAOYSA-N	2.2×10^{-2}		Ma et al. (2010b)	L	369
	2.2×10^{-2}	5300	Fogg and Sangster (2003)	L	
	2.3×10^{-2}		Mackay and Shiu (1981)	L	
	3.3×10^{-2}	6100	Hiatt (2013)	M	
	6.0×10^{-2}		Lee et al. (2012)	M	
	4.0×10^{-2}		Bobadilla et al. (2003)	M	
	2.4×10^{-2}		Destaillats and Charles (2002)	M	
	1.3×10^{-2}	3600	Dewulf et al. (1999)	M	
	1.8×10^{-2}		Altschuh et al. (1999)	M	
	2.2×10^{-2}		De Maagd et al. (1998)	M	12
	2.2×10^{-2}		Shiu and Mackay (1997)	M	
	1.7×10^{-2}	5100	Kondoh and Nakajima (1997)	M	
	2.3×10^{-2}	5700	Alaee et al. (1996)	M	
	2.1×10^{-2}		Zhang and Pawliszyn (1993)	M	
	1.3×10^{-2}		Fendinger and Glotfelty (1990)	M	
	2.7×10^{-2}		Yurteri et al. (1987)	M	12
	2.6×10^{-2}		Webster et al. (1985)	M	
	2.0×10^{-2}		Mackay et al. (1979)	M	
	1.8×10^{-2}		Southworth (1979)	M	
	2.2×10^{-2}	5400	Schwarz and Wasik (1977)	M	
	2.3×10^{-2}		Mackay et al. (2006a)	V	

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.3×10^{-2}		Shiu and Ma (2000)	V	
	3.2×10^{-2}		De Maagd et al. (1998)	V	12
	2.3×10^{-2}		Shiu and Mackay (1997)	V	
	2.0×10^{-2}		Lide and Frederikse (1995)	V	
	2.3×10^{-2}		Abraham et al. (1994a)	V	
	9.0×10^{-3}		Hwang et al. (1992)	V	
	7.2×10^{-3}		Eastcott et al. (1988)	V	
	2.3×10^{-2}		Cabani et al. (1981)	V	
	2.4×10^{-2}		Hine and Mookerjee (1975)	V	
	8.4×10^{-3}		Mackay and Leinonen (1975)	V	
	2.5×10^{-2}	5100	Wauchope and Haque (1972)	V	
	2.3×10^{-2}	5600	Wauchope and Haque (1972)	V	
	1.9×10^{-2}		Bohon and Claussen (1951)	V	
	1.1×10^{-2}	2100	Paasivirta et al. (1999)	T	
	2.1×10^{-2}		Mackay et al. (1979)	T	
	7.1×10^{-3}		Yaws (2003)	X	259
	2.1×10^{-2}	3600	Goldstein (1982)	X	299
	2.7×10^{-2}		McCarty (1980)	X	370
	2.0×10^{-2}		Smith et al. (1993)	C	
	2.0×10^{-2}		Ryan et al. (1988)	C	
	1.8×10^{-2}		Dupeux et al. (2022)	Q	260
	1.3×10^{-1}		Keshavarz et al. (2022)	Q	
	2.4×10^{-2}		Duchowicz et al. (2020)	Q	185
	1.8×10^{-2}		Parnis et al. (2015)	Q	371
	2.7×10^{-2}		Schröder et al. (2013)	Q	372
	1.5×10^{-2}		Schröder et al. (2010)	Q	365
	2.1×10^{-2}		Hilal et al. (2008)	Q	
	4.0×10^{-2}		Modarresi et al. (2007)	Q	68
		5200	Kühne et al. (2005)	Q	
	2.4×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.1×10^{-2}		English and Carroll (2001)	Q	231, 232
	3.3×10^{-4}		Katritzky et al. (1998)	Q	
	5.6×10^{-2}		Russell et al. (1992)	Q	280
	4.3×10^{-2}		Suzuki et al. (1992)	Q	233
	3.2×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	3.4×10^{-2}		Arbuckle (1983)	Q	
	2.2×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	3.6×10^{-2}		MacBean (2012a)	?	
		5400	Kühne et al. (2005)	?	
	8.0×10^{-3}		Yaws and Yang (1992)	?	21
	2.3×10^{-2}		Abraham et al. (1990)	?	
naphthalene-d8 $C_{10}D_8$ [1146-65-2] UFWIBTONFRDIAS-PGRXLJNUSA-N	3.5×10^{-2}	5300	Hiatt (2013)	M	

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methylnaphthalene	2.0×10^{-2}	5800	Brockbank (2013)	L	
$C_{10}H_7CH_3$	2.2×10^{-2}	6100	Fogg and Sangster (2003)	L	
[90-12-0]	2.2×10^{-2}		Mackay and Shiu (1981)	L	
QPUYECUOLPXSFR-UHFFFAOYSA-N	4.4×10^{-2}	5900	Hiatt (2013)	M	
	1.9×10^{-2}		Altschuh et al. (1999)	M	
	2.1×10^{-2}	6100	Bamford et al. (1999a)	M	
	4.1×10^{-2}		Shiu and Mackay (1997)	M	
	1.6×10^{-2}		Fendinger and Glotfelty (1990)	M	
	3.8×10^{-2}		Mackay and Shiu (1981)	M	
	2.8×10^{-2}	4900	Schwarz and Wasik (1977)	M	
	2.2×10^{-2}		Mackay et al. (2006a)	V	
	2.2×10^{-2}		Shiu and Ma (2000)	V	
	2.2×10^{-2}		Shiu and Mackay (1997)	V	
	2.5×10^{-2}		Abraham et al. (1994a)	V	
	2.5×10^{-2}		Eastcott et al. (1988)	V	
	2.2×10^{-2}		Cabani et al. (1981)	V	
	2.2×10^{-2}		Yaws (2003)	X	238
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	Q	
	1.6×10^{-2}		Parnis et al. (2015)	Q	371
	2.3×10^{-2}		Schröder et al. (2013)	Q	372
	1.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.8×10^{-2}		Hilal et al. (2008)	Q	
	3.0×10^{-2}		Modarresi et al. (2007)	Q	68
		5500	Kühne et al. (2005)	Q	
	3.8×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.5×10^{-2}		English and Carroll (2001)	Q	231, 261
	1.2×10^{-3}		Katritzky et al. (1998)	Q	
	2.3×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		5700	Kühne et al. (2005)	?	
	2.2×10^{-2}		Yaws (1999)	?	21
	2.7×10^{-2}		Yaws and Yang (1992)	?	21
1-methylnaphthalene-d10	4.6×10^{-2}	5400	Hiatt (2013)	M	
$C_{10}D_7CD_3$					
[38072-94-5]					
QPUYECUOLPXSFR-UZHHFJDZSA-N					
2-methylnaphthalene	2.0×10^{-2}	5100	Brockbank (2013)	L	
$C_{10}H_7CH_3$	1.8×10^{-2}	5600	Fogg and Sangster (2003)	L	
[91-57-6]	3.5×10^{-2}	5500	Hiatt (2013)	M	
QIMMUPPBPVKWKM-UHFFFAOYSA-N	1.6×10^{-2}		Altschuh et al. (1999)	M	
	1.9×10^{-2}	5400	Bamford et al. (1999a)	M	
	2.2×10^{-2}		De Maagd et al. (1998)	M	12
	5.0×10^{-5}	1200	Hansen et al. (1993)	M	282
	3.1×10^{-2}		Fendinger and Glotfelty (1990)	M	

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.0×10^{-2}		Mackay et al. (2006a)	V	
	2.6×10^{-2}		De Maagd et al. (1998)	V	12
	2.0×10^{-2}		Shiu and Mackay (1997)	V	
	2.4×10^{-2}		Meylan and Howard (1991)	V	
	2.0×10^{-2}		Eastcott et al. (1988)	V	
	2.4×10^{-2}		Mackay and Shiu (1981)	V	
	2.0×10^{-2}		Mackay et al. (1992b)	X	366
	2.3×10^{-2}		Yaws (2003)	X	238
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	Q	
	1.6×10^{-2}		Parnis et al. (2015)	Q	371
	2.2×10^{-2}		Schröder et al. (2013)	Q	372
	1.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.6×10^{-2}		Hilal et al. (2008)	Q	
	2.4×10^{-2}		Modarresi et al. (2007)	Q	68
		5500	Kühne et al. (2005)	Q	
	2.4×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.2×10^{-3}		Katritzky et al. (1998)	Q	
	1.7×10^{-2}		Meylan and Howard (1991)	Q	
	1.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		5700	Kühne et al. (2005)	?	
	2.3×10^{-2}		Yaws (1999)	?	21
	2.0×10^{-2}		Yaws and Yang (1992)	?	21
			Shiu and Ma (2000)	W	362
1-ethylnaphthalene	2.0×10^{-2}	5900	Brockbank (2013)	L	
$C_{10}H_7C_2H_5$	2.6×10^{-2}		Mackay and Shiu (1981)	L	
[1127-76-0]	1.4×10^{-2}		Altschuh et al. (1999)	M	
ZMXIYERNXPIYFR-UHFFFAOYSA-N	2.2×10^{-2}	4800	Schwarz and Wasik (1977)	M	
	2.6×10^{-2}		Mackay et al. (2006a)	V	
	2.7×10^{-2}		Eastcott et al. (1988)	V	
	2.3×10^{-2}		Cabani et al. (1981)	V	
	2.6×10^{-2}		Mackay et al. (1992b)	X	366
	2.0×10^{-2}		Yaws (2003)	X	238
	2.2×10^{-2}		Keshavarz et al. (2022)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	Q	185
	1.9×10^{-2}		Schröder et al. (2013)	Q	372
	1.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.8×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	68
	4.8×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	9.5×10^{-3}		English and Carroll (2001)	Q	231, 232
	2.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.4×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	2.0×10^{-2}		Yaws (1999)	?	21
	2.7×10^{-2}		Yaws and Yang (1992)	?	21

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-ethylnaphthalene	1.2×10^{-2}		Mackay and Shiu (1981)	L	
$C_{10}H_7C_2H_5$	1.8×10^{-2}		Altschuh et al. (1999)	M	
[939-27-5]	1.3×10^{-2}		Mackay et al. (2006a)	V	
RJTJVVYSTUQWNI-UHFFFAOYSA-N	1.6×10^{-2}		Eastcott et al. (1988)	V	
	1.3×10^{-2}		Mackay et al. (1992b)	X	366
	8.8×10^{-3}		Yaws (2003)	X	238
	2.2×10^{-2}		Keshavarz et al. (2022)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	Q	300
	1.9×10^{-2}		Schröder et al. (2013)	Q	372
	3.6×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
	1.9×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	68
	1.2×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.8×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	1.6×10^{-2}		Yaws and Yang (1992)	?	21
1,2,3,4-tetrahydronaphthalene	6.4×10^{-3}	5300	Plyasunov and Shock (2000)	L	
$C_{10}H_{12}$	5.1×10^{-3}	5400	Ashworth et al. (1988)	M	279
(tetralin)	7.3×10^{-3}		Duchowicz et al. (2020)	V	187
[119-64-2]	2.1×10^{-3}		Mackay et al. (1993)	V	
CXWXQJXEFPUFDZ-UHFFFAOYSA-N	5.8×10^{-3}		Yaws (2003)	X	238, 298
	1.2×10^{-2}		Duchowicz et al. (2020)	Q	
	5.8×10^{-3}		HSDB (2015)	Q	100
	3.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	4.3×10^{-3}		Modarresi et al. (2007)	Q	68
		4900	Kühne et al. (2005)	Q	
		5300	Kühne et al. (2005)	?	
	7.2×10^{-3}		Yaws (1999)	?	21, 298
1,2-dimethylnaphthalene	4.8×10^{-2}		Yaws (2003)	X	259
$C_{12}H_{12}$	4.8×10^{-2}		Yaws (2003)	X	238
[573-98-8]	2.6×10^{-2}		Dupeux et al. (2022)	Q	260
QNLZIZAQLLYXTC-UHFFFAOYSA-N	4.2×10^{-2}		Schröder et al. (2013)	Q	372
	1.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
1,3-dimethylnaphthalene	1.7×10^{-2}		Duchowicz et al. (2020)	V	187
$C_{12}H_{12}$	2.6×10^{-2}		Cabani et al. (1981)	V	
[575-41-7]	6.1×10^{-3}		Duchowicz et al. (2020)	Q	
QHJMFSMPSZREIF-UHFFFAOYSA-N	2.0×10^{-2}		Schröder et al. (2013)	Q	372
	2.8×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.9×10^{-2}		Hilal et al. (2008)	Q	
	4.6×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	1.1×10^{-2}		English and Carroll (2001)	Q	231, 232
	1.9×10^{-1}		Nirmalakhandan et al. (1997)	Q	

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.4×10^{-2}		Yaws and Yang (1992)	?	21
1,4-dimethylnaphthalene $C_{12}H_{12}$ [571-58-4] APQSQLNWAIULLK-UHFFFAOYSA-N	2.6×10^{-2}		Duchowicz et al. (2020)	V	187
	3.2×10^{-2}		Mackay et al. (2006a)	V	
	4.7×10^{-2}		Cabani et al. (1981)	V	
	6.1×10^{-3}		Duchowicz et al. (2020)	Q	
	2.0×10^{-2}		Schröder et al. (2013)	Q	372
	2.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.4×10^{-2}		Hilal et al. (2008)	Q	
	3.7×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	1.9×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.3×10^{-2}		Maniere et al. (2011)	?	166
	2.0×10^{-2}		Yaws and Yang (1992)	?	21
1,5-dimethylnaphthalene $C_{12}H_{12}$ [571-61-9] SDDBCEWUYXVGCQ-UHFFFAOYSA-N	2.8×10^{-2}		Shiu and Mackay (1997)	M	
	1.3×10^{-2}		Yaws (2003)	X	238
	2.2×10^{-2}		Keshavarz et al. (2022)	Q	
	6.1×10^{-3}		Duchowicz et al. (2020)	Q	185
	1.4×10^{-2}		Parnis et al. (2015)	Q	371
	2.1×10^{-2}		Schröder et al. (2013)	Q	372
	2.7×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
	3.3×10^{-2}		Hilal et al. (2008)	Q	
	2.4×10^{-2}		Modarresi et al. (2007)	Q	68
	2.9×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.1×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	2.8×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	1.6×10^{-2}		Yaws and Yang (1992)	?	21
1,6-dimethylnaphthalene $C_{12}H_{12}$ [575-43-9] CBMXCNPQDUJNHT-UHFFFAOYSA-N	2.3×10^{-2}		HSDB (2015)	Q	100
	3.8×10^{-2}		Schröder et al. (2013)	Q	372
1,7-dimethylnaphthalene $C_{12}H_{12}$ [575-37-1] SPUWFVKLHHEKGV-UHFFFAOYSA-N	3.9×10^{-2}		Ebert et al. (2023)	?	373
1,8-dimethylnaphthalene $C_{12}H_{12}$ [569-41-5] XAABPYINPXYOLM-UHFFFAOYSA-N	2.6×10^{-2}		Schröder et al. (2013)	Q	372

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-dimethylnaphthalene	1.6×10^{-2}		Mackay et al. (2006a)	V	
$C_{12}H_{12}$	6.4×10^{-2}		Eastcott et al. (1988)	V	
[581-40-8]	4.4×10^{-2}		Cabani et al. (1981)	V	
WWGUMAYGTYQSGA-UHFFFAOYSA-N	1.3×10^{-2}		Yaws (2003)	X	238
	1.1×10^{-2}		Meylan and Howard (1991)	C	
	2.2×10^{-2}		Keshavarz et al. (2022)	Q	
	6.1×10^{-3}		Duchowicz et al. (2020)	Q	300
	2.5×10^{-2}		Schröder et al. (2013)	Q	372
	3.0×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
	3.6×10^{-2}		Hilal et al. (2008)	Q	
	2.0×10^{-2}		Modarresi et al. (2007)	Q	68
	4.6×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.3×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.5×10^{-2}		Meylan and Howard (1991)	Q	
	1.1×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	1.7×10^{-2}		Yaws and Yang (1992)	?	21
2,6-dimethylnaphthalene	7.8×10^{-3}		Mackay et al. (2006a)	V	
$C_{12}H_{12}$	6.2×10^{-2}		Eastcott et al. (1988)	V	
[581-42-0]	3.4×10^{-2}		Cabani et al. (1981)	V	
YGYNBBAUIYTWBF-UHFFFAOYSA-N	2.0×10^{-2}		Schröder et al. (2013)	Q	372
	2.8×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.2×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	68
	3.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.9×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	8.2×10^{-3}		Yaws and Yang (1992)	?	21
2,7-dimethylnaphthalene	2.1×10^{-2}		Schröder et al. (2013)	Q	372
$C_{12}H_{12}$					
[582-16-1]					
LRQYSMQNJLZKPS-UHFFFAOYSA-N					
acenaphthene	5.4×10^{-2}	6500	Schwardt et al. (2021)	L	1
$C_{12}H_{10}$	7.2×10^{-2}	5400	Brockbank (2013)	L	
[83-32-9]	7.2×10^{-2}		Ma et al. (2010b)	L	368
CWRYPZZKDGJXCA-UHFFFAOYSA-N	7.0×10^{-2}		Ma et al. (2010b)	L	369
	5.5×10^{-2}	6500	Fogg and Sangster (2003)	L	
	4.2×10^{-2}		Mackay and Shiu (1981)	L	
	2.6×10^{-1}		Lee et al. (2012)	M	
	5.4×10^{-2}	6600	Bamford et al. (1999a)	M	
	6.2×10^{-2}		Shiu and Mackay (1997)	M	
	1.1×10^{-1}		Zhang and Pawliszyn (1993)	M	
	1.6×10^{-1}		Fendinger and Glotfelty (1990)	M	
	6.4×10^{-3}		Mackay and Shiu (1981)	M	
	4.1×10^{-2}		Warner et al. (1980)	M	

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.8×10^{-2}		Mackay et al. (1979)	M	
	8.2×10^{-2}		Mackay et al. (2006a)	V	
	8.2×10^{-2}		Shiu and Ma (2000)	V	
	8.2×10^{-2}		Shiu and Mackay (1997)	V	
	1.2×10^{-2}		Hwang et al. (1992)	V	
	9.5×10^{-2}		Eastcott et al. (1988)	V	
	8.2×10^{-2}		Cabani et al. (1981)	V	
	1.2×10^{-1}		Hine and Mookerjee (1975)	V	
	1.2×10^{-1}	6000	Wauchope and Haque (1972)	V	
	3.4×10^{-2}	2900	Paasivirta et al. (1999)	T	
	4.1×10^{-2}	2800	Goldstein (1982)	X	299
	5.2×10^{-2}		McCarty (1980)	X	370
	6.4×10^{-2}		HSDB (2015)	C	
	4.1×10^{-2}		Smith et al. (1993)	C	
	4.0×10^{-2}		Ryan et al. (1988)	C	
	4.1×10^{-2}		Shen (1982)	C	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	4.8×10^{-2}		Duchowicz et al. (2020)	Q	
	9.2×10^{-2}		Abraham et al. (2019)	Q	
	3.4×10^{-2}		Parnis et al. (2015)	Q	371
	9.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.9×10^{-2}		Schröder et al. (2010)	Q	365
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	4.4×10^{-2}		Modarresi et al. (2007)	Q	68
		5500	Kühne et al. (2005)	Q	
	6.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	9.9×10^{-2}		Suzuki et al. (1992)	Q	233
	1.1×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	7.9×10^{-2}		Arbuckle (1983)	Q	
	5.4×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		6600	Kühne et al. (2005)	?	
acenaphthylene $C_{12}H_8$ [208-96-8] HXGDTGSAIMULJN-UHFFFAOYSA-N	8.5×10^{-2}	6300	Brockbank (2013)	L	
	8.2×10^{-2}		Ma et al. (2010b)	L	368
	1.0×10^{-1}		Ma et al. (2010b)	L	369
	9.1×10^{-2}	6700	Fogg and Sangster (2003)	L	
	7.9×10^{-2}	6600	Bamford et al. (1999a)	M	
	8.8×10^{-2}		Fendinger and Glotfelty (1990)	M	
	8.7×10^{-2}		Warner et al. (1980)	M	
	8.7×10^{-1}		HSDB (2015)	V	
	1.2×10^{-1}		Mackay et al. (2006a)	V	
	1.2×10^{-1}		Shiu and Mackay (1997)	V	
	1.2×10^{-1}	5000	Paasivirta et al. (1999)	T	
	8.7×10^{-2}		Smith et al. (1993)	C	
	8.4×10^{-2}		Ryan et al. (1988)	C	
	8.7×10^{-2}		Shen (1982)	C	

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	5.7×10^{-2}		Duchowicz et al. (2020)	Q	185
	6.2×10^{-2}		Parnis et al. (2015)	Q	371
	1.1×10^{-1}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	68
		5600	Kühne et al. (2005)	Q	
	8.6×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	8.7×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		6600	Kühne et al. (2005)	?	
			Shiu and Ma (2000)	W	362
1,2,4-trimethylnaphthalene $C_{13}H_{14}$ [2717-42-2] JCNGSJUYPCVGAM-UHFFFAOYSA-N	1.3×10^{-2}		Parnis et al. (2015)	Q	371
1,3,7-trimethylnaphthalene $C_{13}H_{14}$ [2131-38-6] HXDVFWJRDVUZFT-UHFFFAOYSA-N	6.0×10^{-2}		Ebert et al. (2023)	?	373
1,3,8-trimethylnaphthalene $C_{13}H_{14}$ [17057-91-9] XYTKCJHHXQVFCK-UHFFFAOYSA-N	6.7×10^{-2}		Ebert et al. (2023)	?	373
1,4,5-trimethylnaphthalene $C_{13}H_{14}$ [2131-41-1] FSAWRQYDMHSDRN-UHFFFAOYSA-N	1.8×10^{-2}		Mackay et al. (2006a)	V	
	4.3×10^{-2}		Eastcott et al. (1988)	V	
	2.3×10^{-2}		Schröder et al. (2013)	Q	372
1,4,6-trimethylnaphthalene $C_{13}H_{14}$ [2131-42-2] VGKRZAKNKJAKDN-UHFFFAOYSA-N	4.3×10^{-2}		Ebert et al. (2023)	?	373
2,3,6-trimethylnaphthalene $C_{13}H_{14}$ [829-26-5] UNBZRJCHIWTUHB-UHFFFAOYSA-N	2.8×10^{-2}		Ebert et al. (2023)	?	373
1-(1-methylethyl)naphthalene $C_{13}H_{14}$ (1-isopropylnaphthalene) [6158-45-8] PMPBFICDXLLSRM-UHFFFAOYSA-N	3.3×10^{-2}		Schröder et al. (2013)	Q	372

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-(1-methylethyl)naphthalene	1.2×10^{-2}		HSDB (2015)	Q	100
$C_{13}H_{14}$	3.1×10^{-2}		Schröder et al. (2013)	Q	372
(2-isopropylnaphthalene)					
[2027-17-0]					
TVYVQNHYIHAJTD-UHFFFAOYSA-N					
2-ethyl-6-methylnaphthalene	1.2×10^{-2}		Parnis et al. (2015)	Q	371
$C_{13}H_{14}$					
[7372-86-3]					
ZOYUJOHRFWIQTH-UHFFFAOYSA-N					
2,3-benzindene	1.3×10^{-1}	6100	Brockbank (2013)	L	
$C_{13}H_{10}$	1.1×10^{-1}		Ma et al. (2010b)	L	368
(fluorene)	1.1×10^{-1}		Ma et al. (2010b)	L	369
[86-73-7]	1.1×10^{-1}	6000	Fogg and Sangster (2003)	L	
NIHNNTQXNPWCJQ-UHFFFAOYSA-N	1.2×10^{-1}		Mackay and Shiu (1981)	L	
	3.2×10^{-1}		Lee et al. (2012)	M	
	1.0×10^{-1}	6200	Bamford et al. (1999a)	M	
	7.9×10^{-2}	7400	Bamford et al. (1999b)	M	
	1.5×10^{-1}		De Maagd et al. (1998)	M	12
	1.0×10^{-1}		Shiu and Mackay (1997)	M	
	1.6×10^{-1}		Fendinger and Glotfelty (1990)	M	
	9.9×10^{-2}		Mackay and Shiu (1981)	M	
	8.4×10^{-2}		Warner et al. (1980)	M	
	1.3×10^{-1}		Mackay et al. (2006a)	V	
	1.3×10^{-1}		Shiu and Ma (2000)	V	
	1.7×10^{-1}		De Maagd et al. (1998)	V	12
	1.3×10^{-1}		Shiu and Mackay (1997)	V	
	1.5×10^{-2}		Hwang et al. (1992)	V	
	1.1×10^{-1}		Eastcott et al. (1988)	V	
	1.3×10^{-1}		Cabani et al. (1981)	V	
	1.3×10^{-1}	6400	Wauchope and Haque (1972)	V	
	2.3×10^{-2}	3700	Paasivirta et al. (1999)	T	
	8.4×10^{-2}	3000	Goldstein (1982)	X	299
	4.7×10^{-2}		McCarty (1980)	X	370
	9.9×10^{-2}		HSDB (2015)	C	
	8.4×10^{-2}		Smith et al. (1993)	C	
	8.4×10^{-2}		Ryan et al. (1988)	C	
	8.4×10^{-2}		Shen (1982)	C	
	3.2×10^{-1}		Keshavarz et al. (2022)	Q	
	5.7×10^{-2}		Duchowicz et al. (2020)	Q	300
	1.1×10^{-1}		Abraham et al. (2019)	Q	
	1.0×10^{-1}		Parnis et al. (2015)	Q	371
	9.0×10^{-2}		Schröder et al. (2010)	Q	365
	9.2×10^{-2}		Hilal et al. (2008)	Q	
	4.1×10^{-2}		Modarresi et al. (2007)	Q	68
		5100	Kühne et al. (2005)	Q	

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	5.4×10^{-2}		English and Carroll (2001)	Q	231, 275
	2.0×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		5400	Kühne et al. (2005)	?	
	1.2×10^{-1}		Abraham et al. (1990)	?	
1-methyl-9H-fluorene $C_{14}H_{12}$ [1730-37-6] GKEUODMJRFDLJY-UHFFFAOYSA-N	1.5×10^{-1}		Duchowicz et al. (2020)	V	187
	2.9×10^{-2}		Duchowicz et al. (2020)	Q	
2-methyl-9H-fluorene $C_{14}H_{12}$ [1430-97-3] RKJHJMAZNPASHY-UHFFFAOYSA-N	8.6×10^{-2}		Parnis et al. (2015)	Q	371
9-methyl-9H-fluorene $C_{14}H_{12}$ [2523-37-7] ZVEJRZRAUYJYCO-UHFFFAOYSA-N	9.1×10^{-2}		Parnis et al. (2015)	Q	371
1,2,5,6-tetramethylnaphthalene $C_{14}H_{16}$ [2131-43-3] ONIJFQFZCKJNDH-UHFFFAOYSA-N	1.3×10^{-2}		Parnis et al. (2015)	Q	371
1,4,6,7-tetramethylnaphthalene $C_{14}H_{16}$ [13764-18-6] VPSPONOBLZCLIU-UHFFFAOYSA-N	8.6×10^{-2}		Ebert et al. (2023)	?	373
1-methyl-7-(1-methylethyl)-naphthalene $C_{14}H_{16}$ [490-65-3] UZVVHZJKXPCUQU-UHFFFAOYSA-N	1.2×10^{-2}		Parnis et al. (2015)	Q	371
(*E*)-stilbene $C_{14}H_{12}$ (*trans*-1,2-diphenylethene) [103-30-0] PJANXHGTPQOBST-VAWYXSNFSA-N	1.4×10^{-2}		Duchowicz et al. (2020)	V	187
	1.4×10^{-2}		HSDB (2015)	V	
	2.5×10^{-2}		Mackay et al. (2006a)	V	
	2.5×10^{-2}		Mackay et al. (1992b)	X	366
	2.5×10^{-2}		Duchowicz et al. (2020)	Q	
	1.1×10^{-1}		Abraham et al. (2019)	Q	

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
phenanthrene	2.1×10^{-1}	4500	Schwardt et al. (2021)	L	1
$C_{14}H_{10}$	3.4×10^{-1}	7100	Brockbank (2013)	L	1
[85-01-8]	2.3×10^{-1}		Ma et al. (2010b)	L	368
YNPNZTXNASCQKK-UHFFFAOYSA-N	2.3×10^{-1}		Ma et al. (2010b)	L	369
	2.3×10^{-1}	4200	Fogg and Sangster (2003)	L	
	2.5×10^{-1}		Mackay and Shiu (1981)	L	
	1.8×10^{-1}		Lee et al. (2012)	M	
	2.7×10^{-1}	7700	Odabasi et al. (2006)	M	
	2.3×10^{-1}	6000	Bamford et al. (1999a)	M	
	1.6×10^{-1}	7600	Bamford et al. (1999b)	M	
	3.4×10^{-1}		De Maagd et al. (1998)	M	12
	2.8×10^{-1}		Shiu and Mackay (1997)	M	
	2.1×10^{-1}	3800	Alaee et al. (1996)	M	
	2.5×10^{-1}		Zhang and Pawliszyn (1993)	M	
	4.2×10^{-1}		Fendinger and Glotfelty (1990)	M	
	2.7×10^{-1}		Mackay and Shiu (1981)	M	
	2.5×10^{-1}		Mackay et al. (1979)	M	
	1.8×10^{-1}		Southworth (1979)	M	
	3.1×10^{-1}		Mackay et al. (2006a)	V	
	3.1×10^{-1}		Shiu and Ma (2000)	V	
	3.8×10^{-1}		De Maagd et al. (1998)	V	12
	3.1×10^{-1}		Shiu and Mackay (1997)	V	
	3.2×10^{-2}		Hwang et al. (1992)	V	
	2.8×10^{-1}		Eastcott et al. (1988)	V	
	3.2×10^{-1}		Cabani et al. (1981)	V	
	2.0×10^{-1}		Southworth (1979)	V	
	3.9×10^{-1}		Hine and Mookerjee (1975)	V	
	2.8×10^{-1}	6500	Wauchope and Haque (1972)	V	
	9.3×10^{-2}	4900	Paasivirta et al. (1999)	T	
	9.0×10^{-2}		Yaws (2003)	X	259
	9.0×10^{-2}		Yaws (2003)	X	238
	9.3×10^{-2}	4700	Goldstein (1982)	X	299
	7.6×10^{-2}		McCarty (1980)	X	370
	2.5×10^{-1}		Smith et al. (1993)	C	295
	2.5×10^{-1}		Ryan et al. (1988)	C	
	2.5×10^{-1}		Dupeux et al. (2022)	Q	260
	4.3×10^{-1}		Keshavarz et al. (2022)	Q	
	9.2×10^{-2}		Duchowicz et al. (2020)	Q	185
	2.1×10^{-1}		Parnis et al. (2015)	Q	371
	7.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
	1.7×10^{-1}		Schröder et al. (2010)	Q	365
	2.6×10^{-1}		Hilal et al. (2008)	Q	
	6.4×10^{-1}		Modarresi et al. (2007)	Q	68
		4800	Kühne et al. (2005)	Q	
	2.5×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	9.2×10^{-1}		Suzuki et al. (1992)	Q	233

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.8×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	2.6×10^{-1}		Arbuckle (1983)	Q	
	2.3×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		5300	Kühne et al. (2005)	?	
	2.7×10^{-1}		Abraham et al. (1990)	?	
9,10-dihydrophenanthrene	1.2×10^{-1}	7500	Reza and Trejo (2004)	M	
$C_{14}H_{12}$	3.2×10^{-1}		Duchowicz et al. (2020)	V	187
[776-35-2]	5.8×10^{-2}		Duchowicz et al. (2020)	Q	
XXPBFNVKTVJZKF-UHFFFAOYSA-N	9.0×10^{-2}		Schröder et al. (2010)	Q	365
	4.1×10^{-2}		Hilal et al. (2008)	Q	
		5400	Kühne et al. (2005)	Q	
		7500	Kühne et al. (2005)	?	
anthracene	1.8×10^{-1}	4800	Schwardt et al. (2021)	L	1
$C_{14}H_{10}$	3.3×10^{-1}	6700	Brockbank (2013)	L	1
[120-12-7]	2.0×10^{-1}		Ma et al. (2010b)	L	368
MWPLVEDNUUSJAV-UHFFFAOYSA-N	2.0×10^{-1}		Ma et al. (2010b)	L	369
	1.7×10^{-1}	5700	Fogg and Sangster (2003)	L	
	1.7×10^{-1}		Mackay and Shiu (1981)	L	
	1.6×10^{-1}		Lee et al. (2012)	M	
	2.3×10^{-1}	5600	Reza and Trejo (2004)	M	
	1.8×10^{-1}	6000	Bamford et al. (1999a)	M	
	1.5×10^{-1}	6500	Bamford et al. (1999b)	M	
	1.3×10^{-1}		Shiu and Mackay (1997)	M	
	2.0×10^{-1}	3500	Alaee et al. (1996)	M	
	1.1×10^{-1}		Zhang and Pawliszyn (1993)	M	
	5.1×10^{-1}		Fendinger and Glotfelty (1990)	M	
	2.7×10^{-1}		Webster et al. (1985)	M	
	1.4×10^{-2}		Mackay and Shiu (1981)	M	
	1.5×10^{-1}		Southworth (1979)	M	
	2.5×10^{-1}		Mackay et al. (2006a)	V	
	2.5×10^{-1}		Shiu and Ma (2000)	V	
	2.5×10^{-1}		Shiu and Mackay (1997)	V	
	3.0×10^{-2}		Hwang et al. (1992)	V	
	6.1×10^{-1}		Eastcott et al. (1988)	V	
	5.1×10^{-1}		Cabani et al. (1981)	V	
	3.4×10^{-2}		Southworth (1979)	V	
	5.6×10^{-1}		Hine and Mookerjee (1975)	V	
	2.6×10^{1}	7000	Wauchope and Haque (1972)	V	
	4.6×10^{-3}	3100	Paasivirta et al. (1999)	T	
	3.5×10^{-1}	4000	Goldstein (1982)	X	299
	7.0×10^{-3}		McCarty (1980)	X	370
	1.1×10^{-1}		Smith et al. (1993)	C	
	3.7×10^{-2}		Ryan et al. (1988)	C	
	1.0×10^{-1}		Smith et al. (1981a)	C	
	4.3×10^{-1}		Keshavarz et al. (2022)	Q	

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.2×10^{-2}		Duchowicz et al. (2020)	Q	
	1.9×10^{-1}		Parnis et al. (2015)	Q	371
	1.5×10^{-1}		Schröder et al. (2010)	Q	365
	3.3×10^{-1}		Hilal et al. (2008)	Q	
	4.5×10^{-1}		Modarresi et al. (2007)	Q	68
		6400	Kühne et al. (2005)	Q	
	1.7×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	7.0×10^{-1}		Russell et al. (1992)	Q	280
	9.0×10^{-1}		Suzuki et al. (1992)	Q	233
	9.0×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.8×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		5100	Kühne et al. (2005)	?	
9,10-dihydroanthracene $C_{14}H_{12}$ [613-31-0] WPDAVTSOEQEGMS-UHFFFAOYSA-N	1.5×10^{-1}		Schröder et al. (2010)	Q	365
2,3-dihydro-1,1,3,3,5-pentamethyl-1H-indene	7.5×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_{20}$	1.9×10^{-3}		Zhang et al. (2010)	Q	288, 290
[81-03-8]	2.1×10^{-3}		Zhang et al. (2010)	Q	288, 291
NNXHDILUOAXSPU-UHFFFAOYSA-N	3.9×10^{-4}		Zhang et al. (2010)	Q	288, 292
1-methylanthracene $C_{15}H_{12}$ [610-48-0] KZNJSFHJUQDYHE-UHFFFAOYSA-N	1.7×10^{-1}		Parnis et al. (2015)	Q	371
2-methylanthracene	1.6×10^{-2}		Duchowicz et al. (2020)	V	187
$C_{15}H_{12}$	4.7×10^{-2}		Duchowicz et al. (2020)	Q	
[613-12-7] GYMFBYTZOGMSQJ-UHFFFAOYSA-N					
9-methylanthracene	2.5×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{15}H_{12}$	6.1×10^{-1}		Mackay et al. (2006a)	V	
[779-02-2]	9.4×10^{-3}		Eastcott et al. (1988)	V	
CPGPAVAKSZHMBP-UHFFFAOYSA-N	4.7×10^{-2}		Duchowicz et al. (2020)	Q	
	1.9×10^{-1}		Parnis et al. (2015)	Q	371
	4.2×10^{-1}		Hilal et al. (2008)	Q	
9-methyl-phenanthrene $C_{15}H_{12}$ [883-20-5] DALBHIYZSZZWBS-UHFFFAOYSA-N	1.9×10^{-1}		Parnis et al. (2015)	Q	371

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
9-ethylfluorene $C_{15}H_{14}$ [2294-82-8] QBBCCEYJCKGWIK-UHFFFAOYSA-N	7.4×10^{-2}		Parnis et al. (2015)	Q	371
1,7-dimethylfluorene $C_{15}H_{14}$ [442-66-0] NHPVHXMCRWRSNW-UHFFFAOYSA-N	9.1×10^{-2}		Parnis et al. (2015)	Q	371
1-methylphenanthrene $C_{15}H_{12}$ [832-69-9] DOWJXOHBNXRUOD-UHFFFAOYSA-N	2.0×10^{-1}	4600	Bamford et al. (1999a)	M	
	5.8×10^{-1}		Keshavarz et al. (2022)	Q	
	4.7×10^{-2}		Duchowicz et al. (2020)	Q	185
	1.9×10^{-1}		Parnis et al. (2015)	Q	371
	3.3×10^{-1}		Hilal et al. (2008)	Q	
	3.8×10^{-1}		Modarresi et al. (2007)	Q	68
		5200	Kühne et al. (2005)	Q	
	2.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		4600	Kühne et al. (2005)	?	
1,3-diisopropylnaphthalene $C_{16}H_{20}$ [57122-16-4] JDBFIFNXALGSOF-UHFFFAOYSA-N	1.6×10^{-2}		Schröder et al. (2013)	Q	372
1,5-diisopropylnaphthalene $C_{16}H_{20}$ [27351-96-8] GFZWCYSEPXDDRI-UHFFFAOYSA-N	1.6×10^{-2}		Schröder et al. (2013)	Q	372
1,7-diisopropylnaphthalene $C_{16}H_{20}$ [94133-80-9] XNSUVOOWWSAQMZ-UHFFFAOYSA-N	7.8×10^{-3}		Ebert et al. (2023)	?	319
2,6-diisopropylnaphthalene $C_{16}H_{20}$ [24157-81-1] GWLLTEXUIOFAFE-UHFFFAOYSA-N	1.3×10^{-2}		Schröder et al. (2013)	Q	372
2,7-diisopropylnaphthalene $C_{16}H_{20}$ [40458-98-8] YGDMAJYAQCDTNG-UHFFFAOYSA-N	1.3×10^{-2}		Schröder et al. (2013)	Q	372
2-ethylanthracene $C_{16}H_{14}$ [52251-71-5] ZXAGXLDEMUNQSH-UHFFFAOYSA-N	1.9×10^{-1}		Duchowicz et al. (2020)	V	187
	4.7×10^{-2}		Duchowicz et al. (2020)	Q	

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3-dimethylphenanthrene $C_{16}H_{14}$ [16664-45-2] UJUUQKOWULNFNG-UHFFFAOYSA-N	1.7×10^{-1}		Parnis et al. (2015)	Q	371
3,6-dimethylphenanthrene $C_{16}H_{14}$ [1576-67-6] OMIBPZBOAJFEJS-UHFFFAOYSA-N	1.8×10^{-1}		Parnis et al. (2015)	Q	371
2,3-dimethylanthracene $C_{16}H_{14}$ [613-06-9] OGVRJXPGSVLDRD-UHFFFAOYSA-N	2.1×10^{-1}		Parnis et al. (2015)	Q	371
9,10-dimethylanthracene	1.8		Mackay et al. (2006a)	V	
$C_{16}H_{14}$	3.4×10^{-1}		HSDB (2015)	Q	100
[781-43-1]	1.5×10^{-1}		Parnis et al. (2015)	Q	371
JTGMTYWYUZDRBK-UHFFFAOYSA-N					
9-propyl-9H-fluorene $C_{16}H_{16}$ [4037-45-0] ZTBWLZNGULENBG-UHFFFAOYSA-N	6.1×10^{-2}		Parnis et al. (2015)	Q	371
pyrene	5.9×10^{-1}	5500	Schwardt et al. (2021)	L	1
$C_{16}H_{10}$	1.1	6900	Brockbank (2013)	L	1
[129-00-0]	7.5×10^{-1}		Ma et al. (2010b)	L	368
BBEAQIROQSPTKN-UHFFFAOYSA-N	7.5×10^{-1}		Ma et al. (2010b)	L	369
	6.6×10^{-1}	4800	Fogg and Sangster (2003)	L	
	8.3×10^{-1}		Mackay and Shiu (1981)	L	
	4.1×10^{-1}		Lee et al. (2012)	M	
	8.5×10^{-1}	6300	Reza and Trejo (2004)	M	
	2.0		Altschuh et al. (1999)	M	
	5.9×10^{-1}	5500	Bamford et al. (1999a)	M	
	5.0×10^{-1}		De Maagd et al. (1998)	M	12
	1.1		De Maagd et al. (1998)	M	12
	8.3×10^{-1}		Shiu and Mackay (1997)	M	
	9.1×10^{-1}		Mackay and Shiu (1981)	M	
	5.3×10^{-1}		Southworth (1979)	M	
	1.1		Mackay et al. (2006a)	V	
	1.1		Shiu and Ma (2000)	V	
	1.4		De Maagd et al. (1998)	V	12
	1.1		Shiu and Mackay (1997)	V	
	3.6×10^{-2}		Hwang et al. (1992)	V	
	1.1		Eastcott et al. (1988)	V	
	7.6×10^{-1}		Cabani et al. (1981)	V	
	9.4×10^{-1}		Southworth (1979)	V	
	2.2	7600	Wauchope and Haque (1972)	V	

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.4×10^{-1}	5700	Paasivirta et al. (1999)	T	
	1.9		Smith et al. (1993)	C	374
	1.4×10^{-3}		Ryan et al. (1988)	C	
	7.6		Petrasek et al. (1983)	C	
	7.8×10^{-1}		Keshavarz et al. (2022)	Q	
	3.0×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.3		Abraham et al. (2019)	Q	
	4.7×10^{-1}		Parnis et al. (2015)	Q	371
	3.6×10^{-1}		Schröder et al. (2010)	Q	365
	2.3×10^{-1}		Hilal et al. (2008)	Q	
	2.3		Modarresi et al. (2007)	Q	68
		5200	Kühne et al. (2005)	Q	
	8.4×10^{-1}		English and Carroll (2001)	Q	231, 232
	5.4×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	8.3×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		5500	Kühne et al. (2005)	?	
	9.0×10^{-1}		Abraham et al. (1990)	?	
benzo[jk]fluorene	5.8×10^{-1}	5900	Schwardt et al. (2021)	L	1
$C_{16}H_{10}$	7.0×10^{-1}	6900	Brockbank (2013)	L	
(fluoranthene)	6.9×10^{-1}		Ma et al. (2010b)	L	368
[206-44-0]	7.5×10^{-1}		Ma et al. (2010b)	L	369
GVEPBJHOBDJJJI-UHFFFAOYSA-N	5.4×10^{-1}	4800	Fogg and Sangster (2003)	L	
	4.5×10^{-3}		Mackay and Shiu (1981)	L	
	3.4×10^{-1}		Lee et al. (2012)	M	
	5.1×10^{-1}	4900	Bamford et al. (1999a)	M	
	9.1×10^{-1}		De Maagd et al. (1998)	M	12
	1.1	6900	ten Hulscher et al. (1992)	M	
	1.9	8700	Abou-Naccoul et al. (2014)	V	
	1.0		Mackay et al. (2006a)	V	
	1.0		Shiu and Ma (2000)	V	
	1.4		De Maagd et al. (1998)	V	12
	1.0		Shiu and Mackay (1997)	V	
	2.1		McLachlan et al. (1990)	V	375
	1.1		Eastcott et al. (1988)	V	
	4.0×10^{-1}	5400	Paasivirta et al. (1999)	T	
	1.5		Smith et al. (1993)	C	
	1.0		Ryan et al. (1988)	C	
	9.9×10^{-1}		Petrasek et al. (1983)	C	
	7.8×10^{-1}		Keshavarz et al. (2022)	Q	
	3.0×10^{-1}		Duchowicz et al. (2020)	Q	
	1.1		Abraham et al. (2019)	Q	
	5.8×10^{-1}		Parnis et al. (2015)	Q	371
	4.6×10^{-1}		Schröder et al. (2010)	Q	365
	4.4×10^{-1}		Hilal et al. (2008)	Q	
	2.2×10^{-1}		Modarresi et al. (2007)	Q	68
		5100	Kühne et al. (2005)	Q	

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1		Duchowicz et al. (2020)	?	186, 21
		5000	Kühne et al. (2005)	?	
1,2,3,4-tetrahydro-1,1,3,4,4,6-hexamethylnaphthalene	4.2×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_{24}$	1.3×10^{-3}		Zhang et al. (2010)	Q	288, 290
[2084-69-7]	3.2×10^{-3}		Zhang et al. (2010)	Q	288, 291
JIVANURAWUCQIG-UHFFFAOYSA-N	2.7×10^{-4}		Zhang et al. (2010)	Q	288, 292
[2.2]paracyclophane	2.9×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_{16}$	8.4×10^{-2}		Zhang et al. (2010)	Q	288, 290
[1633-22-3]	9.5×10^{-1}		Zhang et al. (2010)	Q	288, 291
OOLUVSIJOMLOCB-UHFFFAOYSA-N	4.3×10^{-2}		Zhang et al. (2010)	Q	288, 292
benzo[*a*]fluorene	3.7×10^{-1}	4400	Bamford et al. (1999a)	M	
$C_{17}H_{12}$	1.1		Keshavarz et al. (2022)	Q	
[238-84-6]	2.2×10^{-1}		Duchowicz et al. (2020)	Q	185
HKMTVMBEALTRRR-UHFFFAOYSA-N	4.6×10^{-1}		Modarresi et al. (2007)	Q	68
		6300	Kühne et al. (2005)	Q	
	3.7×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		4400	Kühne et al. (2005)	?	
			Shiu and Ma (2000)	W	362
1-methylpyrene	3.1		HSDB (2015)	Q	100
$C_{17}H_{12}$	4.5×10^{-1}		Parnis et al. (2015)	Q	371
[2381-21-7]					
KBSPJIWZDWBDGM-UHFFFAOYSA-N					
2-methylpyrene	3.1		HSDB (2015)	Q	100
$C_{17}H_{12}$					
[3442-78-2]					
VIRFPLJXRDHVEI-UHFFFAOYSA-N					
2-methylfluoranthene	5.4×10^{-1}		Parnis et al. (2015)	Q	371
$C_{17}H_{12}$					
[30997-39-8]					
VVRCMNWZFPMXQZ-UHFFFAOYSA-N					
9-n-propylphenanthrene	1.3×10^{-1}		Parnis et al. (2015)	Q	371
$C_{17}H_{16}$					
[17024-03-2]					
PIWHTUVAMGYSIC-UHFFFAOYSA-N					
1,2,6-trimethylphenanthrene	1.8×10^{-1}		Parnis et al. (2015)	Q	371
$C_{17}H_{16}$					
[30436-55-6]					
MYWOJODOMFBVCB-UHFFFAOYSA-N					

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
9-butyl-9H-fluorene $C_{17}H_{18}$ [3952-42-9] RBDADLSAYYPJAN-UHFFFAOYSA-N	5.1×10^{-2}		Parnis et al. (2015)	Q	371
11H-benzo[*b*]fluorene $C_{17}H_{12}$ [243-17-4] HAPOJKSPCGLOOD-UHFFFAOYSA-N	2.5 2.2×10^{-1}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
2,7-dimethylpyrene $C_{18}H_{14}$ [15679-24-0] GSKHIRFMTJUBSM-UHFFFAOYSA-N	2.9 3.9×10^{-1}		HSDB (2015) Parnis et al. (2015)	Q Q	100 371
chrysene $C_{18}H_{12}$ [218-01-9] WDECIBYCCFPHNR-UHFFFAOYSA-N	1.5×10^{1} 2.3 2.7 2.1 1.9 9.4 1.0×10^{1} 1.5×10^{1} 1.5×10^{1} 2.2 2.0×10^{-1} 9.4 4.6×10^{-3} 6.6 1.4 3.6×10^{-1} 2.4 2.0 3.6 5.0 1.9	12000 13000 6400 	Brockbank (2013) Ma et al. (2010b) Ma et al. (2010b) Lee et al. (2012) Bamford et al. (1999a) Zhang and Pawliszyn (1993) HSDB (2015) Mackay et al. (2006a) Shiu and Ma (2000) Eastcott et al. (1988) Paasivirta et al. (1999) Smith et al. (1993) Ryan et al. (1988) Petrasek et al. (1983) Keshavarz et al. (2022) Duchowicz et al. (2020) Parnis et al. (2015) Schröder et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Duchowicz et al. (2020)	L L L M M M V V V V T C C C Q Q Q Q Q Q ?	 368 369 300 371 365 68 186, 21
naphthacene $C_{18}H_{12}$ (2,3-benzanthracene) [92-24-0] IFLREYGFSNHWGE-UHFFFAOYSA-N	2.0×10^{1} 3.6×10^{2} 2.5×10^{2} 3.6×10^{-1} 4.2		Duchowicz et al. (2020) Mackay et al. (2006a) Mackay et al. (1992b) Duchowicz et al. (2020) Ferreira (2001)	V V X Q Q	187 366 12

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
triphenylene	6.4×10^{1}		Duchowicz et al. (2020)	V	187
$C_{18}H_{12}$			Mackay et al. (2006a)	V	293
(benzo[*l*]phenanthrene)	1.0×10^{2}		Mackay et al. (1992b)	X	366
[217-59-4]	3.6×10^{-1}		Duchowicz et al. (2020)	Q	
SLGBZMMZGDRARJ-UHFFFAOYSA-N	8.6		Schröder et al. (2010)	Q	365
	2.9		Hilal et al. (2008)	Q	
	4.7		Modarresi et al. (2007)	Q	68
	3.1		Ferreira (2001)	Q	12
benz[*a*]anthracene	1.4		Ma et al. (2010b)	L	368
$C_{18}H_{12}$	1.6		Ma et al. (2010b)	L	369
[56-55-3]	9.0×10^{-1}	7900	Fogg and Sangster (2003)	L	
DXBHBZVCASKNBY-UHFFFAOYSA-N	1.7		Lee et al. (2012)	M	
	8.2×10^{-1}	8300	Bamford et al. (1999a)	M	
	9.9		Zhang and Pawliszyn (1993)	M	
	1.2		Southworth (1979)	M	
	1.7		Mackay et al. (2006a)	V	
	2.4		Eastcott et al. (1988)	V	
	7.5×10^{1}		Smith and Bomberger (1980)	V	24
	4.0		Southworth (1979)	V	
	1.5×10^{-1}	6100	Paasivirta et al. (1999)	T	
	8.5		Smith et al. (1993)	C	80
	9.8		Ryan et al. (1988)	C	
	8.2×10^{1}		Petrasek et al. (1983)	C	
	1.4		Keshavarz et al. (2022)	Q	
	3.6×10^{-1}		Duchowicz et al. (2020)	Q	
	2.2		Parnis et al. (2015)	Q	371
	1.6		Schröder et al. (2010)	Q	365
	4.4		Hilal et al. (2008)	Q	
	5.0		Modarresi et al. (2007)	Q	68
		6100	Kühne et al. (2005)	Q	
	5.6		Ferreira (2001)	Q	12
	8.2×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		8300	Kühne et al. (2005)	?	
			Shiu and Ma (2000)	W	362
4,5-dimethylpyrene	4.5×10^{-1}		Parnis et al. (2015)	Q	371
$C_{18}H_{14}$					
[15679-25-1]					
MCZKPUHBCIHFBZ-UHFFFAOYSA-N					
3-ethylfluoranthene	4.8×10^{-1}		Parnis et al. (2015)	Q	371
$C_{18}H_{14}$					
[20496-16-6]					
JXUOLJXLPIIRTP-UHFFFAOYSA-N					

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,6,9-tetramethylphenanthrene $C_{18}H_{18}$ [204256-39-3] XFJWRZAPBOJONX-UHFFFAOYSA-N	1.6×10^{-1}		Parnis et al. (2015)	Q	371
1,9-dimethyl-5-ethylphenanthrene $C_{18}H_{18}$ MDZYWNWRMJIOPN-UHFFFAOYSA-N	1.0×10^{-1}		Parnis et al. (2015)	Q	371
1,9-dimethyl-7-ethylphenanthrene $C_{18}H_{18}$ NFFCDFHAMXFVEK-UHFFFAOYSA-N	1.4×10^{-1}		Parnis et al. (2015)	Q	371
1,2,3,4-tetrahydro-5-(1-phenylethyl)-naphthalene	1.6×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{18}H_{20}$	1.0×10^{-1}		Zhang et al. (2010)	Q	288, 290
[60466-61-7]	2.0×10^{-1}		Zhang et al. (2010)	Q	288, 291
TXOHWLOHKUPUKO-UHFFFAOYSA-N	2.9×10^{-2}		Zhang et al. (2010)	Q	288, 292
4-methylchrysene $C_{19}H_{14}$ [3351-30-2] BLVHWJCLSMYFMT-UHFFFAOYSA-N	1.9		Parnis et al. (2015)	Q	371
5-methylchrysene $C_{19}H_{14}$ [3697-24-3] GOHBXWHNJHENRX-UHFFFAOYSA-N	5.2		HSDB (2015)	Q	100
6-methylchrysene $C_{19}H_{14}$ [1705-85-7] ASVDRLYVNFOSCI-UHFFFAOYSA-N	2.2		Parnis et al. (2015)	Q	371
1-propylpyrene $C_{19}H_{16}$ [42211-33-6] HIOZPFGGCXEPAP-UHFFFAOYSA-N	3.2×10^{-1}		Parnis et al. (2015)	Q	371
7-methylbenz[*a*]anthracene $C_{19}H_{14}$ [2541-69-7] DIIFUCUPDHMNIV-UHFFFAOYSA-N	5.2		HSDB (2015)	Q	100
10-methylbenz[*a*]anthracene $C_{19}H_{14}$ [2381-15-9] WUMGYHICFXGLAB-UHFFFAOYSA-N	5.2		HSDB (2015)	Q	100

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
12-methylbenz[*a*]anthracene $C_{19}H_{14}$ [2422-79-9] ACYOLKMEHHTLAB-UHFFFAOYSA-N	5.2		HSDB (2015)	Q	100
6-ethylchrysene $C_{20}H_{16}$ [2732-58-3] ZJSYTTGSPQNXKT-UHFFFAOYSA-N	1.8		Parnis et al. (2015)	Q	371
3,9-dimethylbenz[*a*]anthracene $C_{20}H_{16}$ [316-51-8] DBPDWIZRMPUWRH-UHFFFAOYSA-N	1.9		Parnis et al. (2015)	Q	371
1-butylpyrene $C_{20}H_{18}$ [35980-18-8] UFOTZLIYHMGVAV-UHFFFAOYSA-N	2.8×10^{-1}		Parnis et al. (2015)	Q	371
7,12-dimethyl-benz[*a*]anthracene $C_{20}H_{16}$ [57-97-6] ARSRBNBHOADGJU-UHFFFAOYSA-N	2.6		Duchowicz et al. (2020)	V	187
	5.1×10^{3}		Mackay et al. (2006a)	V	
	9.2×10^{-2}		Duchowicz et al. (2020)	Q	
	4.9		HSDB (2015)	Q	100
	1.5		Parnis et al. (2015)	Q	371
9,10-dimethyl-benz[*a*]anthracene $C_{20}H_{16}$ [58429-99-5] GKVUDAZMZLMNJQ-UHFFFAOYSA-N			Mackay et al. (2006a)	V	293
benzo[*b*]fluoranthene $C_{20}H_{12}$ [205-99-2] FTOVXSOBNPWTSH-UHFFFAOYSA-N	1.5×10^{1}	5400	Brockbank (2013)	L	
	1.5×10^{1}		Ma et al. (2010b)	L	368
	1.5×10^{1}		Ma et al. (2010b)	L	369
	1.5×10^{1}	5400	ten Hulscher et al. (1992)	M	
	1.4×10^{1}	7500	Paasivirta et al. (1999)	T	
	8.3×10^{-1}		Smith et al. (1993)	C	
	1.4		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	185
	6.0		Parnis et al. (2015)	Q	371
	5.6		Hilal et al. (2008)	Q	
	2.1		Modarresi et al. (2007)	Q	68
		4700	Kühne et al. (2005)	Q	
	2.0×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.5×10^{1}		Duchowicz et al. (2020)	?	186, 21
		5400	Kühne et al. (2005)	?	

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benzo[*k*]fluoranthene	1.7×10^{1}		Ma et al. (2010b)	L	368
$C_{20}H_{12}$	1.8×10^{1}		Ma et al. (2010b)	L	369
[207-08-9]	1.0×10^{1}		Lee et al. (2012)	M	
HAXBIWFMXWRORI-UHFFFAOYSA-N	1.7×10^{1}	5900	ten Hulscher et al. (1992)	M	
			Mackay et al. (2006a)	V	293
	8.3×10^{1}		De Maagd et al. (1998)	V	12
	6.2×10^{1}		Shiu and Mackay (1997)	V	
	1.5	6900	Paasivirta et al. (1999)	T	
	9.6×10^{-3}	1900	Goldstein (1982)	X	299
	2.5×10^{-1}		Smith et al. (1993)	C	
	2.6		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	300
	5.9		Parnis et al. (2015)	Q	371
	8.0		Hilal et al. (2008)	Q	
	2.4		Modarresi et al. (2007)	Q	68
		6300	Kühne et al. (2005)	Q	
	2.0×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	1.7×10^{1}		Duchowicz et al. (2020)	?	186, 21
		5800	Kühne et al. (2005)	?	
benzo[*a*]pyrene	4.5	8500	Brockbank (2013)	L	
$C_{20}H_{12}$	2.0×10^{1}		Ma et al. (2010b)	L	368
(benz[*a*]pyrene)	1.3×10^{1}		Ma et al. (2010b)	L	369
[50-32-8]	6.2		Lee et al. (2012)	M	
FMMWHPNWAFZXNH-UHFFFAOYSA-N	1.3×10^{1}		Altschuh et al. (1999)	M	
	2.2×10^{1}	4700	ten Hulscher et al. (1992)	M	
	2.2×10^{1}		Mackay et al. (2006a)	V	
	2.9×10^{1}		De Maagd et al. (1998)	V	12
	2.2×10^{1}		Shiu and Mackay (1997)	V	
	1.3×10^{2}		McLachlan et al. (1990)	V	375
	1.8×10^{1}		Eastcott et al. (1988)	V	
	7.5		Smith and Bomberger (1980)	V	24
	1.9×10^{1}		Southworth (1979)	V	
	8.2×10^{-1}	8200	Paasivirta et al. (1999)	T	
	1.6×10^{-3}	110	Goldstein (1982)	X	299
	2.0×10^{1}		Smith et al. (1993)	C	
	8.2×10^{-4}		Ryan et al. (1988)	C	
	2.6		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	300
	5.1		Parnis et al. (2015)	Q	371
	2.9		Hilal et al. (2008)	Q	
	1.5×10^{1}		Modarresi et al. (2007)	Q	68
		4900	Kühne et al. (2005)	Q	
	2.9×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.2×10^{1}		Duchowicz et al. (2020)	?	186, 21
		4700	Kühne et al. (2005)	?	
			Shiu and Ma (2000)	W	362

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benzo[*e*]pyrene	3.3×10^{1}		Duchowicz et al. (2020)	V	187
$C_{20}H_{12}$	3.3×10^{1}		HSDB (2015)	V	
[192-97-2]	2.1×10^{1}		Mackay et al. (2006a)	V	
TXVHTIQJNYSSKO-UHFFFAOYSA-N	2.7	8300	Paasivirta et al. (1999)	T	
	1.2		Duchowicz et al. (2020)	Q	
	1.5×10^{1}		Ferreira (2001)	Q	12
			Shiu and Ma (2000)	W	362
perylene	2.7		Duchowicz et al. (2020)	V	187
$C_{20}H_{12}$			Mackay et al. (2006a)	V	293
(dibenz[*de*, *kl*]anthracene)	2.3		Riederer (1990)	V	
[198-55-0]	2.5×10^{-1}	6300	Paasivirta et al. (1999)	T	
CSHWQDPOILHKBI-UHFFFAOYSA-N	3.3×10^{2}		Mackay et al. (1992b)	X	366
	1.2		Duchowicz et al. (2020)	Q	
	5.7		Parnis et al. (2015)	Q	371
	2.3		Hilal et al. (2008)	Q	
	1.1×10^{1}		Ferreira (2001)	Q	12
1,2-benzfluoranthene $C_{20}H_{12}$ [203-33-8] OQDXASJSCOTNQS-UHFFFAOYSA-N	6.9		Hilal et al. (2008)	Q	
benzo[*j*]fluoranthene $C_{20}H_{12}$ [205-82-3] KHNYNFUTFKJLDD-UHFFFAOYSA-N	4.9×10^{1}		HSDB (2015)	Q	100
1,3,6-trimethylchrysene $C_{21}H_{18}$ [1586755-28-3] UGLPREDFUVNEMJ-UHFFFAOYSA-N	1.8		Parnis et al. (2015)	Q	371
6-propylchrysene $C_{21}H_{18}$ [6910-41-4] PGBSMHMYMMBHFF-UHFFFAOYSA-N	1.5		Parnis et al. (2015)	Q	371
20-methylcholanthrene	1.9		Duchowicz et al. (2020)	V	187
$C_{21}H_{16}$	1.9		HSDB (2015)	V	
[56-49-5]			Mackay et al. (2006a)	V	293
PPQNQXQZIWHJRB-UHFFFAOYSA-N	3.7×10^{-1}		Duchowicz et al. (2020)	Q	
6-butylchrysene $C_{22}H_{20}$ [6901-71-9] XJQKMLMKECCWEO-UHFFFAOYSA-N	1.3		Parnis et al. (2015)	Q	371

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dibenz[a,h]anthracene	7.0×10^{1}		Duchowicz et al. (2020)	V	187
$C_{22}H_{14}$	1.8×10^{2}	12000	Abou-Naccoul et al. (2014)	V	
[53-70-3]	5.8×10^{3}		Mackay et al. (2006a)	V	
LHRCREOYAASXPZ-UHFFFAOYSA-N	1.3×10^{2}		Eastcott et al. (1988)	V	
	1.2	7800	Paasivirta et al. (1999)	T	
	1.4×10^{2}		Smith et al. (1993)	C	
	1.4		Duchowicz et al. (2020)	Q	
	1.4×10^{2}		HSDB (2015)	Q	100
	2.6×10^{1}		Parnis et al. (2015)	Q	371
	1.2×10^{1}		Hilal et al. (2008)	Q	
	8.3×10^{1}		Ferreira (2001)	Q	12
indeno[1,2,3-cd]pyrene	2.9×10^{1}		Ma et al. (2010b)	L	368
$C_{22}H_{12}$	2.0×10^{1}		Ma et al. (2010b)	L	369
[193-39-5]	2.8×10^{1}	3600	ten Hulscher et al. (1992)	M	
SXQBHARYMNFBPS-UHFFFAOYSA-N	2.5	7400	Paasivirta et al. (1999)	T	
	1.4×10^{2}		Smith et al. (1993)	C	
	4.7		Keshavarz et al. (2022)	Q	
	3.7		Duchowicz et al. (2020)	Q	185
	1.3×10^{1}		Parnis et al. (2015)	Q	371
	5.0		Hilal et al. (2008)	Q	
	9.4		Modarresi et al. (2007)	Q	68
		5100	Kühne et al. (2005)	Q	
	2.8×10^{1}		Duchowicz et al. (2020)	?	186, 21
		3600	Kühne et al. (2005)	?	
benzo[ghi]perylene	3.0×10^{1}		Ma et al. (2010b)	L	368
$C_{22}H_{12}$	2.4×10^{1}		Ma et al. (2010b)	L	369
[191-24-2]	3.0×10^{1}	3200	ten Hulscher et al. (1992)	M	
GYFAGKUZYNFMBN-UHFFFAOYSA-N	1.8×10^{1}		De Maagd et al. (1998)	V	12
	1.3×10^{1}		Shiu and Mackay (1997)	V	
	6.9×10^{1}		Eastcott et al. (1988)	V	
	4.0	9200	Paasivirta et al. (1999)	T	
	1.3×10^{1}		Mackay et al. (1992b)	X	366
	1.8×10^{2}		Smith et al. (1993)	C	
	4.7		Keshavarz et al. (2022)	Q	
	3.7		Duchowicz et al. (2020)	Q	
	1.1×10^{1}		Parnis et al. (2015)	Q	371
	2.6		Hilal et al. (2008)	Q	
	6.1×10^{1}		Modarresi et al. (2007)	Q	68
		3700	Kühne et al. (2005)	Q	
	3.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	3.0×10^{1}		Duchowicz et al. (2020)	?	186, 21
		3300	Kühne et al. (2005)	?	

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benzo[*b*]triphenylene $C_{22}H_{14}$ (dibenz[*a*, *c*]anthracene) [215-58-7] RAASUWZPTOJQAY-UHFFFAOYSA-N	1.9×10^{1} 4.4×10^{3} 1.9×10^{1} 1.4×10^{2}	8600	Abou-Naccoul et al. (2014) Mackay et al. (2006a) Hilal et al. (2008) Ferreira (2001)	V V Q Q	 12
dibenz[*a*, *j*]anthracene $C_{22}H_{14}$ [224-41-9] KLIHYVJAYWCEDM-UHFFFAOYSA-N	8.6×10^{1} 8.3×10^{1}		Hilal et al. (2008) Ferreira (2001)	Q Q	 12
picene $C_{22}H_{14}$ [213-46-7] GBROPGWFBFCKAG-UHFFFAOYSA-N	6.2 7.7×10^{1}		Hilal et al. (2008) Ferreira (2001)	Q Q	 12
benzo[*c*]chrysene $C_{22}H_{14}$ [194-69-4] YZWGEMSQAMDWEM-UHFFFAOYSA-N	8.0×10^{1}		HSDB (2015)	Q	100
benzo[*g*]chrysene $C_{22}H_{14}$ [196-78-1] JZOIZKBKSZMVRV-UHFFFAOYSA-N	8.0×10^{1}		HSDB (2015)	Q	100
dibenzo[*a*, *e*]pyrene $C_{24}H_{14}$ [192-65-4] KGHMWBNEMFNJFZ-UHFFFAOYSA-N	7.0×10^{2}		HSDB (2015)	Q	100
dibenzo[*a*, *h*]pyrene $C_{24}H_{14}$ [189-64-0] RXUSYFJGDZFVND-UHFFFAOYSA-N	7.0×10^{2}		HSDB (2015)	Q	100
dibenzo[*a*, *i*]pyrene $C_{24}H_{14}$ [189-55-9] TUGYIJVAYAHHHM-UHFFFAOYSA-N	7.0×10^{2}		HSDB (2015)	Q	100
coronene $C_{24}H_{12}$ [191-07-1] VPUGDVKSAQVFFS-UHFFFAOYSA-N			Mackay et al. (2006a)	V	293
dibenz[*a*, *e*]aceanthrylene $C_{24}H_{14}$ [5385-75-1] JHOWUOKQHJHGMU-UHFFFAOYSA-N	7.0×10^{2}		HSDB (2015)	Q	100

Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dibenzo[b,k]chrysene $C_{26}H_{16}$ [217-54-9] DHCSBRKYHMINPB-UHFFFAOYSA-N	1.2×10^3		HSDB (2015)	Q	100

A3 Organic species with oxygen (O)

A3.1 Carbon oxides

Table A3.1: Carbon oxides

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
carbon monoxide	9.7×10^{-6}	1300	Burkholder et al. (2019)	L	1
CO	8.0×10^{-6}	1400	Burkholder et al. (2019)	L	71
[630-08-0]	9.7×10^{-6}	1300	Burkholder et al. (2015)	L	1
UGFAIRIUMAVXCW-UHFFFAOYSA-N	8.0×10^{-6}	1400	Burkholder et al. (2015)	L	71
	9.7×10^{-6}	1300	Warneck and Williams (2012)	L	
	9.7×10^{-6}	1300	Sander et al. (2011)	L	1
	9.7×10^{-6}	1300	Sander et al. (2006)	L	1
	9.7×10^{-6}	1300	Fernández-Prini et al. (2003)	L	3
			Cargill (1990)	L	376
	9.4×10^{-6}	1300	Wilhelm et al. (1977)	L	
	9.7×10^{-6}	1300	Rettich et al. (1982)	M	377
	7.0×10^{-6}	1500	Schmidt (1979)	M	33, 34
	7.9×10^{-5}		Meadows and Spedding (1974)	M	
	8.3×10^{-6}		Power and Stegall (1970)	M	14
	7.9×10^{-6}	1200	Douglas (1967)	M	378, 379
	9.4×10^{-6}	1300	Winkler (1901)	M	380
	9.5×10^{-6}	1200	Bunsen (1855a)	M	43
	6.0×10^{-6}		Pierotti (1965)	T	
	1.0×10^{-5}		Hayer et al. (2022)	Q	20
	8.7×10^{-6}		Yaws (1999)	?	21
	9.4×10^{-6}	1300	Yaws et al. (1999)	?	21
	8.4×10^{-6}		Abraham and Weathersby (1994)	?	21
	9.4×10^{-6}	1400	Dean and Lange (1999)	?	381, 23
	8.6×10^{-6}		Yaws and Yang (1992)	?	21
carbon dioxide	3.4×10^{-4}	2300	Burkholder et al. (2019)	L	1
CO_2	2.8×10^{-4}	2600	Burkholder et al. (2019)	L	71
[124-38-9]	3.4×10^{-4}	2300	Burkholder et al. (2015)	L	1
CURLTUGMZLYLDI-UHFFFAOYSA-N	2.8×10^{-4}	2600	Burkholder et al. (2015)	L	71
	3.3×10^{-4}	2400	Sander et al. (2011)	L	1
	3.3×10^{-4}	2400	Sander et al. (2006)	L	1
	3.3×10^{-4}	2300	Fernández-Prini et al. (2003)	L	3
	3.4×10^{-4}	2300	Carroll et al. (1991)	L	
	3.4×10^{-4}	2400	Crovetto (1991)	L	
	3.4×10^{-4}	2300	Yoo et al. (1986)	L	1
	3.4×10^{-4}	2400	Edwards et al. (1978)	L	1
	3.3×10^{-4}	2400	Wilhelm et al. (1977)	L	
	3.4×10^{-4}	2400	Weiss (1974)	L	1
	3.4×10^{-4}	2300	Zheng et al. (1997)	M	382
	3.3×10^{-4}	2400	Murray and Riley (1971)	M	383
	2.4×10^{-4}		Power and Stegall (1970)	M	14
	3.3×10^{-4}	2400	Morrison and Billett (1952)	M	384
	3.3×10^{-4}		Orcutt and Seevers (1937a)	M	

Table A3.1: Carbon oxides (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.3×10^{-4}	2300	Kunerth (1922)	M	
	3.3×10^{-4}	2500	Geffcken (1904)	M	
	3.4×10^{-4}	2400	Bohr (1899)	M	385
	3.4×10^{-4}	2500	Bunsen (1855a)	M	43
	6.5×10^{-4}		Duchowicz et al. (2020)	V	187
	3.4×10^{-4}	2400	Chen et al. (1979)	R	1
	3.1×10^{-4}	2400	Chameides (1984)	T	
	3.3×10^{-4}	2400	Edwards et al. (1975)	T	1
	3.4×10^{-4}		Perry and Chilton (1973)	X	29
	3.4×10^{-4}	2400	Lelieveld and Crutzen (1991)	C	
	3.4×10^{-4}	2400	Pandis and Seinfeld (1989)	C	
	3.9×10^{-4}		Nunn (1958)	C	12
	2.3×10^{-4}		Hayer et al. (2022)	Q	20
	4.0		Duchowicz et al. (2020)	Q	
		2900	Kühne et al. (2005)	Q	
			Scharlin (1996)	E	1, 386
		2400	Kühne et al. (2005)	?	
	4.5×10^{-4}		Yaws (1999)	?	21
	3.3×10^{-4}	2400	Yaws et al. (1999)	?	21
	2.6×10^{-4}		Abraham and Weathersby (1994)	?	21
	3.3×10^{-4}	2400	Dean and Lange (1999)	?	387, 23
	4.5×10^{-4}		Yaws and Yang (1992)	?	21
	3.4×10^{-4}	2400	Seinfeld (1986)	?	21
	3.3×10^{-4}	2400	Hoffmann and Jacob (1984)	?	21
carbon suboxide C_3O_2 [504-64-3] GNEVIACKFGQMHB-UHFFFAOYSA-N	1.1×10^{-2}		Keßel et al. (2017)	M	388

A3.2 Alcohols (ROH)

Table A3.2: Alcohols (ROH)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methanol	2.0	5500	Burkholder et al. (2019)	L	1
CH_3OH	2.0	5500	Burkholder et al. (2015)	L	1
[67-56-1]	2.0	5400	Brockbank (2013)	L	1
OKKJLVBELUTLKV-UHFFFAOYSA-N	2.0	5600	Sander et al. (2011)	L	389, 1
	2.1	5300	Warneck (2006)	L	
	2.2	5200	Sander et al. (2006)	L	
	2.0	5500	Dohnal et al. (2006)	L	1
	1.7	4500	Fogg and Sangster (2003)	L	
	2.1	5400	Plyasunov and Shock (2000)	L	
	3.6×10^{-2}		St-Pierre et al. (2014)	M	174
	2.2	5300	O'Farrell and Waghorne (2010)	M	
	2.1		Vitenberg and Dobryakov (2008)	M	
	7.8×10^{-1}		Helburn et al. (2008)	M	
	2.2	5300	Lin and Chou (2006)	M	
	2.0	5600	Teja et al. (2001)	M	11, 340
	2.6	5900	Zhu et al. (2000)	M	
	2.0	5500	Gupta et al. (2000)	M	
	1.6		Altschuh et al. (1999)	M	
	2.1		Merk and Riederer (1997)	M	
	1.3		Kaneko et al. (1994)	M	14
	2.2		Li and Carr (1993)	M	
	2.6	3900	Pividal et al. (1992)	M	
	2.2	5200	Snider and Dawson (1985)	M	
	2.0		Richon et al. (1985)	M	
	1.3×10^{1}		Mazza (1980)	M	
	2.2		Rytting et al. (1978)	M	
	2.3		Burnett (1963)	M	
	2.3		Butler et al. (1935)	M	390
	7.6×10^{-2}		Abraham and Acree (2007)	V	
	1.8	6200	Fukuchi et al. (2002)	V	
	1.9		Hwang et al. (1992)	V	
	2.8		Riederer (1990)	V	
		5400	Abraham (1984)	V	
	2.2	5700	Glew and Moelwyn-Hughes (1953)	R	
	2.1	5400	Plyasunov et al. (2001)	T	
	1.5		Yaws (2003)	X	259
	1.5		Yaws (2003)	X	238
	1.6	5600	Schaffer and Daubert (1969)	X	299
	2.2		Gaffney and Senum (1984)	X	391
	2.1		Timmermans (1960)	X	392
	1.6		Dupeux et al. (2022)	Q	260
	2.1		Hayer et al. (2022)	Q	20
	5.0×10^{-1}		Keshavarz et al. (2022)	Q	
	2.8		Duchowicz et al. (2020)	Q	185
	3.4×10^{-1}		Wang et al. (2017)	Q	81, 239

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.1		Wang et al. (2017)	Q	81, 240
	6.6		Wang et al. (2017)	Q	81, 241
	2.1		Li et al. (2014)	Q	242
	2.0		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.5		Raventos-Duran et al. (2010)	Q	246
	2.6×10^{-1}		Gharagheizi et al. (2010)	Q	247
	2.0		Hilal et al. (2008)	Q	
	2.9		Modarresi et al. (2007)	Q	68
		6200	Kühne et al. (2005)	Q	
	2.2		Yaffe et al. (2003)	Q	249, 250
	1.1		Yao et al. (2002)	Q	230, 268
	2.6		English and Carroll (2001)	Q	231, 232
	1.6		Katritzky et al. (1998)	Q	
	1.5		Yaws et al. (1997)	Q	
	2.0		Suzuki et al. (1992)	Q	233
	1.8		Nirmalakhandan and Speece (1988)	Q	
	2.4		Taft et al. (1985)	Q	
	2.2		Duchowicz et al. (2020)	?	186, 21
		5000	Kühne et al. (2005)	?	
	1.9		Yaws (1999)	?	21
	1.1		Abraham and Weathersby (1994)	?	21
	1.4		Yaws and Yang (1992)	?	21
	2.2		Abraham et al. (1990)	?	
ethanol	1.9	6400	Burkholder et al. (2019)	L	1
C_2H_5OH	1.9	6400	Burkholder et al. (2015)	L	1
[64-17-5]	1.8	6300	Brockbank (2013)	L	1
LFQSCWFLJHTTHZ-UHFFFAOYSA-N	1.9	6400	Sander et al. (2011)	L	1
	1.9	6300	Warneck (2006)	L	
	2.0	6600	Sander et al. (2006)	L	
	1.8	6300	Dohnal et al. (2006)	L	1
	1.7	5700	Fogg and Sangster (2003)	L	
	1.9	6300	Plyasunov and Shock (2000)	L	
	1.9	6200	Dubowski (1979)	L	1
	1.8	5900	Willey et al. (2017)	M	
	2.2	5500	O'Farrell and Waghorne (2010)	M	
	1.8		Vitenberg and Dobryakov (2008)	M	
	1.9	5800	Falabella et al. (2006)	M	11, 340
	1.9		Straver and de Loos (2005)	M	
			Cheng et al. (2004)	M	330
	1.1		Ueberfeld et al. (2001)	M	
	1.8	5800	Gupta et al. (2000)	M	
	1.3		Altschuh et al. (1999)	M	
	1.0		Eger et al. (1999)	M	14
	1.9		Merk and Riederer (1997)	M	
	8.3×10^{-1}		Kaneko et al. (1994)	M	14
	1.9		Li and Carr (1993)	M	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.1	3900	Pividal et al. (1992)	M	
	1.9		Park et al. (1987)	M	
	1.9	6600	Snider and Dawson (1985)	M	
	2.0		Richon et al. (1985)	M	
	1.9	6000	Jones (1983)	M	1
	6.2		Mazza (1980)	M	
	1.9		Rytting et al. (1978)	M	
	2.3		Rohrschneider (1973)	M	
	2.1		Burnett (1963)	M	
	1.9	6500	Harger et al. (1950)	M	
	1.9		Butler et al. (1935)	M	
	4.7×10^{-2}		Abraham and Acree (2007)	V	
	1.7	6300	Fukuchi et al. (2002)	V	
	1.3		Hwang et al. (1992)	V	
		6300	Abraham (1984)	V	
	1.9	6300	Plyasunov et al. (2001)	T	
	1.4		Yaws (2003)	X	238
	1.5	6400	Schaffer and Daubert (1969)	X	299
	2.0		Gaffney and Senum (1984)	X	391
	1.6		Timmermans (1960)	X	392
	1.7		Hayer et al. (2022)	Q	20
	6.7×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1		Duchowicz et al. (2020)	Q	
	3.1×10^{-1}		Wang et al. (2017)	Q	81, 239
	2.0		Wang et al. (2017)	Q	81, 240
	2.3		Wang et al. (2017)	Q	81, 241
	1.6		Raventos-Duran et al. (2010)	Q	243, 244
	1.6		Raventos-Duran et al. (2010)	Q	245
	1.6		Raventos-Duran et al. (2010)	Q	246
	1.3		Gharagheizi et al. (2010)	Q	247
	1.1		Hilal et al. (2008)	Q	
	1.8		Modarresi et al. (2007)	Q	68
		6500	Kühne et al. (2005)	Q	
	2.0		Yaffe et al. (2003)	Q	249, 250
	1.4		Yao et al. (2002)	Q	230
	1.4		English and Carroll (2001)	Q	231, 232
	1.2		Katritzky et al. (1998)	Q	
	1.3		Yaws et al. (1997)	Q	
	1.4		Russell et al. (1992)	Q	280
	1.4		Suzuki et al. (1992)	Q	233
	1.6		Nirmalakhandan and Speece (1988)	Q	
	2.0		Duchowicz et al. (2020)	?	186, 21
	1.9		Bartelt-Hunt et al. (2008)	?	21
		6400	Kühne et al. (2005)	?	
	1.2		Yaws (1999)	?	21
	8.2×10^{-1}		Abraham and Weathersby (1994)	?	21
	1.2		Yaws and Yang (1992)	?	21

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.9		Abraham et al. (1990)	?	
1-propanol	1.4	6900	Burkholder et al. (2019)	L	393, 1
C_3H_7OH	1.4	6900	Burkholder et al. (2015)	L	394, 1
[71-23-8]	1.5	7000	Brockbank (2013)	L	1, 395
BDERNNFJNOPAEC-UHFFFAOYSA-N	1.4	6900	Sander et al. (2011)	L	396, 1
	1.3	7500	Sander et al. (2006)	L	
	1.4	6900	Dohnal et al. (2006)	L	1
	1.4	6200	Fogg and Sangster (2003)	L	
	1.5	6900	Plyasunov and Shock (2000)	L	
	1.5		Vitenberg and Dobryakov (2008)	M	
	1.2	6200	Falabella et al. (2006)	M	11, 340
	1.5		Straver and de Loos (2005)	M	
	3.2×10^{-1}		van Ruth et al. (2002)	M	14
	3.2×10^{-1}		van Ruth and Villeneuve (2002)	M	14, 363
	6.5×10^{-1}		van Ruth et al. (2001)	M	14
	1.2	6200	Gupta et al. (2000)	M	
	2.7		Altschuh et al. (1999)	M	
	1.5		Merk and Riederer (1997)	M	
	7.2×10^{-1}		Kaneko et al. (1994)	M	14
	1.4		Li and Carr (1993)	M	
	1.3	7500	Snider and Dawson (1985)	M	
	1.8		Richon et al. (1985)	M	
	3.7		Mazza (1980)	M	
	1.5		Rytting et al. (1978)	M	
	1.6		Burnett (1963)	M	
	1.4		Butler et al. (1935)	M	390
	3.1×10^{-2}		Abraham and Acree (2007)	V	
	1.8	7700	Fukuchi et al. (2002)	V	
	8.0×10^{-2}	4500	Djerki and Laub (1988)	V	
		6900	Abraham (1984)	V	
	1.5	6900	Plyasunov et al. (2001)	T	
	1.2		Yaws (2003)	X	259
	1.2		Dupeux et al. (2022)	Q	260
	1.5		Hayer et al. (2022)	Q	20
	9.0×10^{-1}		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	
	2.5×10^{-1}		Wang et al. (2017)	Q	81, 239
	1.3		Wang et al. (2017)	Q	81, 240
	1.2		Wang et al. (2017)	Q	81, 241
	1.2		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.2		Raventos-Duran et al. (2010)	Q	246
	7.0×10^{-1}		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	68
		6900	Kühne et al. (2005)	Q	
	1.2		Yaffe et al. (2003)	Q	249, 273

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1		Yao et al. (2002)	Q	230
	1.2		English and Carroll (2001)	Q	231, 232
	1.7		Katritzky et al. (1998)	Q	
	1.2		Yaws et al. (1997)	Q	
	1.1		Russell et al. (1992)	Q	280
	1.1		Suzuki et al. (1992)	Q	233
	1.2		Nirmalakhandan and Speece (1988)	Q	
	1.3		Duchowicz et al. (2020)	?	186, 21
		7500	Kühne et al. (2005)	?	
	1.3		Yaws (1999)	?	21
	6.0×10^{-1}		Abraham and Weathersby (1994)	?	21
	1.1		Yaws and Yang (1992)	?	21
	1.5		Abraham et al. (1990)	?	
2-propanol	1.2	7100	Burkholder et al. (2019)	L	1
C_3H_7OH	1.2	7100	Burkholder et al. (2015)	L	1
(isopropanol)	1.2	6900	Brockbank (2013)	L	1
[67-63-0]	1.3	7500	Sander et al. (2011)	L	
KFZMGEQAYNKOFK-UHFFFAOYSA-N	1.3	7500	Sander et al. (2006)	L	
	1.2	6200	Fogg and Sangster (2003)	L	
	1.2	7000	Plyasunov and Shock (2000)	L	
	1.1	8400	Hiatt (2013)	M	
	6.8×10^{-1}		Helburn et al. (2008)	M	
	1.3	7300	Lin and Chou (2006)	M	
			Cheng et al. (2004)	M	330
			Cheng et al. (2003)	M	330
	1.8×10^{-1}		Ayuttaya et al. (2001)	M	342
	1.0×10^{-3}		Ayuttaya et al. (2001)	M	343
	5.7×10^{-1}		Ayuttaya et al. (2001)	M	344
	1.1		Kim et al. (2000)	M	
	9.2×10^{-1}		Altschuh et al. (1999)	M	
	1.2		Merk and Riederer (1997)	M	
	5.8×10^{-1}		Kaneko et al. (1994)	M	14
	7.9×10^{-1}	5700	Kolb et al. (1992)	M	278
	1.4		Pividal et al. (1992)	M	81
	9.8×10^{-1}		Yu (1992)	M	12
	1.2	7400	Snider and Dawson (1985)	M	
	2.1		Mazza (1980)	M	
	1.2		Rytting et al. (1978)	M	
	1.2		Butler et al. (1935)	M	
	1.2	7100	Fenclová et al. (2007)	V	1
	1.2	7600	Fukuchi et al. (2002)	V	
	1.7		Hine and Weimar (1965)	R	
	7.6×10^{-1}		Yaws (2003)	X	259
	2.4		Dupeux et al. (2022)	Q	260
	1.2		Hayer et al. (2022)	Q	20
	9.0×10^{-1}		Keshavarz et al. (2022)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.8×10^{-1}		Duchowicz et al. (2020)	Q	185
	2.8×10^{-1}		Wang et al. (2017)	Q	81, 239
	1.0		Wang et al. (2017)	Q	81, 240
	1.2		Wang et al. (2017)	Q	81, 241
	1.2		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.2		Raventos-Duran et al. (2010)	Q	246
	4.3×10^{-1}		Hilal et al. (2008)	Q	
	7.0×10^{-1}		Modarresi et al. (2007)	Q	68
		6900	Kühne et al. (2005)	Q	
			Yaffe et al. (2003)	Q	358
	7.7×10^{-1}		Yao et al. (2002)	Q	230
	1.0		English and Carroll (2001)	Q	231, 275
	1.1		Katritzky et al. (1998)	Q	
	8.9×10^{-1}		Yaws et al. (1997)	Q	
	1.4		Russell et al. (1992)	Q	280
	9.7×10^{-1}		Suzuki et al. (1992)	Q	233
	1.1		Nirmalakhandan and Speece (1988)	Q	
	1.3		Taft et al. (1985)	Q	
	1.2		Duchowicz et al. (2020)	?	186, 21
		6000	Kühne et al. (2005)	?	
	8.0×10^{-1}		Yaws (1999)	?	21
	5.0×10^{-1}		Abraham and Weathersby (1994)	?	21
	8.8×10^{-1}		Yaws and Yang (1992)	?	21
	1.2		Abraham et al. (1990)	?	
glycidol $C_3H_6O_2$ [556-52-5] CTKINSOISVBQLD-UHFFFAOYSA-N	1.7×10^{3}		HSDB (2015)	Q	100
1-butanol C_4H_9OH [71-36-3] LRHPLDYGYMQRHN-UHFFFAOYSA-N	1.2	7500	Burkholder et al. (2019)	L	1
	1.2	7500	Burkholder et al. (2015)	L	1
	1.2	7500	Brockbank (2013)	L	1
	1.2	7500	Sander et al. (2011)	L	1
	1.3	7200	Sander et al. (2006)	L	
	1.2	7500	Dohnal et al. (2006)	L	1
	1.1	6300	Fogg and Sangster (2003)	L	
	1.2	7400	Plyasunov and Shock (2000)	L	
	1.0	7000	Wu et al. (2022a)	M	
	2.0		Chao et al. (2017)	M	
	1.0	6800	Shunthirasingham et al. (2013)	M	
	1.3		Vitenberg and Dobryakov (2008)	M	
	1.1	6000	Lei et al. (2007)	M	397
	8.2×10^{-1}	6200	Falabella et al. (2006)	M	11, 340
	9.4×10^{-1}	6100	Hovorka et al. (2002)	M	11
	4.5×10^{-1}		van Ruth et al. (2002)	M	14
	4.4×10^{-1}		van Ruth and Villeneuve (2002)	M	14, 363

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.8×10^{-1}		van Ruth et al. (2001)	M	14
	1.1		Kim et al. (2000)	M	
	8.2×10^{-1}	6200	Gupta et al. (2000)	M	
	1.2		Altschuh et al. (1999)	M	
	5.5×10^{-1}		Eger et al. (1999)	M	14
	1.1		Merk and Riederer (1997)	M	
	1.4×10^{-1}		Chaintreau et al. (1995)	M	
	5.1×10^{-1}		Kaneko et al. (1994)	M	14
	1.1		Li and Carr (1993)	M	
	6.1×10^{-1}	5600	Kolb et al. (1992)	M	278
	1.2	7200	Snider and Dawson (1985)	M	
	5.3×10^{-1}		Friant and Suffet (1979)	M	38
	1.2		Rytting et al. (1978)	M	
	1.1		Amoore and Buttery (1978)	M	
	1.1		Buttery et al. (1969)	M	
	1.4		Burnett (1963)	M	
	1.2		Butler et al. (1935)	M	390
	1.1		Chao et al. (2017)	V	
	1.1		Mackay et al. (2006c)	V	
	7.3×10^{-1}		Mackay et al. (1995)	V	
	8.3×10^{-1}		Hwang et al. (1992)	V	
	2.2×10^{-1}	4700	Djerki and Laub (1988)	V	
		7400	Abraham (1984)	V	
	1.2		Amoore and Buttery (1978)	V	
	1.2		Butler et al. (1935)	V	
	1.2		Yaws (2003)	X	259
	9.4×10^{-1}		Dupeux et al. (2022)	Q	260
	1.9		Hayer et al. (2022)	Q	20
	1.2		Keshavarz et al. (2022)	Q	
	1.3		Duchowicz et al. (2020)	Q	185
	2.0×10^{-1}		Wang et al. (2017)	Q	81, 239
	9.1×10^{-1}		Wang et al. (2017)	Q	81, 240
	1.3		Wang et al. (2017)	Q	81, 241
	1.2		Li et al. (2014)	Q	242
	9.4×10^{-1}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	5.6×10^{-1}		Hilal et al. (2008)	Q	
	1.0		Modarresi et al. (2007)	Q	68
		7200	Kühne et al. (2005)	Q	
	1.2		Yaffe et al. (2003)	Q	249, 273
	1.1		Yao et al. (2002)	Q	230
	9.5×10^{-1}		English and Carroll (2001)	Q	231, 261
	1.8		Katritzky et al. (1998)	Q	
	1.1		Yaws et al. (1997)	Q	
	8.6×10^{-1}		Russell et al. (1992)	Q	280

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.4×10^{-1}		Suzuki et al. (1992)	Q	233
	9.9×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	1.1		Duchowicz et al. (2020)	?	186, 21
		6900	Kühne et al. (2005)	?	
	1.1		Yaws (1999)	?	21
	1.2		Abraham et al. (1990)	?	
	1.8		Mackay and Yeun (1983)	?	
2-butanol	1.1	7600	Burkholder et al. (2019)	L	1
$C_4H_{10}O$	1.1	7600	Burkholder et al. (2015)	L	1
(*sec*-butanol)	9.5×10^{-1}	7600	Brockbank (2013)	L	1
[78-92-2]	1.1	7300	Sander et al. (2011)	L	
BTANRVKWQNVYAZ-UHFFFAOYSA-N	1.1	7300	Sander et al. (2006)	L	
	1.0	7400	Fogg and Sangster (2003)	L	
	9.9×10^{-1}	7600	Plyasunov and Shock (2000)	L	
	8.3×10^{-1}		Merk and Riederer (1997)	M	
	1.1	7300	Snider and Dawson (1985)	M	
	9.8×10^{-1}		Rytting et al. (1978)	M	
	9.6×10^{-1}		Butler et al. (1935)	M	
	9.5×10^{-1}	7600	Fenclová et al. (2007)	V	1
	1.1		Mackay et al. (2006c)	V	
	1.1		Mackay et al. (1995)	V	
	9.1×10^{-1}	7500	Cabani et al. (1975b)	T	
	6.7×10^{-1}		Yaws (2003)	X	259
	1.1		Dupeux et al. (2022)	Q	260
	1.2		Hayer et al. (2022)	Q	20
	1.2		Keshavarz et al. (2022)	Q	
	5.1×10^{-1}		Duchowicz et al. (2020)	Q	300
	2.3×10^{-1}		Wang et al. (2017)	Q	81, 239
	8.9×10^{-1}		Wang et al. (2017)	Q	81, 240
	7.3×10^{-1}		Wang et al. (2017)	Q	81, 241
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	3.9×10^{-1}		Hilal et al. (2008)	Q	
	4.9×10^{-1}		Modarresi et al. (2007)	Q	68
		7200	Kühne et al. (2005)	Q	
	1.2		Yaffe et al. (2003)	Q	249, 250
	6.2×10^{-1}		Yao et al. (2002)	Q	230
	8.4×10^{-1}		English and Carroll (2001)	Q	231, 232
	5.7×10^{-1}		Katritzky et al. (1998)	Q	
	1.2		Yaws et al. (1997)	Q	
	7.7×10^{-1}		Suzuki et al. (1992)	Q	233
	9.0×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	1.1		Duchowicz et al. (2020)	?	186, 21
		7100	Kühne et al. (2005)	?	
	1.2		Yaws (1999)	?	21

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.9×10^{-1}		Abraham et al. (1990)	?	
2-methyl-1-propanol	8.3×10^{-1}	7200	Burkholder et al. (2019)	L	1
$C_4H_{10}O$	8.3×10^{-1}	7200	Burkholder et al. (2015)	L	1
(isobutanol)	8.0×10^{-1}	7400	Brockbank (2013)	L	1
[78-83-1]	1.0		Sander et al. (2011)	L	
ZXEKIIBDNHEJCQ-UHFFFAOYSA-N	1.0		Sander et al. (2006)	L	
	8.5×10^{-1}	7200	Plyasunov and Shock (2000)	L	
	1.2		Chao et al. (2017)	M	
	2.2×10^{-1}		Kim and Kim (2014)	M	
			Cheng et al. (2004)	M	330
	6.7×10^{-1}	6100	Hovorka et al. (2002)	M	11
	1.1		Altschuh et al. (1999)	M	
	3.7×10^{-1}		Shiu and Mackay (1997)	M	
	7.8×10^{-1}		Merk and Riederer (1997)	M	
	4.4×10^{-1}		Kaneko et al. (1994)	M	14
	1.0		Snider and Dawson (1985)	M	
	8.0×10^{-1}		Rytting et al. (1978)	M	
	8.3×10^{-1}		Butler et al. (1935)	M	
	9.2×10^{-1}		Chao et al. (2017)	V	
	7.6×10^{-1}	7200	Fenclová et al. (2007)	V	1
	7.3×10^{-1}		Mackay et al. (2006c)	V	
	7.3×10^{-1}		Shiu and Mackay (1997)	V	
	7.3×10^{-1}		Mackay et al. (1995)	V	
	1.2		Keshavarz et al. (2022)	Q	
	5.1×10^{-1}		Duchowicz et al. (2020)	Q	
	2.3×10^{-1}		Wang et al. (2017)	Q	81, 239
	9.1×10^{-1}		Wang et al. (2017)	Q	81, 240
	7.6×10^{-1}		Wang et al. (2017)	Q	81, 241
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	5.1×10^{-1}		Hilal et al. (2008)	Q	
	6.1×10^{-1}		Modarresi et al. (2007)	Q	68
		7200	Kühne et al. (2005)	Q	
	3.7×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	6.2×10^{-1}		Yao et al. (2002)	Q	230
	5.7×10^{-1}		English and Carroll (2001)	Q	231, 232
	1.8		Katritzky et al. (1998)	Q	
	8.3×10^{-1}		Yaws et al. (1997)	Q	
	7.7×10^{-1}		Suzuki et al. (1992)	Q	233
	8.4×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	1.0		Duchowicz et al. (2020)	?	186, 21
		8100	Kühne et al. (2005)	?	
	8.4×10^{-1}		Yaws (1999)	?	21
	3.1×10^{-1}		Abraham and Weathersby (1994)	?	21
	8.0×10^{-1}		Abraham et al. (1990)	?	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.6×10^{-1}		Mackay and Yeun (1983)	?	
2-methyl-2-propanol	7.9×10^{-1}	7600	Brockbank (2013)	L	1
$C_4H_{10}O$	6.9×10^{-1}	8300	Sander et al. (2011)	L	
(*tert*-butanol)	6.9×10^{-1}	8300	Sander et al. (2006)	L	
[75-65-0]	7.9×10^{-1}	7700	Plyasunov and Shock (2000)	L	
DKGAVHZHDRPRBM-UHFFFAOYSA-N	1.4	7900	Hiatt (2013)	M	
	1.1		Altschuh et al. (1999)	M	
	8.1×10^{-1}		Merk and Riederer (1997)	M	
			Koga (1995)	M	398
	6.8×10^{-1}	8300	Snider and Dawson (1985)	M	
	7.6×10^{-1}		Rytting et al. (1978)	M	
	8.3×10^{-1}		Butler et al. (1935)	M	
	8.0×10^{-1}	7700	Fenclová et al. (2007)	V	1
	2.4×10^{-1}		Yaws (2003)	X	259
	8.0×10^{-1}	6500	Pankow et al. (1996)	C	
	2.0		Dupeux et al. (2022)	Q	260
	1.2		Keshavarz et al. (2022)	Q	
	2.2×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.6×10^{-1}		Wang et al. (2017)	Q	81, 239
	6.6×10^{-1}		Wang et al. (2017)	Q	81, 240
	1.1		Wang et al. (2017)	Q	81, 241
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	4.1×10^{-1}		Modarresi et al. (2007)	Q	68
		7200	Kühne et al. (2005)	Q	
	7.9×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.9×10^{-1}		Yao et al. (2002)	Q	230
	9.0×10^{-1}		English and Carroll (2001)	Q	231, 232
	7.5×10^{-1}		Katritzky et al. (1998)	Q	
	7.3×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	3.0×10^{-1}		Yaws et al. (1997)	Q	
	6.1×10^{-1}		Suzuki et al. (1992)	Q	233
	7.0×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	1.1		Duchowicz et al. (2020)	?	186, 21
		8300	Kühne et al. (2005)	?	
	5.7×10^{-1}		Yaws (1999)	?	21
	7.7×10^{-1}		Abraham et al. (1990)	?	
			Burkholder et al. (2019)	W	399
			Burkholder et al. (2015)	W	400

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-pentanol	8.6×10^{-1}	7400	Brockbank (2013)	L	1
$C_5H_{11}OH$	1.0	7900	Dohnal et al. (2006)	L	1
(amyl alcohol)	8.9×10^{-1}	7800	Plyasunov and Shock (2000)	L	
[71-41-0]	8.1×10^{-1}	7100	Shunthirasingham et al. (2013)	M	
AMQJEAYHLZJPGS-UHFFFAOYSA-N	7.5×10^{-1}	6100	Lei et al. (2007)	M	397
	9.4×10^{-1}	6800	Falabella et al. (2006)	M	11, 340
	9.5×10^{-1}	6900	Gupta et al. (2000)	M	
	7.7×10^{-1}		Merk and Riederer (1997)	M	
	4.2×10^{-1}		Kaneko et al. (1994)	M	14
	8.4×10^{-1}		Li and Carr (1993)	M	
	9.0×10^{-1}		Rytting et al. (1978)	M	
	7.8×10^{-1}		Butler et al. (1935)	M	
	8.3×10^{-1}		Mackay et al. (2006c)	V	
	8.3×10^{-1}		Mackay et al. (1995)	V	
	6.1×10^{-1}	4900	Djerki and Laub (1988)	V	
		7800	Abraham (1984)	V	
	7.8×10^{-1}		Amoore and Buttery (1978)	V	
	7.6×10^{-1}		Butler et al. (1935)	V	
	7.6×10^{-1}		Yaws (2003)	X	259
	7.3×10^{-1}		Dupeux et al. (2022)	Q	260
	1.6		Keshavarz et al. (2022)	Q	
	1.4		Duchowicz et al. (2020)	Q	
	1.8×10^{-1}		Wang et al. (2017)	Q	81, 239
	6.6×10^{-1}		Wang et al. (2017)	Q	81, 240
	9.1×10^{-1}		Wang et al. (2017)	Q	81, 241
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	4.5×10^{-1}		Hilal et al. (2008)	Q	
	7.6×10^{-1}		Modarresi et al. (2007)	Q	68
		7600	Kühne et al. (2005)	Q	
	7.9×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	5.3×10^{-1}		Yao et al. (2002)	Q	230
	7.7×10^{-1}		English and Carroll (2001)	Q	231, 232
	1.3		Katritzky et al. (1998)	Q	
	7.7×10^{-1}		Yaws et al. (1997)	Q	
	6.2×10^{-1}		Russell et al. (1992)	Q	360
	6.5×10^{-1}		Suzuki et al. (1992)	Q	233
	7.9×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	7.6×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		7700	Kühne et al. (2005)	?	
	7.7×10^{-1}		Yaws (1999)	?	21
	8.1×10^{-1}		Yaws and Yang (1992)	?	21
	9.0×10^{-1}		Abraham et al. (1990)	?	
	9.6×10^{-1}		Mackay and Yeun (1983)	?	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-pentanol	6.7×10^{-1}	7900	Brockbank (2013)	L	1
$C_5H_{12}O$	6.5×10^{-1}	8000	Plyasunov and Shock (2000)	L	
(*sec*-pentanol)	7.1×10^{-1}	8000	Fenclová et al. (2010)	M	1
[6032-29-7]	3.0×10^{-1}		van Ruth et al. (2002)	M	14
JYVLIDXNZAXMDK-UHFFFAOYSA-N	2.6×10^{-1}		van Ruth and Villeneuve (2002)	M	14, 363
	2.3×10^{-1}		van Ruth et al. (2001)	M	14
	6.6×10^{-1}		Merk and Riederer (1997)	M	
	6.7×10^{-1}		Butler et al. (1935)	M	
	6.6×10^{-1}		Mackay et al. (2006c)	V	
	6.6×10^{-1}		Mackay et al. (1995)	V	
	6.5×10^{-1}		Yaws (2003)	X	259
	7.6×10^{-1}		Dupeux et al. (2022)	Q	260
	1.6		Keshavarz et al. (2022)	Q	
	5.3×10^{-1}		Duchowicz et al. (2020)	Q	
	1.8×10^{-1}		Wang et al. (2017)	Q	81, 239
	6.3×10^{-1}		Wang et al. (2017)	Q	81, 240
	6.2×10^{-1}		Wang et al. (2017)	Q	81, 241
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	3.1×10^{-1}		Hilal et al. (2008)	Q	
	3.5×10^{-1}		Modarresi et al. (2007)	Q	68
		7600	Kühne et al. (2005)	Q	
	6.7×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	6.4×10^{-1}		Yao et al. (2002)	Q	230
	7.0×10^{-1}		English and Carroll (2001)	Q	231, 261
	9.0×10^{-1}		Katritzky et al. (1998)	Q	
	6.5×10^{-1}		Yaws et al. (1997)	Q	
	5.8×10^{-1}		Suzuki et al. (1992)	Q	233
	7.2×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	6.7×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		7900	Kühne et al. (2005)	?	
	6.5×10^{-1}		Yaws (1999)	?	21
	6.7×10^{-1}		Abraham et al. (1990)	?	
3-pentanol	6.0×10^{-1}	7600	Brockbank (2013)	L	1
$C_5H_{12}O$	5.5×10^{-1}		Plyasunov and Shock (2000)	L	
[584-02-1]	6.4×10^{-1}	8000	Fenclová et al. (2010)	M	1
AQIXEPGDORPWBJ-UHFFFAOYSA-N	5.0×10^{-1}		Duchowicz et al. (2020)	V	187
	6.3×10^{-1}	7900	Cabani et al. (1975b)	T	
	5.3×10^{-1}		Duchowicz et al. (2020)	Q	
	1.8×10^{-1}		Wang et al. (2017)	Q	81, 239
	6.6×10^{-1}		Wang et al. (2017)	Q	81, 240
	2.3×10^{-1}		Wang et al. (2017)	Q	81, 241
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	3.2×10^{-1}		Hilal et al. (2008)	Q	
	5.2×10^{-1}		Modarresi et al. (2007)	Q	68
		7600	Kühne et al. (2005)	Q	
	6.7×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	6.1×10^{-1}		Yao et al. (2002)	Q	230
	7.0×10^{-1}		English and Carroll (2001)	Q	231, 232
	5.0×10^{-1}		Katritzky et al. (1998)	Q	
	7.7×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	5.2×10^{-1}		Yaws et al. (1997)	Q	
		7500	Kühne et al. (2005)	?	
	5.3×10^{-1}		Yaws (1999)	?	21
	6.2×10^{-1}		Abraham et al. (1990)	?	
2-methyl-1-butanol	7.6×10^{-1}	7900	Brockbank (2013)	L	1
$C_5H_{12}O$	7.1×10^{-1}		Plyasunov and Shock (2000)	L	
[137-32-6]	7.8×10^{-1}	7700	Fenclová et al. (2010)	M	1
QPRQEDXDYOZYLA-UHFFFAOYSA-N	3.3×10^{-1}		Kaneko et al. (1994)	M	14
	7.0×10^{-1}		Butler et al. (1935)	M	
	8.4×10^{-1}		Yaws (2003)	X	259
	4.6×10^{-1}		Dupeux et al. (2022)	Q	260
	1.6		Keshavarz et al. (2022)	Q	
	5.3×10^{-1}		Duchowicz et al. (2020)	Q	300
	1.8×10^{-1}		Wang et al. (2017)	Q	81, 239
	7.6×10^{-1}		Wang et al. (2017)	Q	81, 240
	5.5×10^{-1}		Wang et al. (2017)	Q	81, 241
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	3.9×10^{-1}		Hilal et al. (2008)	Q	
	5.9×10^{-1}		Modarresi et al. (2007)	Q	68
		7600	Kühne et al. (2005)	Q	
	7.0×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	4.7×10^{-1}		English and Carroll (2001)	Q	231, 275
	1.9		Katritzky et al. (1998)	Q	
	8.3×10^{-1}		Yaws et al. (1997)	Q	
	6.0×10^{-1}		Suzuki et al. (1992)	Q	233
	6.9×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	7.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		6800	Kühne et al. (2005)	?	
	8.4×10^{-1}		Yaws (1999)	?	21
	7.0×10^{-1}		Abraham et al. (1990)	?	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(*S*)-2-methyl-1-butanol $C_5H_{12}O$ [1565-80-6] QPRQEDXDYOZYLA-RXMQYKEDSA-N	3.9×10^{-1}		Hilal et al. (2008)	Q	
3-methyl-1-butanol	8.2×10^{-1}	8000	Brockbank (2013)	L	1
$C_5H_{12}O$	7.0×10^{-1}		Plyasunov and Shock (2000)	L	
(isopentanol)	6.7×10^{-1}	6900	Ammari and Schroen (2019)	M	11
[123-51-3]	8.2×10^{-1}	7700	Fenclová et al. (2010)	M	1
PHTQWCKDNZKARW-UHFFFAOYSA-N	3.3×10^{-1}		van Ruth et al. (2002)	M	14
	3.2×10^{-1}		van Ruth and Villeneuve (2002)	M	14, 363
	3.2×10^{-1}		van Ruth et al. (2001)	M	14
	7.5×10^{-1}		Yaws (2003)	X	259
	7.1×10^{-1}		Dupeux et al. (2022)	Q	260
	1.6		Keshavarz et al. (2022)	Q	
	1.2×10^{-1}		Abney (2021)	Q	401
	5.3×10^{-1}		Duchowicz et al. (2020)	Q	300
	1.8×10^{-1}		Wang et al. (2017)	Q	81, 239
	7.4×10^{-1}		Wang et al. (2017)	Q	81, 240
	1.3		Wang et al. (2017)	Q	81, 241
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	4.6×10^{-1}		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	68
		7600	Kühne et al. (2005)	Q	
	6.1×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	7.0×10^{-1}		Yao et al. (2002)	Q	230
	4.7×10^{-1}		English and Carroll (2001)	Q	231, 232
	6.9×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	7.4×10^{-1}		Yaws et al. (1997)	Q	
	7.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		8200	Kühne et al. (2005)	?	
	7.4×10^{-1}		Yaws (1999)	?	21
	7.0×10^{-1}		Abraham et al. (1990)	?	
2-methyl-2-butanol	6.5×10^{-1}	7900	Brockbank (2013)	L	1
$C_5H_{12}O$	7.1×10^{-1}	8200	Plyasunov and Shock (2000)	L	
(*tert*-pentanol)	7.2×10^{-1}	8200	Fenclová et al. (2010)	M	1
[75-85-4]	7.0×10^{-1}		Merk and Riederer (1997)	M	
MSXVEPNJUHWQHW-UHFFFAOYSA-N	7.1×10^{-1}		Butler et al. (1935)	M	
	1.6		Keshavarz et al. (2022)	Q	
	2.3×10^{-1}		Duchowicz et al. (2020)	Q	
	1.2×10^{-1}		Wang et al. (2017)	Q	81, 239
	6.6×10^{-1}		Wang et al. (2017)	Q	81, 240
	4.8×10^{-1}		Wang et al. (2017)	Q	81, 241
	7.2×10^{-1}		HSDB (2015)	Q	100

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	2.7×10^{-1}		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	68
		7600	Kühne et al. (2005)	Q	
	7.9×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	2.8×10^{-1}		Yao et al. (2002)	Q	230
	7.5×10^{-1}		English and Carroll (2001)	Q	231, 232
	6.9×10^{-1}		Katritzky et al. (1998)	Q	
	6.1×10^{-1}		Yaws et al. (1997)	Q	
	5.0×10^{-1}		Suzuki et al. (1992)	Q	233
	6.0×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	7.2×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		7200	Kühne et al. (2005)	?	
	5.6×10^{-2}		Yaws (1999)	?	21
	7.2×10^{-1}		Abraham et al. (1990)	?	
3-methyl-2-butanol	5.1×10^{-1}	7600	Brockbank (2013)	L	1
$C_5H_{12}O$	5.4×10^{-1}	7800	Fenclová et al. (2010)	M	1
[598-75-4]	5.6×10^{-1}		Duchowicz et al. (2020)	V	187
MXLMTQWGSQIYOW-UHFFFAOYSA-N	2.1×10^{-1}		Duchowicz et al. (2020)	Q	
	2.1×10^{-1}		Wang et al. (2017)	Q	81, 239
	6.9×10^{-1}		Wang et al. (2017)	Q	81, 240
	4.2×10^{-1}		Wang et al. (2017)	Q	81, 241
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	3.1×10^{-1}		Hilal et al. (2008)	Q	
	7.1×10^{-1}		Modarresi et al. (2007)	Q	68
		7600	Kühne et al. (2005)	Q	
	6.1×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	4.5×10^{-1}		Katritzky et al. (1998)	Q	
	5.4×10^{-1}		Yaws et al. (1997)	Q	
		7500	Kühne et al. (2005)	?	
	5.5×10^{-1}		Yaws (1999)	?	21
2,2-dimethyl-1-propanol	3.0×10^{-1}	7800	Brockbank (2013)	L	1, 402
$C_5H_{12}O$	1.9×10^{-1}		Duchowicz et al. (2020)	V	187
[75-84-3]	1.9×10^{-1}		HSDB (2015)	V	
KPSSIOMAKSHJJG-UHFFFAOYSA-N	5.7×10^{-1}		Yaws (2003)	X	259
	3.7×10^{-1}		Dupeux et al. (2022)	Q	260
	2.3×10^{-1}		Duchowicz et al. (2020)	Q	
	1.2×10^{-1}		Wang et al. (2017)	Q	81, 239
	5.9×10^{-1}		Wang et al. (2017)	Q	81, 240
	3.0×10^{-1}		Wang et al. (2017)	Q	81, 241
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	3.1×10^{-1}		Hilal et al. (2008)	Q	
	5.7×10^{-1}		Modarresi et al. (2007)	Q	68
		7600	Kühne et al. (2005)	Q	
	4.9×10^{-1}		Saxena and Hildemann (1996)	E	403
		7900	Kühne et al. (2005)	?	
1-hexanol	7.6×10^{-1}	7800	Brockbank (2013)	L	1
$C_6H_{14}O$	6.6×10^{-1}	8200	Plyasunov and Shock (2000)	L	
[111-27-3]	5.7×10^{-1}	7300	Shunthirasingham et al. (2013)	M	
ZSIAUFGUXNUGDI-UHFFFAOYSA-N	5.1×10^{-1}	6100	Lei et al. (2007)	M	397
	3.9×10^{-1}	5800	Falabella et al. (2006)	M	11, 340
	3.8×10^{-1}		Souchon et al. (2004)	M	
	2.5×10^{-1}		van Ruth et al. (2002)	M	14
	7.3×10^{-1}		van Ruth and Villeneuve (2002)	M	14, 363
	1.6×10^{-1}		van Ruth et al. (2001)	M	14
	3.9×10^{-1}	5800	Gupta et al. (2000)	M	
	9.8×10^{-1}		Altschuh et al. (1999)	M	
	3.5×10^{-1}		Eger et al. (1999)	M	14
	5.8×10^{-1}		Merk and Riederer (1997)	M	
	6.4×10^{-1}		Li and Carr (1993)	M	
	6.9×10^{-1}		Rytting et al. (1978)	M	
	5.8×10^{-1}		Buttery et al. (1969)	M	
	5.3×10^{-1}		Mackay et al. (2006c)	V	
	5.3×10^{-1}		Mackay et al. (1995)	V	
	7.6×10^{-1}		Hwang et al. (1992)	V	
	1.7	5100	Djerki and Laub (1988)	V	
		8200	Abraham (1984)	V	
	6.4×10^{-1}		Hine and Mookerjee (1975)	V	
	6.4×10^{-1}		Butler et al. (1935)	V	
	5.2×10^{-1}		Yaws (2003)	X	259
	5.8×10^{-1}		Dupeux et al. (2022)	Q	260
	2.1×10^{-1}		Keshavarz et al. (2022)	Q	
	1.4		Duchowicz et al. (2020)	Q	300
	1.4×10^{-1}		Wang et al. (2017)	Q	81, 239
	5.0×10^{-1}		Wang et al. (2017)	Q	81, 240
	8.5×10^{-1}		Wang et al. (2017)	Q	81, 241
	6.4×10^{-1}		Li et al. (2014)	Q	242
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	3.7×10^{-1}		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	68
		7900	Kühne et al. (2005)	Q	
	4.1×10^{-1}		Yao et al. (2002)	Q	230, 268

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.2×10^{-1}		English and Carroll (2001)	Q	231, 232
	1.5		Katritzky et al. (1998)	Q	
	4.7×10^{-1}		Yaws et al. (1997)	Q	
	3.9×10^{-1}		Russell et al. (1992)	Q	280
	5.1×10^{-1}		Suzuki et al. (1992)	Q	233
	6.2×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	5.8×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		8400	Kühne et al. (2005)	?	
	4.7×10^{-1}		Yaws (1999)	?	21
	5.3×10^{-1}		Yaws and Yang (1992)	?	21
	6.9×10^{-1}		Abraham et al. (1990)	?	
2-hexanol	3.9×10^{-1}	8100	Brockbank (2013)	L	1
$C_6H_{14}O$	5.2×10^{-1}		Plyasunov and Shock (2000)	L	
[626-93-7]	4.8×10^{-1}		Merk and Riederer (1997)	M	
QNVRIHYSUZMSGM-UHFFFAOYSA-N	4.0×10^{-1}		Duchowicz et al. (2020)	V	187
	4.2×10^{-1}		Yaws (2003)	X	259
	7.3×10^{-1}		Dupeux et al. (2022)	Q	260
	5.4×10^{-1}		Duchowicz et al. (2020)	Q	
	1.7×10^{-1}		Wang et al. (2017)	Q	81, 239
	4.6×10^{-1}		Wang et al. (2017)	Q	81, 240
	5.6×10^{-1}		Wang et al. (2017)	Q	81, 241
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	2.5×10^{-1}		Hilal et al. (2008)	Q	
	2.8×10^{-1}		Modarresi et al. (2007)	Q	68
	4.0×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.8×10^{-1}		Yao et al. (2002)	Q	230
	1.1		Katritzky et al. (1998)	Q	
	4.2×10^{-1}		Yaws et al. (1997)	Q	
	4.2×10^{-1}		Yaws (1999)	?	21
3-hexanol	3.7×10^{-1}	8400	Brockbank (2013)	L	1
$C_6H_{14}O$	4.2×10^{-1}	8400	Plyasunov and Shock (2000)	L	
[623-37-0]	2.5×10^{-1}		Duchowicz et al. (2020)	V	187
ZOCHHNOQQHDWHG-UHFFFAOYSA-N	2.3×10^{-1}		Meylan and Howard (1991)	V	
	2.0×10^{-1}		Hine and Mookerjee (1975)	V	
	3.9×10^{-1}	8400	Cabani et al. (1975b)	T	
	2.2×10^{-1}		Yaws (2003)	X	238
	5.4×10^{-1}		Duchowicz et al. (2020)	Q	
	1.7×10^{-1}		Wang et al. (2017)	Q	81, 239
	5.3×10^{-1}		Wang et al. (2017)	Q	81, 240
	2.5×10^{-1}		Wang et al. (2017)	Q	81, 241
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.0×10^{-1}		Gharagheizi et al. (2010)	Q	247
	2.8×10^{-1}		Hilal et al. (2008)	Q	
	4.1×10^{-1}		Modarresi et al. (2007)	Q	68
	4.0×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	5.8×10^{-1}		English and Carroll (2001)	Q	231, 232
	4.1×10^{-1}		Yaws et al. (1997)	Q	
	4.8×10^{-1}		Suzuki et al. (1992)	Q	233
	5.6×10^{-1}		Meylan and Howard (1991)	Q	
	6.0×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	3.9×10^{-1}		Abraham et al. (1990)	?	
2-methyl-1-pentanol	4.6×10^{-1}		Plyasunov and Shock (2000)	L	
$C_6H_{14}O$	2.3×10^{-1}		Duchowicz et al. (2020)	V	187
[105-30-6]	2.3×10^{-1}		HSDB (2015)	V	
PFNHSEQQEPMLNI-UHFFFAOYSA-N	5.4×10^{-1}		Duchowicz et al. (2020)	Q	
	1.7×10^{-1}		Wang et al. (2017)	Q	81, 239
	6.0×10^{-1}		Wang et al. (2017)	Q	81, 240
	5.5×10^{-1}		Wang et al. (2017)	Q	81, 241
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	4.4×10^{-1}		Hilal et al. (2008)	Q	
	4.6×10^{-1}		Modarresi et al. (2007)	Q	68
	3.1×10^{-1}		Yaws et al. (1997)	Q	
	3.1×10^{-1}		Yaws (1999)	?	21
3-methyl-1-pentanol	7.5×10^{-1}	8600	Brockbank (2013)	L	1
$C_6H_{14}O$	1.7×10^{-1}		Wang et al. (2017)	Q	81, 239
[589-35-5]	6.8×10^{-1}		Wang et al. (2017)	Q	81, 240
IWTBVKIGCDZRPL-UHFFFAOYSA-N	9.6×10^{-1}		Wang et al. (2017)	Q	81, 241
	3.3×10^{-1}		Gharagheizi et al. (2012)	Q	
	3.8×10^{-1}		Hilal et al. (2008)	Q	
2-methyl-2-pentanol	2.8×10^{-1}		Duchowicz et al. (2020)	V	187
$C_6H_{14}O$	3.1×10^{-1}		Hine and Mookerjee (1975)	V	
[590-36-3]	2.4×10^{-1}		Duchowicz et al. (2020)	Q	
WFRBDWRZVBPBDO-UHFFFAOYSA-N	1.0×10^{-1}		Wang et al. (2017)	Q	81, 239
	5.1×10^{-1}		Wang et al. (2017)	Q	81, 240
	3.9×10^{-1}		Wang et al. (2017)	Q	81, 241
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	3.2×10^{-1}		Hilal et al. (2008)	Q	
	7.7×10^{-1}		Modarresi et al. (2007)	Q	68
	2.9×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	6.2×10^{-1}		English and Carroll (2001)	Q	231, 232
	6.7×10^{-1}		Katritzky et al. (1998)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.0×10^{-1}		Yaws et al. (1997)	Q	
	3.9×10^{-1}		Suzuki et al. (1992)	Q	233
	4.7×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	3.1×10^{-1}		Abraham et al. (1990)	?	
3-methyl-2-pentanol	5.0×10^{-1}		Plyasunov and Shock (2000)	L	
$C_6H_{14}O$	1.7×10^{-1}		Wang et al. (2017)	Q	81, 239
[565-60-6]	8.1×10^{-1}		Wang et al. (2017)	Q	81, 240
ZXNBBWHRUSXUFZ-UHFFFAOYSA-N	3.6×10^{-1}		Wang et al. (2017)	Q	81, 241
	4.0×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	2.8×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-2-pentanol	2.2×10^{-1}	7300	Brockbank (2013)	L	1
$C_6H_{14}O$	3.5×10^{-1}		Plyasunov and Shock (2000)	L	
[108-11-2]	2.1×10^{-1}		Meylan and Howard (1991)	V	
WVYWICLMDOOCFB-UHFFFAOYSA-N	2.2×10^{-1}		Hine and Mookerjee (1975)	V	
	2.1×10^{-1}		Keshavarz et al. (2022)	Q	
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	
	1.7×10^{-1}		Wang et al. (2017)	Q	81, 239
	5.6×10^{-1}		Wang et al. (2017)	Q	81, 240
	4.7×10^{-1}		Wang et al. (2017)	Q	81, 241
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	2.6×10^{-1}		Hilal et al. (2008)	Q	
	2.8×10^{-1}		Modarresi et al. (2007)	Q	68
		7900	Kühne et al. (2005)	Q	
	2.3×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	5.3×10^{-1}		Katritzky et al. (1998)	Q	
	1.9×10^{-1}		Yaws et al. (1997)	Q	
	4.0×10^{-1}		Suzuki et al. (1992)	Q	233
	5.6×10^{-1}		Meylan and Howard (1991)	Q	
	4.8×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	2.2×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		8700	Kühne et al. (2005)	?	
	2.1×10^{-1}		Yaws (1999)	?	21, 404
	2.2×10^{-1}		Abraham et al. (1990)	?	
2-methyl-3-pentanol	2.9×10^{-1}		Hine and Mookerjee (1975)	V	
$C_6H_{14}O$	1.7×10^{-1}		Wang et al. (2017)	Q	81, 239
[565-67-3]	6.9×10^{-1}		Wang et al. (2017)	Q	81, 240
ISTJMQSHILQAEC-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	81, 241
	3.3×10^{-1}		Hilal et al. (2008)	Q	
	5.8×10^{-1}		Modarresi et al. (2007)	Q	68
	2.9×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	3.7×10^{-1}		English and Carroll (2001)	Q	231, 275
	3.7×10^{-1}		Yaws et al. (1997)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.2×10^{-1}		Suzuki et al. (1992)	Q	233
	5.2×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	2.9×10^{-1}		Abraham et al. (1990)	?	
3-methyl-3-pentanol	2.4×10^{-1}	7300	Brockbank (2013)	L	1
$C_6H_{14}O$	4.7×10^{-1}		Plyasunov and Shock (2000)	L	
[77-74-7]	4.8×10^{-1}		Merk and Riederer (1997)	M	
FRDAATYAJDYRNW-UHFFFAOYSA-N	5.6×10^{-1}		Duchowicz et al. (2020)	V	187
	2.4×10^{-1}		Duchowicz et al. (2020)	Q	
	1.0×10^{-1}		Wang et al. (2017)	Q	81, 239
	5.5×10^{-1}		Wang et al. (2017)	Q	81, 240
	2.8×10^{-1}		Wang et al. (2017)	Q	81, 241
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	2.1×10^{-1}		Hilal et al. (2008)	Q	
	3.3×10^{-1}		Modarresi et al. (2007)	Q	68
	2.9×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	5.6×10^{-1}		Katritzky et al. (1998)	Q	
	7.0×10^{-1}		Yaws et al. (1997)	Q	
2-ethyl-1-butanol	5.4×10^{-1}		Plyasunov and Shock (2000)	L	
$C_6H_{14}O$	1.9×10^{-1}		Duchowicz et al. (2020)	V	187
[97-95-0]	5.4×10^{-1}		Duchowicz et al. (2020)	Q	
TZYRSLHNPKPEFV-UHFFFAOYSA-N	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	4.7×10^{-1}		Hilal et al. (2008)	Q	
	5.5×10^{-1}		Modarresi et al. (2007)	Q	68
	3.5×10^{-1}		Yao et al. (2002)	Q	230
	2.0		Katritzky et al. (1998)	Q	
	4.8×10^{-1}		Yaws et al. (1997)	Q	
	4.8×10^{-1}		Yaws (1999)	?	21
2,2-dimethyl-1-butanol	1.0×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O$	5.4×10^{-1}		Wang et al. (2017)	Q	81, 240
[1185-33-7]	2.7×10^{-1}		Wang et al. (2017)	Q	81, 241
XRMVWAKMXZNZIL-UHFFFAOYSA-N	4.0×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	2.8×10^{-1}		Yaws et al. (1997)	Q	
2,3-dimethyl-1-butanol	1.7×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O$	9.1×10^{-1}		Wang et al. (2017)	Q	81, 240
[19550-30-2]	5.1×10^{-1}		Wang et al. (2017)	Q	81, 241
SXSWMAUXEHKFGX-UHFFFAOYSA-N	8.2×10^{-1}		Yaws et al. (1997)	Q	
	4.2×10^{-1}		Suzuki et al. (1992)	Q	405, 233
	4.7×10^{-1}		Nirmalakhandan and Speece (1988)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-dimethyl-2-butanol	3.8×10^{-1}		Plyasunov and Shock (2000)	L	
$C_6H_{14}O$	9.9×10^{-1}		Duchowicz et al. (2020)	V	187
[594-60-5]	3.0×10^{-1}		Hine and Mookerjee (1975)	V	406
IKECULIHBUCAKR-UHFFFAOYSA-N	9.3×10^{-2}		Duchowicz et al. (2020)	Q	
	1.2×10^{-1}		Wang et al. (2017)	Q	81, 239
	6.3×10^{-1}		Wang et al. (2017)	Q	81, 240
	3.0×10^{-1}		Wang et al. (2017)	Q	81, 241
	2.0×10^{-1}		Hilal et al. (2008)	Q	
	2.4×10^{-1}		Modarresi et al. (2007)	Q	68
	1.0		Yaffe et al. (2003)	Q	249, 250
	6.0×10^{-1}		Katritzky et al. (1998)	Q	
3,3-dimethyl-1-butanol	1.0×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O$	5.6×10^{-1}		Wang et al. (2017)	Q	81, 240
[624-95-3]	1.6		Wang et al. (2017)	Q	81, 241
DUXCSEISVMREAX-UHFFFAOYSA-N	2.4×10^{-1}		Gharagheizi et al. (2012)	Q	
3,3-dimethyl-2-butanol	1.2×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O$	5.3×10^{-1}		Wang et al. (2017)	Q	81, 240
[464-07-3]	2.0×10^{-1}		Wang et al. (2017)	Q	81, 241
DFOXKPDFWGNLJU-UHFFFAOYSA-N	5.6×10^{-1}		HSDB (2015)	Q	100
	4.0×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	4.9×10^{-1}		Yaws et al. (1997)	Q	
2,2-bis(hydroxymethyl)-1-butanol	1.2×10^{6}		Duchowicz et al. (2020)	V	187
$C_6H_{14}O_3$	8.8×10^{5}		Duchowicz et al. (2020)	Q	
[77-99-6]					
ZJCCRDAZUWHFQH-UHFFFAOYSA-N					
1-heptanol	5.3×10^{-1}	8200	Brockbank (2013)	L	1
$C_7H_{16}O$	5.4×10^{-1}	8600	Plyasunov and Shock (2000)	L	
[111-70-6]	3.8×10^{-1}	7200	Shunthirasingham et al. (2013)	M	
BBMCTIGTTCKYKF-UHFFFAOYSA-N	3.6×10^{-1}	6300	Lei et al. (2007)	M	397
	8.6×10^{-1}		Altschuh et al. (1999)	M	
	1.8×10^{-1}		Shiu and Mackay (1997)	M	
	6.2×10^{-1}		Mackay et al. (2006c)	V	
	6.2×10^{-1}		Shiu and Mackay (1997)	V	
	6.2×10^{-1}		Mackay et al. (1995)	V	
	4.6	5300	Djerki and Laub (1988)	V	
	4.9×10^{-1}	8700	Abraham (1984)	V	
	5.3×10^{-1}		Hine and Mookerjee (1975)	V	
	5.2×10^{-1}		Butler et al. (1935)	V	
	5.2×10^{-1}		Yaws (2003)	X	259
	4.6×10^{-1}		Dupeux et al. (2022)	Q	260
	2.8×10^{-1}		Keshavarz et al. (2022)	Q	
	1.4		Duchowicz et al. (2020)	Q	
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	245

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	3.0×10^{-1}		Hilal et al. (2008)	Q	
	7.3×10^{-1}		Modarresi et al. (2007)	Q	68
		8300	Kühne et al. (2005)	Q	
	1.9×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.9×10^{-1}		Yao et al. (2002)	Q	230
	5.0×10^{-1}		English and Carroll (2001)	Q	231, 232
	1.3		Katritzky et al. (1998)	Q	
	5.2×10^{-1}		Yaws et al. (1997)	Q	
	1.8×10^{-1}		Russell et al. (1992)	Q	280
	3.9×10^{-1}		Suzuki et al. (1992)	Q	233
	5.0×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	3.8×10^{-1}		Rumble (2021)	?	407
	5.2×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		9400	Kühne et al. (2005)	?	
	5.2×10^{-1}		Yaws (1999)	?	21
	8.5×10^{-1}		Yaws and Yang (1992)	?	21
	5.0×10^{-1}		Abraham et al. (1990)	?	
2-heptanol	3.3×10^{-1}	8700	Brockbank (2013)	L	1
$C_7H_{16}O$	4.1×10^{-1}		Plyasunov and Shock (2000)	L	
[543-49-7]	1.8×10^{-1}		Duchowicz et al. (2020)	V	187
CETWDUZRCINIHU-UHFFFAOYSA-N	1.2×10^{-1}		Yaws (2003)	X	259
	1.2×10^{-1}		Yaws (2003)	X	238, 38
	5.8×10^{-1}		Dupeux et al. (2022)	Q	260
	5.5×10^{-1}		Duchowicz et al. (2020)	Q	
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-1}		Gharagheizi et al. (2010)	Q	247
	2.0×10^{-1}		Hilal et al. (2008)	Q	
	2.5×10^{-1}		Modarresi et al. (2007)	Q	68
	2.6×10^{-1}		Yao et al. (2002)	Q	230
	1.2×10^{-1}		Yaws et al. (1997)	Q	
	1.7×10^{-1}		Yaws (1999)	?	21, 38
3-heptanol	3.2×10^{-1}	9100	Brockbank (2013)	L	1
$C_7H_{16}O$	3.1×10^{-1}		Plyasunov and Shock (2000)	L	
[589-82-2]	3.5×10^{-1}		Duchowicz et al. (2020)	V	187
RZKSECIXORKHQS-UHFFFAOYSA-N	5.5×10^{-1}		Duchowicz et al. (2020)	Q	
	1.3×10^{-1}		Wang et al. (2017)	Q	81, 239
	4.1×10^{-1}		Wang et al. (2017)	Q	81, 240
	2.2×10^{-1}		Wang et al. (2017)	Q	81, 241
	1.9×10^{-1}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	246

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.0×10^{-1}		Modarresi et al. (2007)	Q	68
	3.7×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	5.3×10^{-1}		Katritzky et al. (1998)	Q	
	2.1×10^{-1}		Yaws et al. (1997)	Q	
4-heptanol $C_7H_{16}O$ [589-55-9] YVBCULSIZWMTFY-UHFFFAOYSA-N	3.4×10^{-1}	9100	Plyasunov and Shock (2000)	L	
	3.5×10^{-1}	9100	Cabani et al. (1975b)	T	
	1.8×10^{-1}		Gharagheizi et al. (2012)	Q	
	2.2×10^{-1}		Yaws et al. (1997)	Q	
2-methyl-1-hexanol $C_7H_{16}O$ [624-22-6] LCFKURIJYIJNRU-UHFFFAOYSA-N	6.9×10^{-1}	11000	Hiatt (2013)	M	
	1.7×10^{-1}		Yaws et al. (1997)	Q	
3-methyl-1-hexanol $C_7H_{16}O$ [13231-81-7] YGZVAQICDGBHMD-UHFFFAOYSA-N	1.3×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-1-hexanol $C_7H_{16}O$ [818-49-5] YNPVNLWKVZZBTM-UHFFFAOYSA-N	1.3×10^{-1}		Yaws et al. (1997)	Q	
5-methyl-1-hexanol $C_7H_{16}O$ [627-98-5] ZVHAANQOQZVVFD-UHFFFAOYSA-N	2.8×10^{-1}		Yaws et al. (1997)	Q	
2-methyl-2-hexanol $C_7H_{16}O$ [625-23-0] KRIMXCDMVRMCTC-UHFFFAOYSA-N	9.1×10^{-2}		Wang et al. (2017)	Q	81, 239
	4.0×10^{-1}		Wang et al. (2017)	Q	81, 240
	3.8×10^{-1}		Wang et al. (2017)	Q	81, 241
	6.7×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	6.4×10^{-1}		Yaws et al. (1997)	Q	
3-methyl-2-hexanol $C_7H_{16}O$ [2313-65-7] IRLSKJITMWPWNY-UHFFFAOYSA-N	1.5×10^{-1}		Yaws (2003)	X	238
	1.7×10^{-1}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-1}		Gharagheizi et al. (2010)	Q	247
	4.9×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-2-hexanol $C_7H_{16}O$ [2313-61-3] KZUBXUKRWLMPIO-UHFFFAOYSA-N	1.6×10^{-1}		Wang et al. (2017)	Q	81, 239
	5.1×10^{-1}		Wang et al. (2017)	Q	81, 240
	4.7×10^{-1}		Wang et al. (2017)	Q	81, 241
	5.0×10^{-1}		Yaws et al. (1997)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5-methyl-2-hexanol	1.6×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O$	4.3×10^{-1}		Wang et al. (2017)	Q	81, 240
[627-59-8]	5.9×10^{-1}		Wang et al. (2017)	Q	81, 241
ZDVJGWXFXGJSIU-UHFFFAOYSA-N	2.4×10^{-1}		Gharagheizi et al. (2012)	Q	
	4.2×10^{-1}		Yaws et al. (1997)	Q	
2-methyl-3-hexanol	5.8×10^{-1}		Yaws et al. (1997)	Q	
$C_7H_{16}O$					
[617-29-8]					
RGRUUTLDBCWYBL-UHFFFAOYSA-N					
3-methyl-3-hexanol	9.1×10^{-2}		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O$	4.7×10^{-1}		Wang et al. (2017)	Q	81, 240
[597-96-6]	2.6×10^{-1}		Wang et al. (2017)	Q	81, 241
KYWJZCSJMOILIZ-UHFFFAOYSA-N	9.2×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	7.7×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-3-hexanol	1.1×10^{-1}		Yaws (2003)	X	238
$C_7H_{16}O$	1.0×10^{-1}		Gharagheizi et al. (2012)	Q	
[615-29-2]	1.3×10^{-1}		Gharagheizi et al. (2010)	Q	247
NZPGYIBESMMUFU-UHFFFAOYSA-N	5.2×10^{-1}		Yaws et al. (1997)	Q	
5-methyl-3-hexanol	1.6×10^{-1}		Yaws (2003)	X	238
$C_7H_{16}O$	1.5×10^{-1}		Gharagheizi et al. (2012)	Q	
[623-55-2]	1.2×10^{-1}		Gharagheizi et al. (2010)	Q	247
RGCZULIFYUPTAR-UHFFFAOYSA-N	5.4×10^{-1}		Yaws et al. (1997)	Q	
2-ethyl-1-pentanol	1.0×10^{-1}		Yaws (2003)	X	238
$C_7H_{16}O$	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
[27522-11-8]	1.1×10^{-1}		Gharagheizi et al. (2010)	Q	247
UKFQWAVMIMCNEH-UHFFFAOYSA-N	3.4×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-1-pentanol	9.1×10^{-2}		Yaws (2003)	X	238
$C_7H_{16}O$	1.7×10^{-1}		Gharagheizi et al. (2012)	Q	
[66225-51-2]	1.2×10^{-1}		Gharagheizi et al. (2010)	Q	247
DVEFUHVVWJONKR-UHFFFAOYSA-N	3.4×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-2-pentanol	1.1×10^{-1}		Yaws (2003)	X	238
$C_7H_{16}O$	1.7×10^{-1}		Gharagheizi et al. (2012)	Q	
[609-27-8]	1.2×10^{-1}		Gharagheizi et al. (2010)	Q	247
NEHRITNOSGFGGS-UHFFFAOYSA-N	4.9×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-3-pentanol	3.0×10^{-1}		Plyasunov and Shock (2000)	L	
$C_7H_{16}O$	1.2		Yaffe et al. (2003)	Q	249, 250
[597-49-9]	1.1		Yaws et al. (1997)	Q	
XKIRHOWVQWCYBT-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2-dimethyl-1-pentanol	9.6×10^{-2}		Yaws (2003)	X	238
$C_7H_{16}O$	5.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[2370-12-9]	1.1×10^{-1}		Gharagheizi et al. (2010)	Q	247
QTOMCRXZFDHJOL-UHFFFAOYSA-N	3.3×10^{-1}		Yaws et al. (1997)	Q	
2,3-dimethyl-1-pentanol	3.6×10^{-1}		Yaws et al. (1997)	Q	
$C_7H_{16}O$					
[10143-23-4]					
MIBBFRQOCRYDDB-UHFFFAOYSA-N					
2,4-dimethyl-1-pentanol	9.4×10^{-2}		Yaws (2003)	X	238
$C_7H_{16}O$	9.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[6305-71-1]	1.0×10^{-1}		Gharagheizi et al. (2010)	Q	247
OVOVDHYEOQJKMD-UHFFFAOYSA-N	3.3×10^{-1}		Yaws et al. (1997)	Q	
3,3-dimethyl-1-pentanol	3.5×10^{-1}		Yaws et al. (1997)	Q	
$C_7H_{16}O$					
[19264-94-9]					
IFDHMBHPLKHMOY-UHFFFAOYSA-N					
3,4-dimethyl-1-pentanol	1.6×10^{-1}		Yaws (2003)	X	238
$C_7H_{16}O$	1.6×10^{-1}		Gharagheizi et al. (2012)	Q	
[6570-87-2]	1.1×10^{-1}		Gharagheizi et al. (2010)	Q	247
SVJNECJVNWTYQG-UHFFFAOYSA-N	3.5×10^{-1}		Yaws et al. (1997)	Q	
4,4-dimethyl-1-pentanol	8.5×10^{-2}		Yaws (2003)	X	238
$C_7H_{16}O$	1.4×10^{-1}		Gharagheizi et al. (2012)	Q	
[3121-79-7]	1.1×10^{-1}		Gharagheizi et al. (2010)	Q	247
OWCNPTHAWPMOJU-UHFFFAOYSA-N	3.8×10^{-1}		Yaws et al. (1997)	Q	
2,3-dimethyl-2-pentanol	9.2×10^{-1}		Yaffe et al. (2003)	Q	249, 250
$C_7H_{16}O$	8.6×10^{-1}		Yaws et al. (1997)	Q	
[4911-70-0]					
YRSIFCHKXFKNME-UHFFFAOYSA-N					
2,4-dimethyl-2-pentanol	4.0×10^{-1}		Yaffe et al. (2003)	Q	249, 273
$C_7H_{16}O$	5.7×10^{-1}		Yaws et al. (1997)	Q	
[625-06-9]					
FMLSQAUAAGVTJO-UHFFFAOYSA-N					
3,3-dimethyl-2-pentanol	9.0×10^{-2}		Yaws (2003)	X	238
$C_7H_{16}O$	1.0×10^{-1}		Gharagheizi et al. (2012)	Q	
[19781-24-9]	1.2×10^{-1}		Gharagheizi et al. (2010)	Q	247
FCUOIGTWJDBTHR-UHFFFAOYSA-N	5.5×10^{-1}		Yaws et al. (1997)	Q	
3,4-dimethyl-2-pentanol	1.8×10^{-1}		Gharagheizi et al. (2012)	Q	
$C_7H_{16}O$	4.7×10^{-1}		Yaws et al. (1997)	Q	
[64502-86-9]					
SODKTKJZYBOMMT-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,4-dimethyl-2-pentanol $C_7H_{16}O$ [6144-93-0] OIBKGNPMOMMSSI-UHFFFAOYSA-N	6.8×10^{-1}		Yaws et al. (1997)	Q	
2,2-dimethyl-3-pentanol $C_7H_{16}O$ [3970-62-5] HMSVXZJWPVIVIV-UHFFFAOYSA-N	4.0×10^{-1} 4.0×10^{-1}		Yaffe et al. (2003) Yaws et al. (1997)	Q Q	249, 250
2,3-dimethyl-3-pentanol $C_7H_{16}O$ [595-41-5] RFZHJHSNHYIRNE-UHFFFAOYSA-N	9.2×10^{-1} 9.2×10^{-1}		Yaffe et al. (2003) Yaws et al. (1997)	Q Q	249, 250
2,4-dimethyl-3-pentanol $C_7H_{16}O$ [600-36-2] BAYAKMPRFGNNFW-UHFFFAOYSA-N	4.0×10^{-1} 3.8×10^{-1}		Yaffe et al. (2003) Yaws et al. (1997)	Q Q	249, 250
2-ethyl-2-methyl-1-butanol $C_7H_{16}O$ [18371-13-6] KMWHQWJVSALJAW-UHFFFAOYSA-N	4.3×10^{-1}		Yaws et al. (1997)	Q	
2-ethyl-3-methyl-1-butanol $C_7H_{16}O$ [32444-34-1] OXFFPTMSBXBVLZ-UHFFFAOYSA-N	3.8×10^{-1}		Yaws et al. (1997)	Q	
2,2,3-trimethyl-1-butanol $C_7H_{16}O$ [55505-23-2] FAMOAJMEFGYSNY-UHFFFAOYSA-N	8.3×10^{-2} 6.2×10^{-2} 1.0×10^{-1} 4.3×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	238 247
2,3,3-trimethyl-1-butanol $C_7H_{16}O$ [36794-64-6] IWWVOLGZHKFWKK-UHFFFAOYSA-N	7.9×10^{-2} 1.0×10^{-1} 1.0×10^{-1} 4.0×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	238 247
2,3,3-trimethyl-2-butanol $C_7H_{16}O$ [594-83-2] OKXVARYIKDXAEO-UHFFFAOYSA-N	2.7×10^{-1}		Yaws et al. (1997)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-octanol	3.4×10^{-1}	9000	Brockbank (2013)	L	1
$C_8H_{18}O$	4.1×10^{-1}	8900	Plyasunov and Shock (2000)	L	
[111-87-5]	1.7×10^{-1}	7000	Wu et al. (2022a)	M	
KBPLFHHGFOOTCA-UHFFFAOYSA-N	2.1×10^{-1}	6900	Shunthirasingham et al. (2013)	M	
	1.9×10^{-1}	6000	Lei et al. (2007)	M	397
	6.5×10^{-1}		Altschuh et al. (1999)	M	
	2.7×10^{-1}		Eger et al. (1999)	M	14
	4.0×10^{-1}		Buttery et al. (1969)	M	
	3.8×10^{-1}		Mackay et al. (2006c)	V	
	2.4×10^{-1}		Mackay et al. (1995)	V	
		8900	Abraham (1984)	V	
	4.1×10^{-1}		Hine and Mookerjee (1975)	V	
	4.1×10^{-1}		Butler et al. (1935)	V	
	3.9×10^{-1}		Yaws (2003)	X	259
	3.6×10^{-1}		Dupeux et al. (2022)	Q	260
	3.8×10^{-1}		Keshavarz et al. (2022)	Q	
	1.4		Duchowicz et al. (2020)	Q	300
	3.3×10^{-1}		Savary et al. (2014)	Q	
	4.1×10^{-1}		Li et al. (2014)	Q	242
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	2.5×10^{-1}		Hilal et al. (2008)	Q	
	5.6×10^{-1}		Modarresi et al. (2007)	Q	68
		8600	Kühne et al. (2005)	Q	
	3.2×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	2.6×10^{-1}		Yao et al. (2002)	Q	230
	4.0×10^{-1}		English and Carroll (2001)	Q	231, 261
	1.2		Katritzky et al. (1998)	Q	
	3.9×10^{-1}		Yaws et al. (1997)	Q	
	3.0×10^{-1}		Suzuki et al. (1992)	Q	233
	3.9×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	4.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		7700	Kühne et al. (2005)	?	
	3.9×10^{-1}		Yaws (1999)	?	21
	6.2×10^{-1}		Yaws and Yang (1992)	?	21
	4.0×10^{-1}		Abraham et al. (1990)	?	
2-octanol	2.7×10^{-1}	9600	Brockbank (2013)	L	1
$C_8H_{18}O$	3.5×10^{-1}		Plyasunov and Shock (2000)	L	
[123-96-6]	2.7×10^{-1}		HSDB (2015)	V	
SJWFXCIHNDVPSH-UHFFFAOYSA-N	2.7×10^{-1}		Meylan and Howard (1991)	V	
	9.6×10^{-1}		Yaws (2003)	X	259
	4.2×10^{-1}		Dupeux et al. (2022)	Q	260
	3.8×10^{-1}		Keshavarz et al. (2022)	Q	
	5.6×10^{-1}		Duchowicz et al. (2020)	Q	300

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	1.7×10^{-1}		Hilal et al. (2008)	Q	
	2.0×10^{-1}		Modarresi et al. (2007)	Q	68
	3.0×10^{-1}		Yaws et al. (1997)	Q	
	3.2×10^{-1}		Meylan and Howard (1991)	Q	
	8.0×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	9.6×10^{-1}		Yaws (1999)	?	21
3-octanol	3.2×10^{-1}		Plyasunov and Shock (2000)	L	
$C_8H_{18}O$	1.2×10^{-1}	8300	Wu et al. (2022a)	M	
[589-98-0]	1.3×10^{-1}		Yaws (2003)	X	238
NMRPBPVERJPACX-UHFFFAOYSA-N	1.1×10^{-1}		Wang et al. (2017)	Q	81, 239
	3.2×10^{-1}		Wang et al. (2017)	Q	81, 240
	2.3×10^{-1}		Wang et al. (2017)	Q	81, 241
	1.2×10^{-1}		Gharagheizi et al. (2012)	Q	
	7.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
	3.1×10^{-1}		Yaws et al. (1997)	Q	
4-octanol	1.3×10^{-1}		Gharagheizi et al. (2012)	Q	
$C_8H_{18}O$	2.9×10^{-1}		Yaws et al. (1997)	Q	
[589-62-8]					
WOFPPJOZXUTRAU-UHFFFAOYSA-N					
2-methyl-1-heptanol	9.1×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	5.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[60435-70-3]	7.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
QZESEQBMSFFHRY-UHFFFAOYSA-N	3.4×10^{-1}		Yaws et al. (1997)	Q	408
3-methyl-1-heptanol	8.9×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	7.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
[1070-32-2]	2.1×10^{-1}		Yaws et al. (1997)	Q	
MUPPEBVXFKNMCI-UHFFFAOYSA-N					
4-methyl-1-heptanol	9.3×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	7.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
[817-91-4]	2.3×10^{-1}		Yaws et al. (1997)	Q	
LLUQZGDMUIMPTC-UHFFFAOYSA-N					
5-methyl-1-heptanol	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
$C_8H_{18}O$	2.1×10^{-1}		Yaws et al. (1997)	Q	
[7212-53-5]					
KFARNLMRENFOHE-UHFFFAOYSA-N					
6-methyl-1-heptanol	1.1×10^{-1}		Duchowicz et al. (2020)	V	187
$C_8H_{18}O$	1.1×10^{-1}		HSDB (2015)	V	
[1653-40-3]	5.6×10^{-1}		Duchowicz et al. (2020)	Q	
BWDBEAQIHAEVLV-UHFFFAOYSA-N	2.0×10^{-1}		Yaws et al. (1997)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-2-heptanol $C_8H_{18}O$ [625-25-2] ACBMYYVZWKYLIP-UHFFFAOYSA-N	5.1×10^{-1}		Yaws et al. (1997)	Q	
3-methyl-2-heptanol	7.8×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	9.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[31367-46-1]	7.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
SZERMVMTUUAYML-UHFFFAOYSA-N	3.9×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-2-heptanol	1.6×10^{-1}		Gharagheizi et al. (2012)	Q	
$C_8H_{18}O$	3.4×10^{-1}		Yaws et al. (1997)	Q	
[56298-90-9] GUHWHNUGIGOSCN-UHFFFAOYSA-N					
5-methyl-2-heptanol	1.0×10^{-1}		Yaws (2003)	X	238
$C_8H_{18}O$	1.7×10^{-1}		Gharagheizi et al. (2012)	Q	
[54630-50-1]	7.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
FYMBAYNKBWGEIK-UHFFFAOYSA-N	3.3×10^{-1}		Yaws et al. (1997)	Q	
6-methyl-2-heptanol	1.6×10^{-1}		Gharagheizi et al. (2012)	Q	
$C_8H_{18}O$	3.3×10^{-1}		Yaws et al. (1997)	Q	
[4730-22-7] FCOUHTHQYOMLJT-UHFFFAOYSA-N					
2-methyl-3-heptanol $C_8H_{18}O$ [18720-62-2] QGVFLDUEHSIZIG-UHFFFAOYSA-N	3.8×10^{-1}		Yaws et al. (1997)	Q	
3-methyl-3-heptanol $C_8H_{18}O$ [5582-82-1] PQOSNJHBSNZITJ-UHFFFAOYSA-N	2.9×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-3-heptanol	7.4×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	4.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[14979-39-6]	8.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
BKQICAFAUMRYLZ-UHFFFAOYSA-N	5.3×10^{-1}		Yaws et al. (1997)	Q	
5-methyl-3-heptanol	8.7×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	6.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[18720-65-5]	7.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
SECKOSOTZOBWEI-UHFFFAOYSA-N	5.6×10^{-1}		Yaws et al. (1997)	Q	
6-methyl-3-heptanol	8.8×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	7.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[18720-66-6]	7.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
MNBIBGDICHMQFN-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-4-heptanol $C_8H_{18}O$ [21570-35-4] QXPLZEKPCGUWEM-UHFFFAOYSA-N	3.9×10^{-1}		Yaws et al. (1997)	Q	
3-methyl-4-heptanol $C_8H_{18}O$ [1838-73-9] JMRDKKYZLXDPLN-UHFFFAOYSA-N	8.2×10^{-2} 6.2×10^{-2} 8.2×10^{-2} 4.1×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	238 247
4-methyl-4-heptanol $C_8H_{18}O$ [598-01-6] IQXKGRKRIRMQCQ-UHFFFAOYSA-N	4.5×10^{-1}		Yaws et al. (1997)	Q	
2-ethyl-1-hexanol $C_8H_{18}O$ [104-76-7] YIWUKEYIRIRTPP-UHFFFAOYSA-N	4.6×10^{-1} 1.5×10^{-1} 3.7×10^{-1} 3.8×10^{-1} 5.6×10^{-1} 7.0×10^{-2} 2.5×10^{-1} 3.1×10^{-1} 3.1×10^{-1} 3.1×10^{-1} 4.0×10^{-1} 1.1×10^{-1} 4.3×10^{-1} 4.2×10^{-2}	7200	Plyasunov and Shock (2000) Wu et al. (2022a) Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Gharagheizi et al. (2012) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Yao et al. (2002) Yaws et al. (1997) Yaws (1999)	L M V V Q Q Q Q Q Q Q Q Q ?	 187 272, 244 245 246 68 230, 268 21
3-ethyl-1-hexanol $C_8H_{18}O$ [41065-95-6] LWWJDXKGQVEZKT-UHFFFAOYSA-N	7.0×10^{-2} 9.5×10^{-2} 7.5×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
4-ethyl-1-hexanol $C_8H_{18}O$ [66576-32-7] RLGDVTUGYZAYIX-UHFFFAOYSA-N	7.0×10^{-2} 9.5×10^{-2} 7.5×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
2,2-dimethyl-1-hexanol $C_8H_{18}O$ [2370-13-0] GSSDZVRLQDXOPL-UHFFFAOYSA-N	4.9×10^{-1}		Yaws et al. (1997)	Q	
2,3-dimethyl-1-hexanol $C_8H_{18}O$ HIYTVAULOHUDEC-UHFFFAOYSA-N	7.0×10^{-2} 5.5×10^{-2} 6.8×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4-dimethyl-1-hexanol	6.9×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	5.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[3965-59-1]	6.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
GDRBQWCGBCJTLB-UHFFFAOYSA-N	4.6×10^{-1}		Yaws et al. (1997)	Q	
2,5-dimethyl-1-hexanol	6.5×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	6.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[6886-16-4]	6.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
OBOHUKJIPIBYTA-UHFFFAOYSA-N	4.1×10^{-1}		Yaws et al. (1997)	Q	
3,3-dimethyl-1-hexanol	5.7×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	1.0×10^{-1}		Gharagheizi et al. (2012)	Q	
[10524-70-6]	7.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
RAKYQWCHMSXUEG-UHFFFAOYSA-N					
3,4-dimethyl-1-hexanol	6.3×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	9.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[66576-57-6]	7.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
QVFKMROLPSPCIX-UHFFFAOYSA-N					
3,5-dimethyl-1-hexanol	6.1×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
[13501-73-0]	7.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
WETBJXIDTZXCBL-UHFFFAOYSA-N	3.6×10^{-1}		Yaws et al. (1997)	Q	
4,4-dimethyl-1-hexanol	5.6×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	1.0×10^{-1}		Gharagheizi et al. (2012)	Q	
[6481-95-4]	7.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
VZWIUKUDEGQHIO-UHFFFAOYSA-N					
4,5-dimethyl-1-hexanol	6.2×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	1.0×10^{-1}		Gharagheizi et al. (2012)	Q	
[60564-76-3]	7.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
QABJATQYUASJEM-UHFFFAOYSA-N					
5,5-dimethyl-1-hexanol	5.6×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	1.0×10^{-1}		Gharagheizi et al. (2012)	Q	
[2768-18-5]	7.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
QYFVEEMPFRRFNN-UHFFFAOYSA-N					
3-ethyl-2-hexanol	7.7×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	1.0×10^{-1}		Gharagheizi et al. (2012)	Q	
[24448-19-9]	7.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
YBQZSEZVMFENOM-UHFFFAOYSA-N	5.6×10^{-1}		Yaws et al. (1997)	Q	
4-ethyl-2-hexanol	7.7×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	1.5×10^{-1}		Gharagheizi et al. (2012)	Q	
ALAPJJMGVQNJIU-UHFFFAOYSA-N	7.7×10^{-2}		Gharagheizi et al. (2010)	Q	247

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-dimethyl-2-hexanol $C_8H_{18}O$ [19550-03-9] BFKOEFFCVFMWPF-UHFFFAOYSA-N	7.0×10^{-1}		Yaws et al. (1997)	Q	
2,4-dimethyl-2-hexanol $C_8H_{18}O$ [42328-76-7] RTRZHEPXWQXCCI-UHFFFAOYSA-N	8.9×10^{-1}		Yaws et al. (1997)	Q	
2,5-dimethyl-2-hexanol $C_8H_{18}O$ [3730-60-7] JPUIYNHIEXIFMV-UHFFFAOYSA-N	8.5×10^{-1}		Yaws et al. (1997)	Q	
3,3-dimethyl-2-hexanol $C_8H_{18}O$ [22025-20-3] LTTHCWFPLXSQOD-UHFFFAOYSA-N	7.5×10^{-2} 5.5×10^{-2} 7.8×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
3,4-dimethyl-2-hexanol $C_8H_{18}O$ [19550-05-1] LBJWJHMCZHKLQU-UHFFFAOYSA-N	6.8×10^{-2} 1.1×10^{-1} 7.7×10^{-2} 5.2×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	238 247
3,5-dimethyl-2-hexanol $C_8H_{18}O$ [66576-27-0] VGGMROOHXNLMTP-UHFFFAOYSA-N	8.1×10^{-2} 8.1×10^{-2} 7.7×10^{-2} 7.0×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	238 247
4,4-dimethyl-2-hexanol $C_8H_{18}O$ CJGWLHDFPXIKQX-UHFFFAOYSA-N	7.2×10^{-2} 1.3×10^{-1} 7.4×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
4,5-dimethyl-2-hexanol $C_8H_{18}O$ KHSOOQUMPPYGAW-UHFFFAOYSA-N	7.9×10^{-2} 1.3×10^{-1} 7.5×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
5,5-dimethyl-2-hexanol $C_8H_{18}O$ [31841-77-7] NMSUCVXVCHZTEH-UHFFFAOYSA-N	6.7×10^{-2} 1.4×10^{-1} 7.4×10^{-2} 6.0×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	238 247
3-ethyl-3-hexanol $C_8H_{18}O$ [597-76-2] WNDLTOTUHMHNOC-UHFFFAOYSA-N	7.2×10^{-1}		Yaws et al. (1997)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-ethyl-3-hexanol	1.3×10^{-1}		Yaws (2003)	X	238
$C_8H_{18}O$	8.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
[19780-44-0]	6.3×10^{-1}		Yaws et al. (1997)	Q	
BOJLCKCCKQMGKD-UHFFFAOYSA-N					
2,2-dimethyl-3-hexanol	6.2×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	3.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[4209-90-9]	8.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
PFHLGQKVKALLMD-UHFFFAOYSA-N	7.8×10^{-1}		Yaws et al. (1997)	Q	
2,3-dimethyl-3-hexanol	7.4×10^{-1}		Yaws et al. (1997)	Q	
$C_8H_{18}O$					
[4166-46-5]					
CGWJMIUMPDDHQC-UHFFFAOYSA-N					
2,4-dimethyl-3-hexanol	7.0×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	3.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[13432-25-2]	8.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
UCRQJBCLZKHOGX-UHFFFAOYSA-N	7.0×10^{-1}		Yaws et al. (1997)	Q	
2,5-dimethyl-3-hexanol	7.2×10^{-1}		Yaws et al. (1997)	Q	
$C_8H_{18}O$					
[19550-07-3]					
SNKTZHPOKPYBPT-UHFFFAOYSA-N					
3,4-dimethyl-3-hexanol	8.6×10^{-1}		Yaws et al. (1997)	Q	
$C_8H_{18}O$					
[19550-08-4]					
FJXOYCIYKQJAAF-UHFFFAOYSA-N					
3,5-dimethyl-3-hexanol	8.9×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	1.4×10^{-1}		Gharagheizi et al. (2012)	Q	
[4209-91-0]	7.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
INMGJWCKWKKMPN-UHFFFAOYSA-N	8.6×10^{-1}		Yaws et al. (1997)	Q	
4,4-dimethyl-3-hexanol	7.2×10^{-1}		Yaws et al. (1997)	Q	
$C_8H_{18}O$					
[19550-09-5]					
BARKHVPKOOSMNW-UHFFFAOYSA-N					
4,5-dimethyl-3-hexanol	8.7×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	4.9×10^{-2}		Gharagheizi et al. (2012)	Q	
UAVZZCGGBCLHIP-UHFFFAOYSA-N	7.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
5,5-dimethyl-3-hexanol	8.4×10^{-1}		Yaws et al. (1997)	Q	
$C_8H_{18}O$					
[66576-31-6]					
NPZRPUOKIPAIEL-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-propyl-1-pentanol $C_8H_{18}O$ [58175-57-8] LASHFHLFDRTERB-UHFFFAOYSA-N	4.1×10^{-1}		Yaws et al. (1997)	Q	
2-ethyl-2-methyl-1-pentanol $C_8H_{18}O$ [5970-63-8] VZCOFGHOKLEMPL-UHFFFAOYSA-N	4.3×10^{-1}		Yaws et al. (1997)	Q	
2-ethyl-3-methyl-1-pentanol $C_8H_{18}O$ ALPFTHGDLMTYRM-UHFFFAOYSA-N	6.7×10^{-2} 6.0×10^{-2} 6.8×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
2-ethyl-4-methyl-1-pentanol $C_8H_{18}O$ [106-67-2] QCHSJPKDWOFACC-UHFFFAOYSA-N	4.4×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-2-methyl-1-pentanol $C_8H_{18}O$ VWQDMMBTEFDWNM-UHFFFAOYSA-N	6.9×10^{-2} 5.7×10^{-2} 6.8×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
3-ethyl-3-methyl-1-pentanol $C_8H_{18}O$ [10524-71-7] XYUCPYMMHKJJSS-UHFFFAOYSA-N	6.3×10^{-2} 8.4×10^{-2} 7.2×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
3-ethyl-4-methyl-1-pentanol $C_8H_{18}O$ [38514-13-5] RWIFVESHBHTZEM-UHFFFAOYSA-N	6.9×10^{-2} 8.3×10^{-2} 7.0×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
2,2,3-trimethyl-1-pentanol $C_8H_{18}O$ [57409-53-7] GBONVOIRPAJSLA-UHFFFAOYSA-N	4.7×10^{-1}		Yaws et al. (1997)	Q	
2,2,4-trimethyl-1-pentanol $C_8H_{18}O$ [123-44-4] CWPPDTVYIJETDF-UHFFFAOYSA-N	5.6×10^{-1}		Yaws et al. (1997)	Q	
2,3,3-trimethyl-1-pentanol $C_8H_{18}O$ LFRFDOWJBYDJGD-UHFFFAOYSA-N	5.7×10^{-2} 6.0×10^{-2} 6.7×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
2,3,4-trimethyl-1-pentanol $C_8H_{18}O$ [6570-88-3] PAZDSSMTPLLLIR-UHFFFAOYSA-N	5.5×10^{-2} 7.3×10^{-2} 6.3×10^{-2} 3.6×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	238 247

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4,4-trimethyl-1-pentanol $C_8H_{18}O$ [16325-63-6] ZNRVRWHPZZOTIE-UHFFFAOYSA-N	5.2×10^{-2} 5.2×10^{-1}		Gharagheizi et al. (2012) Yaws et al. (1997)	Q Q	
3,3,4-trimethyl-1-pentanol $C_8H_{18}O$ OIPMJJVCOSACDS-UHFFFAOYSA-N	6.2×10^{-2} 7.6×10^{-2} 6.9×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
3,4,4-trimethyl-1-pentanol $C_8H_{18}O$ [16325-64-7] FQNYRSRCONKFCN-UHFFFAOYSA-N	6.2×10^{-2} 7.6×10^{-2} 6.9×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
3-ethyl-2-methyl-2-pentanol $C_8H_{18}O$ [19780-63-3] FRUMTAZIGSJVOJ-UHFFFAOYSA-N	7.4×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-4-methyl-2-pentanol $C_8H_{18}O$ [66576-23-6] PFRFNYYIOSQSDD-UHFFFAOYSA-N	7.6×10^{-2} 9.1×10^{-2} 7.7×10^{-2} 6.3×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	238 247
2,3,3-trimethyl-2-pentanol $C_8H_{18}O$ [23171-85-9] FBWWGYIEJGQWJP-UHFFFAOYSA-N	8.0×10^{-2} 1.2×10^{-1} 6.8×10^{-2} 7.0×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	238 247
2,3,4-trimethyl-2-pentanol $C_8H_{18}O$ [66576-26-9] FTPXXARYDFWPGE-UHFFFAOYSA-N	7.2×10^{-2} 1.7×10^{-1} 6.9×10^{-2} 7.4×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	238 247
2,4,4-trimethyl-2-pentanol $C_8H_{18}O$ [690-37-9] BSYJHYLAMMJNRC-UHFFFAOYSA-N	9.9×10^{-1}		Yaws et al. (1997)	Q	
3,3,4-trimethyl-2-pentanol $C_8H_{18}O$ [19411-41-7] BOBYQFFCQPQLOB-UHFFFAOYSA-N	6.3×10^{-2} 6.5×10^{-2} 7.5×10^{-2} 6.1×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	238 247
3,4,4-trimethyl-2-pentanol $C_8H_{18}O$ [10575-56-1] MXDGSCZQIMQLII-UHFFFAOYSA-N	7.4×10^{-1}		Yaws et al. (1997)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-2-methyl-3-pentanol	7.5×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	8.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[597-05-7]	7.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
DMHIJUVUPKCGLJ-UHFFFAOYSA-N	7.0×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-3-methyl-2-pentanol	7.5×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	5.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[66576-22-5]	7.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
SLBLSROGXMXPPF-UHFFFAOYSA-N					
2,2,3-trimethyl-3-pentanol	1.2		Yaffe et al. (2003)	Q	249, 250
$C_8H_{18}O$	1.1		Yaws et al. (1997)	Q	
[7294-05-5]					
KLIHWYNSISMOMR-UHFFFAOYSA-N					
2,2,4-trimethyl-3-pentanol	8.9×10^{-1}		Yaws et al. (1997)	Q	
$C_8H_{18}O$					
[5162-48-1]					
AXINNNJHLJWMTC-UHFFFAOYSA-N					
2,3,4-trimethyl-3-pentanol	6.4×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	7.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[3054-92-0]	7.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
PLSMHHUFDLYURK-UHFFFAOYSA-N	7.6×10^{-1}		Yaws et al. (1997)	Q	
3-methyl-2-(1-methylethyl)-1-butanol	6.6×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	5.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[18593-92-5]	6.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
IDGDEUZERZKYHG-UHFFFAOYSA-N	4.9×10^{-1}		Yaws et al. (1997)	Q	
2,2,3,3-tetramethyl-1-butanol	5.0×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66576-24-7]	6.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
OCTRJUXIYWWVAR-UHFFFAOYSA-N					
2,2-diethyl-1-butanol	6.5×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	3.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[13023-60-4]	7.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
CBHXDVOSUKFRBE-UHFFFAOYSA-N					
2,3-dimethyl-2-ethyl-1-butanol	6.0×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	3.7×10^{-2}		Gharagheizi et al. (2012)	Q	
YPIJDMPDVZUWJO-UHFFFAOYSA-N	6.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
3,3-dimethyl-2-ethyl-1-butanol	6.0×10^{-2}		Yaws (2003)	X	238
$C_8H_{18}O$	5.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[66576-56-5]	6.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
WOVMYJCSCISMAU-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-(hexyloxy)-ethanol	3.2		Duchowicz et al. (2020)	V	187
$C_8H_{18}O_2$	8.4		Duchowicz et al. (2020)	Q	
[112-25-4]					
UPGSWASWQBLSKZ-UHFFFAOYSA-N					
1-nonanol	2.7×10^{-1}	9300	Brockbank (2013)	L	1
$C_9H_{20}O$	1.1×10^{-1}	6300	Shunthirasingham et al. (2013)	M	
[143-08-8]	1.4×10^{-1}	6200	Lei et al. (2007)	M	409, 397
ZWRUINPWMLAQRD-UHFFFAOYSA-N	3.2×10^{-1}		Duchowicz et al. (2020)	V	187
	3.2×10^{-1}		HSDB (2015)	V	
	2.8×10^{-1}		Abraham (1984)	V	
	3.8×10^{-1}		Yaws (2003)	X	259
	3.5×10^{-1}		Dupeux et al. (2022)	Q	260
	5.4×10^{-1}		Abney (2021)	Q	401
	1.4		Duchowicz et al. (2020)	Q	
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	5.1×10^{-1}		Modarresi et al. (2007)	Q	68
	3.2×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.4×10^{-1}		Yao et al. (2002)	Q	230
	1.0		Katritzky et al. (1998)	Q	
	3.1×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	3.2×10^{-1}		Yaws et al. (1997)	Q	
	3.0×10^{-1}		Yaws (1999)	?	21
	5.9×10^{-1}		Yaws and Yang (1992)	?	21
	2.9×10^{-1}		Abraham et al. (1990)	?	
2-nonanol	2.1×10^{-1}	11000	Brockbank (2013)	L	1
$C_9H_{20}O$	6.5×10^{-2}		van Ruth et al. (2002)	M	14
[628-99-9]	4.9×10^{-1}		van Ruth and Villeneuve (2002)	M	14, 363
NGDNVOAEIVQRFH-UHFFFAOYSA-N	6.9×10^{-2}		van Ruth et al. (2001)	M	14
	2.0×10^{-1}		Duchowicz et al. (2020)	V	187
	5.6×10^{-1}		Duchowicz et al. (2020)	Q	
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	2.2×10^{-1}		Modarresi et al. (2007)	Q	68
	2.1×10^{-1}		Yao et al. (2002)	Q	230
	5.4×10^{-1}		Yaws et al. (1997)	Q	
	2.0×10^{-1}		Yaws (1999)	?	21, 81

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-nonanol	5.2×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	9.6×10^{-2}		Wang et al. (2017)	Q	81, 239
[624-51-1]	2.6×10^{-1}		Wang et al. (2017)	Q	81, 240
GYSCXPVAKHVAAY-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	81, 241
	8.4×10^{-2}		Gharagheizi et al. (2012)	Q	
	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
	3.0×10^{-1}		Yaws et al. (1997)	Q	
4-nonanol	5.4×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	8.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[5932-79-6]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
IXUOEGRSQCCEHB-UHFFFAOYSA-N	3.1×10^{-1}		Yaws et al. (1997)	Q	
5-nonanol	5.2×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	8.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[623-93-8]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
FCBBRODPXVPZAH-UHFFFAOYSA-N	2.9×10^{-1}		Yaws et al. (1997)	Q	
2-methyl-1-octanol	4.8×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[818-81-5]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
IGVGCQGTEINVOH-UHFFFAOYSA-N					
3-methyl-1-octanol	4.8×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	6.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[38514-02-2]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
CLFSZAMBOZSCOS-UHFFFAOYSA-N					
4-methyl-1-octanol	4.8×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	6.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[38514-03-3]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
MWWKESKJRHQWEF-UHFFFAOYSA-N					
5-methyl-1-octanol	4.8×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	6.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[38514-04-4]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
CGCDFYUPZXVGIX-UHFFFAOYSA-N					
6-methyl-1-octanol	4.3×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
[38514-05-5]	2.1×10^{-1}		Yaws et al. (1997)	Q	
WWRGKAMABZHMCN-UHFFFAOYSA-N					
7-methyl-1-octanol	4.3×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
[2430-22-0]	2.1×10^{-1}		Yaws et al. (1997)	Q	
QDTDKYHPHANITQ-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-2-octanol	5.7×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	1.7×10^{-1}		Gharagheizi et al. (2012)	Q	
[628-44-4]	5.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
KBCNUEXDHWDIFX-UHFFFAOYSA-N	4.8×10^{-1}		Yaws et al. (1997)	Q	
3-methyl-2-octanol	6.0×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[27644-49-1]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
WQADSKJNOTZWML-UHFFFAOYSA-N					
5-methyl-2-octanol	6.0×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	8.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-81-5]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
IWFICVXFFNDWOJ-UHFFFAOYSA-N					
7-methyl-2-octanol	6.0×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	8.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-83-7]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
NOEKZKTXHKNMAQ-UHFFFAOYSA-N					
2-methyl-3-octanol	5.7×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[26533-34-6]	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
DIVBBSLQUDHECU-UHFFFAOYSA-N	4.1×10^{-1}		Yaws et al. (1997)	Q	
3-methyl-3-octanol	5.4×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.8×10^{-2}		Yaws (2003)	X	238
[5340-36-3]	1.3×10^{-1}		Gharagheizi et al. (2012)	Q	
JEWXYDDSLPIBBO-UHFFFAOYSA-N	1.6×10^{-1}		Gharagheizi et al. (2012)	Q	
	5.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
	5.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
	3.6×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-3-octanol	5.6×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-80-4]	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
XPWBBDBJJRZCPW-UHFFFAOYSA-N					
6-methyl-3-octanol	5.6×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	6.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[40225-75-0]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
MFYHIHFYDULUQP-UHFFFAOYSA-N					
7-methyl-3-octanol	5.6×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	6.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-84-8]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
IDCFJIMYNKBKMB-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-4-octanol	5.7×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	6.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[40575-41-5]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
BIAVIOIDPRPYJK-UHFFFAOYSA-N	4.1×10^{-1}		Yaws et al. (1997)	Q	
3-methyl-4-octanol	6.1×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[26533-35-7]	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
MJOKZMZDONULOD-UHFFFAOYSA-N	4.6×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-4-octanol	5.5×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	1.2×10^{-1}		Gharagheizi et al. (2012)	Q	
[23418-37-3]	5.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
RXSIKQJQLQRQQY-UHFFFAOYSA-N	4.5×10^{-1}		Yaws et al. (1997)	Q	
5-methyl-4-octanol	5.9×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[59734-23-5]	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
YLTHHPQUTLMNIF-UHFFFAOYSA-N					
6-methyl-4-octanol	5.9×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-82-6]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
KFRCBGHGDZSOJV-UHFFFAOYSA-N					
7-methyl-4-octanol	5.9×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[33933-77-6]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
KJMBBHZOLRRVMV-UHFFFAOYSA-N					
2-ethyl-1-heptanol	4.9×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[817-60-7]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
QNJAZNNWHWYOEO-UHFFFAOYSA-N					
3-ethyl-1-heptanol	4.2×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
[3525-25-5]	2.0×10^{-1}		Yaws et al. (1997)	Q	
VRZRVMXNGMZLDB-UHFFFAOYSA-N					
5-ethyl-1-heptanol	4.9×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
[998-65-2]					
GOJBFVJUMYSMJJ-UHFFFAOYSA-N					
3-ethyl-2-heptanol	5.9×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	7.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[19780-39-3]	5.8×10^{-2}		Gharagheizi et al. (2012)	Q	
MMQDVLWWGWJSFS-UHFFFAOYSA-N	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	247

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-3-heptanol	5.4×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	8.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[19780-41-7]	5.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
XKRZDNKKANUBPV-UHFFFAOYSA-N	4.3×10^{-1}		Yaws et al. (1997)	Q	
4-ethyl-4-heptanol	5.7×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	7.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[597-90-0]	5.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
GNROHGFUVTWFNG-UHFFFAOYSA-N	4.7×10^{-1}		Yaws et al. (1997)	Q	
2,2-dimethyl-1-heptanol	4.5×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	2.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[14250-79-4]	4.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
WENIXZFPXMQPQQ-UHFFFAOYSA-N	3.2×10^{-1}		Yaws et al. (1997)	Q	
4,6-dimethyl-1-heptanol	5.9×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[820-05-3]	4.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
GCBXGQPBCBPHSP-UHFFFAOYSA-N					
6,6-dimethyl-1-heptanol	5.4×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[65769-10-0]	4.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
IOFUAVGBFVXDAO-UHFFFAOYSA-N					
2,3-dimethyl-2-heptanol	5.0×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	1.3×10^{-1}		Gharagheizi et al. (2012)	Q	
[66794-00-1]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
PQSMEVPHTJECDZ-UHFFFAOYSA-N					
2,4-dimethyl-2-heptanol	5.0×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
[65822-93-7]					
VORBOMMQBCSRQF-UHFFFAOYSA-N					
2,5-dimethyl-2-heptanol	5.0×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
[1561-18-8]					
LVIFBEPHIBJBEU-UHFFFAOYSA-N					
2,6-dimethyl-2-heptanol	5.9×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	1.4×10^{-1}		Gharagheizi et al. (2012)	Q	
[13254-34-7]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
HGDVHRITTGWMJK-UHFFFAOYSA-N	5.8×10^{-1}		Yaws et al. (1997)	Q	
4,6-dimethyl-2-heptanol	4.4×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	1.2×10^{-1}		Gharagheizi et al. (2012)	Q	
[51079-52-8]	4.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
YYUGBYFBCFRGNZ-UHFFFAOYSA-N	3.1×10^{-1}		Yaws et al. (1997)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5,6-dimethyl-2-heptanol	4.6×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	1.2×10^{-1}		Gharagheizi et al. (2012)	Q	
[58795-24-7]	4.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
ONBXNGYZXZBRJA-UHFFFAOYSA-N	3.2×10^{-1}		Yaws et al. (1997)	Q	
2,2-dimethyl-3-heptanol	5.3×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	2.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[19549-70-3]	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
QENWAAAGDINHGE-UHFFFAOYSA-N					
2,3-dimethyl-3-heptanol	5.7×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	7.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[19549-71-4]	5.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
JIEGVNXCNNWVPH-UHFFFAOYSA-N	5.4×10^{-1}		Yaws et al. (1997)	Q	
2,6-dimethyl-3-heptanol	6.1×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	3.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[19549-73-6]	5.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
XZDMJRIWJSNEGC-UHFFFAOYSA-N	5.2×10^{-1}		Yaws et al. (1997)	Q	
3,5-dimethyl-3-heptanol	5.4×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
[19549-74-7]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
NOSOEGQGQOMHBF-UHFFFAOYSA-N					
2,2-dimethyl-4-heptanol	5.7×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-99-5]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
ZIKNXBYJTDTRQA-UHFFFAOYSA-N	5.4×10^{-1}		Yaws et al. (1997)	Q	
2,4-dimethyl-4-heptanol	5.9×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	9.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[19549-77-0]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
QKRRAXACNUNGCF-UHFFFAOYSA-N	5.7×10^{-1}		Yaws et al. (1997)	Q	
2,5-dimethyl-4-heptanol	1.6×10^{-1}		Yaws et al. (1997)	Q	
$C_9H_{20}O$					
NXLQTSHQSAVKJB-UHFFFAOYSA-N					
2,6-dimethyl-4-heptanol	1.0×10^{-1}	9300	Brockbank (2013)	L	1
$C_9H_{20}O$	7.7×10^{-2}		Duchowicz et al. (2020)	V	187
[108-82-7]	8.6×10^{-2}		Duchowicz et al. (2020)	Q	
HXQPUEQDBSPXTE-UHFFFAOYSA-N	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	1.7×10^{-1}		Hilal et al. (2008)	Q	
	3.7×10^{-1}		Modarresi et al. (2007)	Q	68
	1.6×10^{-1}		Katritzky et al. (1998)	Q	
	1.7×10^{-1}		Yaws et al. (1997)	Q	
	1.7×10^{-1}		Yaws (1999)	?	21

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3-dimethyl-4-heptanol	5.5×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	2.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[19549-78-1]	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
UGAZGYFCTFGQQH-UHFFFAOYSA-N	2.2×10^{-1}		Yaws et al. (1997)	Q	
3,5-dimethyl-4-heptanol	5.0×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	3.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[19549-79-2]	5.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
ZKXITRNXHWEQJU-UHFFFAOYSA-N					
3,6-dimethyl-3-heptanol	6.8×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	1.0×10^{-1}		Gharagheizi et al. (2012)	Q	
[1573-28-0]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
HVPGGLNDHUWMLS-UHFFFAOYSA-N					
2-ethyl-3-methyl-1-hexanol	4.9×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	3.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[66794-04-5]	4.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
DXXCMAAACWSRPE-UHFFFAOYSA-N					
2-ethyl-4-methyl-1-hexanol	4.7×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[66794-06-7]	4.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
NRZVENBFUFCASY-UHFFFAOYSA-N	1.2×10^{-1}		Yaws et al. (1997)	Q	
2-ethyl-5-methyl-1-hexanol	4.9×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	3.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[66794-07-8]	4.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
KVJOUCNJVQBRAO-UHFFFAOYSA-N					
3-ethyl-1-methyl-1-hexanol	5.0×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	1.2×10^{-1}		Gharagheizi et al. (2012)	Q	
YNZQSDTXBBBFQH-UHFFFAOYSA-N	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
3-ethyl-2-methyl-1-hexanol	1.3×10^{-1}		Yaws et al. (1997)	Q	
$C_9H_{20}O$					
[66794-01-2]					
UDZCUJOKBNABRS-UHFFFAOYSA-N					
3,3,5-trimethyl-1-hexanol	4.1×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[1484-87-3]	4.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
HRXNWQMMTLLJJQ-UHFFFAOYSA-N					
3,4,4-trimethyl-1-hexanol	4.2×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-73-5]	4.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
OLRPKAJSAOYYCY-UHFFFAOYSA-N	1.4×10^{-1}		Yaws et al. (1997)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,5,5-trimethyl-1-hexanol	4.1×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[3452-97-9]	4.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
BODRLKRKPXBDBN-UHFFFAOYSA-N	1.3×10^{-1}		Yaws et al. (1997)	Q	
4,5,5-trimethyl-1-hexanol	3.4×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	7.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-75-7]	4.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
IECJUMYEWJOKHM-UHFFFAOYSA-N	9.4×10^{-2}		Yaws et al. (1997)	Q	
2-propyl-1-hexanol	5.8×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	3.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[817-46-9]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
JSUXZEJWGVYJJG-UHFFFAOYSA-N					
3-propyl-1-hexanol	5.8×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-85-9]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
MHJIVMDBOGBUHH-UHFFFAOYSA-N					
3-ethyl-2-methyl-2-hexanol	5.3×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	1.2×10^{-1}		Gharagheizi et al. (2012)	Q	
[66794-02-3]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
HTOYXTGJEOUKPM-UHFFFAOYSA-N	2.1×10^{-1}		Yaws et al. (1997)	Q	
2,3,4-trimethyl-2-hexanol	3.7×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
[21102-13-6]					
JTOONBKGYWVPOY-UHFFFAOYSA-N					
2,4,4-trimethyl-2-hexanol	3.4×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66793-91-7]					
QMEHJTXRYVSFES-UHFFFAOYSA-N					
2,4,5-trimethyl-2-hexanol	3.7×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66793-93-9]					
CIVZBWYMPDUPSQ-UHFFFAOYSA-N					
2,5,5-trimethyl-2-hexanol	3.4×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66793-71-3]					
ASOCSFZHADJKFU-UHFFFAOYSA-N					
3-ethyl-2-methyl-3-hexanol	4.8×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	6.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[66794-03-4]	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
VUMFTWNZYFBYEB-UHFFFAOYSA-N	1.7×10^{-1}		Yaws et al. (1997)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-4-methyl-3-hexanol	5.2×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[51200-80-7]	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
YOCLWWFBEJQTBM-UHFFFAOYSA-N					
3-ethyl-5-methyl-3-hexanol	5.8×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	6.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[597-77-3]	5.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
RMBUNHOAKTUXTC-UHFFFAOYSA-N	2.5×10^{-1}		Yaws et al. (1997)	Q	
4-ethyl-2-methyl-3-hexanol	5.7×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	2.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[33943-21-4]	5.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
GBUYIUMHXYBONU-UHFFFAOYSA-N					
4-ethyl-3-methyl-3-hexanol	5.2×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	8.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[66794-05-6]	5.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
DUGZCTGTSJAPCV-UHFFFAOYSA-N					
2,2,3-trimethyl-3-hexanol	4.8×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[5340-41-0]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
DHNHHYWBZNQHGN-UHFFFAOYSA-N	2.4×10^{-1}		Yaws et al. (1997)	Q	
2,2,4-trimethyl-3-hexanol	5.7×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66793-89-3]	2.7×10^{-1}		Yaws et al. (1997)	Q	
YMBVVPXERVAJTB-UHFFFAOYSA-N					
2,2,5-trimethyl-3-hexanol	6.6×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
[3970-60-3]	3.4×10^{-1}		Yaws et al. (1997)	Q	
UCLXUUYVWJKXIK-UHFFFAOYSA-N					
2,3,4-trimethyl-3-hexanol	6.0×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66793-90-6]					
LTKHKGAPVGSECA-UHFFFAOYSA-N					
2,3,5-trimethyl-3-hexanol	6.0×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
[65927-60-8]					
ZVKQNIUBLJYSGN-UHFFFAOYSA-N					
2,4,4-trimethyl-3-hexanol	5.5×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66793-92-8]	2.5×10^{-1}		Yaws et al. (1997)	Q	
PDIVDRVTPZNRDZ-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,5,5-trimethyl-3-hexanol	5.7×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	2.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-72-4]	5.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
NPUIBFBNZSKEAP-UHFFFAOYSA-N					
3,4,4-trimethyl-3-hexanol	5.5×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66793-74-6]	2.9×10^{-1}		Yaws et al. (1997)	Q	
QWJDXMFJOMPTCV-UHFFFAOYSA-N					
3,5,5-trimethyl-3-hexanol	5.5×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66810-87-5]					
HGGJNDQMXCTKCR-UHFFFAOYSA-N					
4-methyl-2-propyl-1-pentanol	5.0×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[54004-41-0]	4.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
IGSWOIOCVJEQRH-UHFFFAOYSA-N	1.3×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-2-(1-methylethyl)-1-pentanol	5.0×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	3.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[55505-24-3]	4.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
CBHPZSADBWMIGE-UHFFFAOYSA-N	1.6×10^{-1}		Yaws et al. (1997)	Q	
2-ethyl-2,4-dimethyl-1-pentanol	4.4×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	2.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-98-4]	4.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
JIZZVMCXCCJUHI-UHFFFAOYSA-N	1.5×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-2,2-dimethyl-1-pentanol	4.5×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	2.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-95-1]	4.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
HEQYMZTUSVDQBW-UHFFFAOYSA-N					
2,3,3,4-tetramethyl-2-pentanol	3.9×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	8.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-86-0]	4.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
HLWCPAJEXXTJHY-UHFFFAOYSA-N					
2,3,4,4-tetramethyl-2-pentanol	3.9×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	1.3×10^{-1}		Gharagheizi et al. (2012)	Q	
[66793-87-1]	4.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
DBCCRNKDJIOKIO-UHFFFAOYSA-N					
3,3,4,4-tetramethyl-2-pentanol	3.9×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-88-2]	4.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
AIQOKYGLKGGWOI-UHFFFAOYSA-N	2.0×10^{-1}		Yaws et al. (1997)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3-diethyl-2-pentanol	4.5×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-94-0]	5.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
IENXYHLNFHBNRR-UHFFFAOYSA-N					
2,3-dimethyl-3-ethyl-2-pentanol	3.7×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
[66793-97-3]	4.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
AVQHNUMJCWRCBA-UHFFFAOYSA-N					
4,4-dimethyl-3-ethyl-2-pentanol	4.1×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	7.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[21102-09-0]	4.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
YGQDLQQRBCOMKJ-UHFFFAOYSA-N					
3-ethyl-2,2-dimethyl-3-pentanol	4.8×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	3.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-96-2]	5.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
CFWIFHZJKFFDFU-UHFFFAOYSA-N	2.3×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-2,4-dimethyl-3-pentanol	4.9×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	4.8×10^{-2}		Yaws (2003)	X	238
[3970-59-0]	3.7×10^{-2}		Gharagheizi et al. (2012)	Q	
PZPYIRQFCOFLGJ-UHFFFAOYSA-N	3.6×10^{-2}		Gharagheizi et al. (2012)	Q	
	5.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
	5.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.1×10^{-1}		Yaws et al. (1997)	Q	
2,2,3,4-tetramethyl-3-pentanol	4.4×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	3.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[29772-39-2]	4.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
KNTFAYXQHRNXSM-UHFFFAOYSA-N	2.3×10^{-1}		Yaws et al. (1997)	Q	
2,2,4,4-tetramethyl-3-pentanol	5.0×10^{-2}		Yaws (2003)	X	238
$C_9H_{20}O$	5.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
[14609-79-1]	2.8×10^{-1}		Yaws et al. (1997)	Q	
WFJSIIHYYLHRHB-UHFFFAOYSA-N					
1-decanol	2.0×10^{-1}	9200	Brockbank (2013)	L	1, 410
$C_{10}H_{22}O$	7.6×10^{-2}	6600	Shunthirasingham et al. (2013)	M	
[112-30-1]	6.5×10^{-2}	5300	Lei et al. (2007)	M	397
MWKFXSUHUHTGQN-UHFFFAOYSA-N	3.1×10^{-1}		Altschuh et al. (1999)	M	
	1.9×10^{-1}		Abraham (1984)	V	
	2.1×10^{-1}		Yaws (2003)	X	259
	2.8×10^{-1}		Dupeux et al. (2022)	Q	260
	1.3×10^{-1}		Keshavarz et al. (2022)	Q	
	1.5		Duchowicz et al. (2020)	Q	
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	2.0×10^{-1}		Hilal et al. (2008)	Q	
	4.6×10^{-1}		Modarresi et al. (2007)	Q	68
	2.1×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.2×10^{-1}		Yao et al. (2002)	Q	230
	9.9×10^{-1}		Katritzky et al. (1998)	Q	
	2.4×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	2.1×10^{-1}		Yaws et al. (1997)	Q	
	3.1×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	4.4×10^{-2}		Maniere et al. (2011)	?	242, 166
	2.1×10^{-1}		Yaws (1999)	?	21
	3.7×10^{-1}		Yaws and Yang (1992)	?	21
	1.9×10^{-1}		Abraham et al. (1990)	?	
2-decanol $C_{10}H_{22}O$ [1120-06-5] ACUZDYFTRHEKOS-UHFFFAOYSA-N	5.4×10^{-1}		Yaws et al. (1997)	Q	
3-decanol $C_{10}H_{22}O$ [1565-81-7] ICEQLCZWZXUUIJ-UHFFFAOYSA-N	3.8×10^{-2}		Yaws (2003)	X	238
	7.8×10^{-2}		Wang et al. (2017)	Q	81, 239
	2.1×10^{-1}		Wang et al. (2017)	Q	81, 240
	2.0×10^{-1}		Wang et al. (2017)	Q	81, 241
	7.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
4-decanol $C_{10}H_{22}O$ [2051-31-2] DTDMYWXTWWFLGJ-UHFFFAOYSA-N	3.8×10^{-2}		Yaws (2003)	X	238
	7.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
	5.3×10^{-1}		Yaws et al. (1997)	Q	
5-decanol $C_{10}H_{22}O$ [5205-34-5] SZMNDOUFZGODBR-UHFFFAOYSA-N	4.5×10^{-2}		Yaws (2003)	X	238
	6.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
	7.3×10^{-1}		Yaws et al. (1997)	Q	
2-methyl-1-nonanol $C_{10}H_{22}O$ [40589-14-8] BEGNRPGEHZBNKK-UHFFFAOYSA-N	3.0×10^{-2}		Yaws (2003)	X	238
	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
	3.4×10^{-1}		Yaws et al. (1997)	Q	
2-methyl-2-nonanol $C_{10}H_{22}O$ [10297-57-1] VREDNSVJXRJXRI-UHFFFAOYSA-N	2.9×10^{-2}		Yaws (2003)	X	238
	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	247

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-3-nonanol	3.6×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[26533-33-5]	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
OFIYMUXECPHIPZ-UHFFFAOYSA-N	5.7×10^{-1}		Yaws et al. (1997)	Q	
2-methyl-4-nonanol	3.6×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	5.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[26533-31-3]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
IBHHTADZYDLHPM-UHFFFAOYSA-N					
2-methyl-5-nonanol	3.6×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	5.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[29843-62-7]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
RLQVUGAVOCBRNQ-UHFFFAOYSA-N					
3-methyl-1-nonanol	3.5×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[22663-64-5]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
BXQPYGLPOMTAPU-UHFFFAOYSA-N					
3-methyl-2-nonanol	3.2×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	5.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[60671-32-1]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
QCBDLZKDRUKOFS-UHFFFAOYSA-N					
3-methyl-3-nonanol	3.2×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
[21078-72-8]	4.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
VZBFPIMCUSPDLS-UHFFFAOYSA-N					
3-methyl-5-nonanol	3.6×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	5.1×10^{-2}		Gharagheizi et al. (2012)	Q	
QRZAYHZIHWIJHD-UHFFFAOYSA-N	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
4-methyl-1-nonanol	3.1×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[1489-47-0]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
HECVGHIJHFNAIL-UHFFFAOYSA-N					
4-methyl-4-nonanol	3.2×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
[23418-38-4]	4.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
GDCOAKPWVJCNGI-UHFFFAOYSA-N					
5-methyl-1-nonanol	3.5×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[2768-16-3]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
DBJSFYCKLLBKGB-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5-methyl-2-nonanol	3.2×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	8.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[66731-95-1]	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
KZTLXVUOEODDMR-UHFFFAOYSA-N					
5-methyl-3-nonanol	3.6×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	5.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-43-5]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
CCSZLOPBDJWYHV-UHFFFAOYSA-N					
5-methyl-4-nonanol	3.6×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-44-6]	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
BFYIAYZULSQBFQ-UHFFFAOYSA-N					
5-methyl-5-nonanol	4.9×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	9.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[33933-78-7]	4.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
AGSIGVZAVLOKLP-UHFFFAOYSA-N					
6-methyl-2-nonanol	3.2×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	8.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-60-8]	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
OYTRLQQQIHEJFE-UHFFFAOYSA-N					
7-methyl-1-nonanol	3.5×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[33234-93-4]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
BJKXZCGJAOWNTN-UHFFFAOYSA-N					
7-methyl-2-nonanol	3.2×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66256-61-9]					
GCOBJHFUTQUABB-UHFFFAOYSA-N					
7-methyl-4-nonanol	3.6×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	5.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[26981-98-6]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
KLZAWUYSXUGWGQ-UHFFFAOYSA-N					
8-methyl-1-nonanol	1.8×10^{-1}		HSDB (2015)	Q	100
$C_{10}H_{22}O$					
(isodecanol)					
[25339-17-7]					
PLLBRTOLHQQAQQ-UHFFFAOYSA-N					
8-methyl-2-nonanol	3.2×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	8.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[14779-92-1]	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
ZVZKLBCGIYWGOU-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2-dimethyl-1-octanol	3.3×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	1.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[2370-14-1]	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
KEXGXAGJHHCTKD-UHFFFAOYSA-N	5.7×10^{-1}		Yaws et al. (1997)	Q	
2,2-dimethyl-3-octanol	3.9×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	1.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[19841-72-6]	4.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
AZIWNYAWODSERA-UHFFFAOYSA-N					
2,2-dimethyl-4-octanol	4.2×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-52-6]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
IVLDCRDTRQCTIY-UHFFFAOYSA-N	1.0		Yaws et al. (1997)	Q	
2,3-dimethyl-3-octanol	4.2×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[19781-10-3]	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
AWHYRPPRRQITHX-UHFFFAOYSA-N	1.0		Yaws et al. (1997)	Q	
2,4-dimethyl-2-octanol	2.7×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
[18675-20-2]					
WHJCLXRXPLJSSV-UHFFFAOYSA-N					
2,4-dimethyl-4-octanol	4.1×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	6.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[33933-79-8]	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
VRFMFHBPJUSGFK-UHFFFAOYSA-N					
2,5-dimethyl-4-octanol	4.5×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	2.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-53-7]	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
VIHAZZPWGKHJQE-UHFFFAOYSA-N					
2,6-dimethyl-1-octanol	3.5×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	2.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[62417-08-7]	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
ZKWASVBZSAGDBI-UHFFFAOYSA-N					
2,6-dimethyl-2-octanol	2.7×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
[18479-57-7]					
WRFXXJKURVTLSY-UHFFFAOYSA-N					
2,6-dimethyl-4-octanol	3.5×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-54-8]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
ZFOGJEKQQNVCFB-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,7-dimethyl-2-octanol	2.7×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
[42007-73-8]					
JJZZVQICFJITMO-UHFFFAOYSA-N					
2,7-dimethyl-3-octanol	4.3×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	2.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-55-9]	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
VFUOFVONEDBLIJ-UHFFFAOYSA-N	9.0×10^{-1}		Yaws et al. (1997)	Q	
2,7-dimethyl-4-octanol	2.3×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[19781-11-4]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
FRJOBNOTOHIMIH-UHFFFAOYSA-N					
3,4-dimethyl-4-octanol	4.1×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-30-0]	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
JEBZCASOCDXENQ-UHFFFAOYSA-N					
3,5-dimethyl-3-octanol	4.0×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	7.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[56065-42-0]	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
DMIBTMSBSULJMT-UHFFFAOYSA-N					
3,6-dimethyl-3-octanol	4.0×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	6.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[151-19-9]	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
NPHCXUPGMINOPP-UHFFFAOYSA-N	9.6×10^{-1}		Yaws et al. (1997)	Q	
3,6-dimethyl-4-octanol	4.5×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	2.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-31-1]	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
XFUFFAQPWAGSDK-UHFFFAOYSA-N					
3,7-dimethyl-1-octanol	3.3×10^{-2}		Yaws (2003)	X	259
$C_{10}H_{22}O$	3.3×10^{-2}		Yaws (2003)	X	238
(pelargol)	3.7×10^{-1}		Dupeux et al. (2022)	Q	260
[106-21-8]	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
PRNCMAKCNVRZFX-UHFFFAOYSA-N	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
	5.0×10^{-1}		Yaws et al. (1997)	Q	
3,7-dimethyl-2-octanol	3.0×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	5.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[15340-96-2]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
XCWMPEYBKUYTLZ-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,7-dimethyl-3-octanol	3.7×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	7.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[78-69-3]	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
DLHQZZUEERVIGQ-UHFFFAOYSA-N	8.5×10^{-1}		Yaws et al. (1997)	Q	
4,5-dimethyl-1-octanol	3.3×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-32-2]	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
UQKHXPAWOMZBLN-UHFFFAOYSA-N					
4,6-dimethyl-1-octanol	3.3×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-33-3]	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
JOWDWXPTKVUHBV-UHFFFAOYSA-N					
4,6-dimethyl-4-octanol	4.1×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	6.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[56065-43-1]	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
QJVDAQVYZBSYCB-UHFFFAOYSA-N					
4,7-dimethyl-1-octanol	3.3×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-34-4]	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
UWAGZVFFZJGLJU-UHFFFAOYSA-N					
4,7-dimethyl-4-octanol	4.0×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	6.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[19781-13-6]	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
OTISWHNJCUMBFI-UHFFFAOYSA-N	9.6×10^{-1}		Yaws et al. (1997)	Q	
7,7-dimethyl-1-octanol	3.0×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-35-5]	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
RYFZXYQQFYLUHM-UHFFFAOYSA-N					
2-ethyl-1-octanol	3.9×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	2.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[20592-10-3]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
HTRVTKUOKQWGMO-UHFFFAOYSA-N					
3-ethyl-1-octanol	3.9×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-36-6]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
VXOCEIUJVCHLRR-UHFFFAOYSA-N					
3-ethyl-3-octanol	3.9×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	5.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[2051-32-3]	4.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
NPQPNSNHYJTUSA-UHFFFAOYSA-N	7.7×10^{-1}		Yaws et al. (1997)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-4-octanol	4.8×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	2.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[63126-48-7]	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
WXJDPIWUPZLVSF-UHFFFAOYSA-N					
4-ethyl-4-octanol	4.3×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[38395-42-5]	4.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
OYBUBRUQIKTRET-UHFFFAOYSA-N					
6-ethyl-3-octanol	4.3×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[19781-27-2]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
JWZFCOOWAQHCBP-UHFFFAOYSA-N					
2,2,3-trimethyl-3-heptanol	3.7×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	2.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[29772-40-5]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
GCLFPNQSLCWZAQ-UHFFFAOYSA-N	1.1		Yaws et al. (1997)	Q	
2,2,4-trimethyl-4-heptanol	4.1×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
[57233-31-5]	1.3		Yaws et al. (1997)	Q	
KNACVESXMPHLNM-UHFFFAOYSA-N					
2,2,5-trimethyl-4-heptanol	4.4×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66256-42-6]					
JHHGGYCQTXZCTL-UHFFFAOYSA-N					
2,2,6-trimethyl-3-heptanol	3.8×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	1.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-43-7]	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
AXUPPSSNJCYJOX-UHFFFAOYSA-N					
2,2,6-trimethyl-4-heptanol	4.4×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66256-44-8]					
ITTQYDBLGDGLMB-UHFFFAOYSA-N					
2,3,6-trimethyl-3-heptanol	3.8×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[58046-40-5]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
BAZNZYUOJWCTIQ-UHFFFAOYSA-N					
2,4,5-trimethyl-4-heptanol	4.4×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66256-46-0]					
RCSCLTAIPNDFGC-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4,6-trimethyl-2-heptanol	3.6×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	1.0×10^{-1}		Gharagheizi et al. (2012)	Q	
[66256-47-1]	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
VUZHXHGZVRACMM-UHFFFAOYSA-N					
2,4,6-trimethyl-4-heptanol	4.4×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
[60836-07-9]	1.3		Yaws et al. (1997)	Q	
QSVYJSJPLCSACO-UHFFFAOYSA-N					
2,5,6-trimethyl-2-heptanol	3.6×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
[66256-48-2]	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
LQQYOLMGDBGEBC-UHFFFAOYSA-N	9.3×10^{-1}		Yaws et al. (1997)	Q	
3,3,6-trimethyl-4-heptanol	4.4×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
LTDMOZOPTDNTLG-UHFFFAOYSA-N					
3,5,5-trimethyl-3-heptanol	3.1×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	7.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-50-6]	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
WOUVARFKMJIYBY-UHFFFAOYSA-N	8.6×10^{-1}		Yaws et al. (1997)	Q	
4,6,6-trimethyl-2-heptanol	3.6×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[51079-79-9]	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
FHQUDZUTAZYJRH-UHFFFAOYSA-N					
3-(1-methylethyl)-1-heptanol	3.1×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[38514-15-7]	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
NTGBCQFKKOCODF-UHFFFAOYSA-N	4.4×10^{-1}		Yaws et al. (1997)	Q	
4-(1-methylethyl)-4-heptanol	4.2×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[51200-82-9]	4.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
OHSMKBPEDBXYDU-UHFFFAOYSA-N	1.0		Yaws et al. (1997)	Q	
3-ethyl-2-methyl-3-heptanol	4.0×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-37-7]	4.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
GYCRUUSYQLIIBA-UHFFFAOYSA-N	9.3×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-5-methyl-3-heptanol	4.0×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.8×10^{-2}		Gharagheizi et al. (2012)	Q	
FGJMKJVRSBVZPS-UHFFFAOYSA-N	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	247

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5-ethyl-4-methyl-3-heptanol	4.4×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	2.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[66731-94-0]	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
XVSHXHABYNUHNI-UHFFFAOYSA-N					
2-propyl-1-heptanol	3.3×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[10042-59-8]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
YLQLIQIAXYRMDL-UHFFFAOYSA-N	4.0×10^{-1}		Yaws et al. (1997)	Q	
4-propyl-4-heptanol	4.2×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[2198-72-3]	4.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
SJTPBRMACCDJPZ-UHFFFAOYSA-N	9.0×10^{-1}		Yaws et al. (1997)	Q	
2,2,3,4-tetramethyl-3-hexanol	3.1×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	2.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-63-1]	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
SAFMWGCEQYLRLS-UHFFFAOYSA-N	9.6×10^{-1}		Yaws et al. (1997)	Q	
2,2,4,4-tetramethyl-3-hexanol	3.2×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	6.7×10^{-3}		Gharagheizi et al. (2012)	Q	
[66256-65-3]	4.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
LKAPNEGVXBMYKE-UHFFFAOYSA-N	1.0		Yaws et al. (1997)	Q	
2,2,5,5-tetramethyl-3-hexanol	4.6×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
[55073-86-4]	1.7		Yaws et al. (1997)	Q	
CFEYPBVKHMZCFR-UHFFFAOYSA-N					
2,3,4,4-tetramethyl-2-hexanol	3.2×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	6.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-66-4]	3.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
IELWGTFQRBDDCZ-UHFFFAOYSA-N	1.0		Yaws et al. (1997)	Q	
2,3,4,4-tetramethyl-3-hexanol	2.5×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	2.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-67-5]	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
ZQFIWHOYWCJIHU-UHFFFAOYSA-N	7.3×10^{-1}		Yaws et al. (1997)	Q	
2,3,5,5-tetramethyl-3-hexanol	2.5×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	6.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[5396-09-8]	3.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
KTSYBVKVNWGHBC-UHFFFAOYSA-N					
2,4,4,5-tetramethyl-3-hexanol	2.8×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	1.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-68-6]	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
VVRHXTVKOHXZJX-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3,5,5-tetramethyl-2-hexanol	3.2×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	2.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-69-7]	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
USWOQOMRDCYQMW-UHFFFAOYSA-N					
3,4,4,5-tetramethyl-3-hexanol	2.5×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-39-1]	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
UHJJSHWWLQIIOU-UHFFFAOYSA-N	7.0×10^{-1}		Yaws et al. (1997)	Q	
3,4,5,5-tetramethyl-3-hexanol	2.9×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	5.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-40-4]	3.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
LBLUJHQRJVUQJR-UHFFFAOYSA-N	8.8×10^{-1}		Yaws et al. (1997)	Q	
2,4-dimethyl-4-ethyl-3-hexanol	4.0×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66719-48-0]					
NLGGBBOPZSANIC-UHFFFAOYSA-N					
2-butyl-1-hexanol	4.4×10^{-1}		Yaws et al. (1997)	Q	
$C_{10}H_{22}O$					
[2768-15-2]					
LAPPDPWPIZBBJY-UHFFFAOYSA-N					
4-ethyl-2,2-dimethyl-3-hexanol	4.0×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66719-47-9]	1.1		Yaws et al. (1997)	Q	
UOYRABPBVGDJLW-UHFFFAOYSA-N					
4-methyl-2-(1-methylethyl)-1-hexanol	3.7×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	1.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-41-3]	3.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
VHGVOODVCUKVCL-UHFFFAOYSA-N	7.3×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-2-propyl-1-hexanol	3.6×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	2.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-62-0]	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
VZXWJVFQXZUFQS-UHFFFAOYSA-N	5.7×10^{-1}		Yaws et al. (1997)	Q	
5,5-dimethyl-2-ethyl-1-hexanol	2.7×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	2.7×10^{-2}		Gharagheizi et al. (2012)	Q	
DXDJMJLAABGHOH-UHFFFAOYSA-N	3.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
5,5-dimethyl-3-ethyl-3-hexanol	3.7×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	4.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[5340-62-5]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
FVVBGHIXYRKNGT-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5-methyl-2-(1-methylethyl)-1-hexanol	3.0×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	2.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[2051-33-4]	3.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
SFIQHFBITUEIBP-UHFFFAOYSA-N	4.8×10^{-1}		Yaws et al. (1997)	Q	
2-methyl-3-(1-methylethyl)-3-hexanol	4.3×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.7×10^{-2}		Yaws (2003)	X	238
(2,4-dimethyl-3-propyl-3-pentanol)	2.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[51200-81-8]	1.7×10^{-2}		Gharagheizi et al. (2012)	Q	
GGOIYPAZTVTJBE-UHFFFAOYSA-N	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
	9.6×10^{-1}		Yaws et al. (1997)	Q	
	1.2		Yaws et al. (1997)	Q	
2,2,3,4,4-pentamethyl-3-pentanol	2.4×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	1.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[5857-69-2]	3.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
UYFZQUABCZILAI-UHFFFAOYSA-N	8.9×10^{-1}		Yaws et al. (1997)	Q	
2,3-dimethyl-2-*tert*-butyl-1-butanol	3.0×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[81931-81-9]	3.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
WQRJEFGWAMKEBO-UHFFFAOYSA-N					
2,4-dimethyl-3-(1-methylethyl)-3-pentanol	3.2×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	1.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[51200-83-0]	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
IFXNWIUSZUHIDG-UHFFFAOYSA-N	8.9×10^{-1}		Yaws et al. (1997)	Q	
3,4-dimethyl-3-isopropyl-2-pentanol	4.0×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66719-50-4]					
DNBJFVXHMLZKHP-UHFFFAOYSA-N					
4,4-dimethyl-3-isopropyl-1-pentanol	4.3×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	3.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66719-51-5]					
DQWFOEIWLQBIFY-UHFFFAOYSA-N					
3-ethyl-2,2,4-trimethyl-3-pentanol	3.1×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	1.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-41-5]	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
CHZVHXPAKQDRSE-UHFFFAOYSA-N	9.9×10^{-1}		Yaws et al. (1997)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methyl-2-(2-methylpropyl)-1-pentanol	3.5×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{22}O$	2.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[22417-45-4]	3.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
FXXCTCCAZGTNNO-UHFFFAOYSA-N	6.6×10^{-1}		Yaws et al. (1997)	Q	
1-undecanol	1.4×10^{-1}		Brockbank (2013)	L	
$C_{11}H_{24}O$	2.2×10^{-1}		Yaws (2003)	X	259
[112-42-5]	2.1×10^{-1}		Dupeux et al. (2022)	Q	260
KJIOQYGWTQBHNH-UHFFFAOYSA-N	1.4×10^{-1}		HSDB (2015)	Q	100
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	1.7×10^{-1}		Yao et al. (2002)	Q	230
	2.2×10^{-1}		Yaws et al. (1997)	Q	
	3.0×10^{-1}		Yaws (1999)	?	21
2-undecanol	1.2×10^{-1}		Yaws (2003)	X	259
$C_{11}H_{24}O$	2.3×10^{-1}		Dupeux et al. (2022)	Q	260
[1653-30-1]					
XMUJIPOFTAHSOK-UHFFFAOYSA-N					
3-undecanol	6.0×10^{-2}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{24}O$	1.7×10^{-1}		Wang et al. (2017)	Q	81, 240
[6929-08-4]	1.6×10^{-1}		Wang et al. (2017)	Q	81, 241
HCARCYFXWDRVBZ-UHFFFAOYSA-N					
1-dodecanol	1.2×10^{-1}		Brockbank (2013)	L	
$C_{12}H_{26}O$	4.4×10^{-1}		Altschuh et al. (1999)	M	
[112-53-8]	1.4×10^{-1}	9800	Abraham (1984)	V	
LQZZUXJYWNFBMV-UHFFFAOYSA-N	1.9×10^{-1}		Yaws (2003)	X	259
	1.8×10^{-1}		Dupeux et al. (2022)	Q	260
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.5		Duchowicz et al. (2020)	Q	185
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.5×10^{-1}		Hilal et al. (2008)	Q	
	3.5×10^{-1}		Modarresi et al. (2007)	Q	68
	2.1×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	1.6×10^{-1}		Yao et al. (2002)	Q	230, 268
	1.9×10^{-1}		Yaws et al. (1997)	Q	
	4.4×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	1.9×10^{-1}		Yaws (1999)	?	21
	1.1×10^{-1}		Yaws and Yang (1992)	?	21
3-dodecanol	4.8×10^{-2}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{26}O$	1.5×10^{-1}		Wang et al. (2017)	Q	81, 240
[10203-30-2]	1.5×10^{-1}		Wang et al. (2017)	Q	81, 241
OKDGZLITBCRLLJ-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,6,8-trimethyl-4-nonanol	1.0×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_{26}O$	1.1×10^{-1}		Zhang et al. (2010)	Q	288, 290
[123-17-1]	6.0×10^{-2}		Zhang et al. (2010)	Q	288, 291
LFEHSRSSAGQWNI-UHFFFAOYSA-N	2.6×10^{-2}		Zhang et al. (2010)	Q	288, 292
1-tridecanol	1.2×10^{-1}		Yaws (2003)	X	259
$C_{13}H_{28}O$	1.5×10^{-1}		Dupeux et al. (2022)	Q	260
[112-70-9]	7.6×10^{-2}		HSDB (2015)	Q	100
XFRVVPUIAFSTFO-UHFFFAOYSA-N	1.3×10^{-1}		Yao et al. (2002)	Q	230
	1.2×10^{-1}		Yaws et al. (1997)	Q	
	1.8×10^{-1}		Yaws (1999)	?	21
1-tetradecanol	6.2×10^{-2}		Duchowicz et al. (2020)	V	187
$C_{14}H_{30}O$	6.2×10^{-2}		HSDB (2015)	V	
[112-72-1]	2.2×10^{-1}		Abraham (1984)	R	
HLZKNKRTKFSKGZ-UHFFFAOYSA-N	9.4×10^{-2}		Yaws (2003)	X	259
	1.2×10^{-1}		Dupeux et al. (2022)	Q	260
	1.5		Duchowicz et al. (2020)	Q	
	6.2×10^{-2}		Hilal et al. (2008)	Q	
	2.7×10^{-1}		Modarresi et al. (2007)	Q	68
	9.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	6.6×10^{-2}		Yao et al. (2002)	Q	230
	9.5×10^{-2}		Yaws et al. (1997)	Q	
	9.5×10^{-2}		Yaws (1999)	?	21
	3.9×10^{3}		Yaws and Yang (1992)	?	21, 411
2-tetradecanol	1.7×10^{-1}		Gharagheizi et al. (2012)	Q	
$C_{14}H_{30}O$					
[4706-81-4]					
BRGJIIMZXMWMCC-UHFFFAOYSA-N					
1-pentadecanol	2.2×10^{-1}		Abraham (1984)	V	
$C_{15}H_{32}O$	2.5×10^{-2}		Yaws (2003)	X	238
[629-76-5]	8.9×10^{-2}		Gharagheizi et al. (2012)	Q	
REIUXOLGHVXAEO-UHFFFAOYSA-N	2.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.5×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.5×10^{-1}		Yaws et al. (1997)	Q	
	3.0×10^{3}		Yaws and Yang (1992)	?	21, 412
1-hexadecanol	2.1×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{16}H_{34}O$	2.1×10^{-1}		HSDB (2015)	V	
(cetyl alcohol)	3.5×10^{-1}		Abraham (1984)	R	
[124-29-8]	6.4×10^{-2}		Yaws (2003)	X	238
BXWNKGSJHAJOGX-UHFFFAOYSA-N	1.5		Duchowicz et al. (2020)	Q	
	7.4×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	68

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.5×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	1.0×10^{-1}		Yaws et al. (1997)	Q	
	1.0×10^{-1}		Yaws (1999)	?	21
	5.9×10^{-1}		Yaws and Yang (1992)	?	21
2-hexadecanol $C_{16}H_{34}O$ [14852-31-4] FVDRFBGMOWJEOR-UHFFFAOYSA-N	1.6×10^{-2}		Yaws (2003)	X	238
	1.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
1-heptadecanol $C_{17}H_{36}O$ [1454-85-9] GOQYKNQRPGWPLP-UHFFFAOYSA-N	4.5×10^{-2}		Yaws (2003)	X	238
	7.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
	4.6×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	4.5×10^{-2}		Yaws et al. (1997)	Q	
	1.2×10^{1}		Yaws and Yang (1992)	?	21
2-heptadecanol $C_{17}H_{36}O$ [16813-18-6] ZNYQHFLBAPNPRC-UHFFFAOYSA-N	8.7×10^{-3}		Yaws (2003)	X	238
	1.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
1-octadecanol $C_{18}H_{38}O$ [112-92-5] GLDOVTGHNKAZLK-UHFFFAOYSA-N	1.2×10^{-2}		Duchowicz et al. (2020)	V	187
	1.2×10^{-2}		HSDB (2015)	V	
	3.8×10^{-1}		Abraham (1984)	R	
	1.5		Duchowicz et al. (2020)	Q	
	2.5×10^{-2}		Hilal et al. (2008)	Q	
	1.7×10^{-1}		Modarresi et al. (2007)	Q	68
	3.1×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	3.1×10^{-3}		Yaws et al. (1997)	Q	
	1.2×10^{-2}		Yaws (1999)	?	21, 413
	9.1×10^{-1}		Yaws and Yang (1992)	?	21, 413
1-nonadecanol $C_{19}H_{40}O$ [1454-84-8] XGFDHKJUZCCPKQ-UHFFFAOYSA-N	9.9×10^{-2}		Yaws et al. (1997)	Q	
1-eicosanol $C_{20}H_{42}O$ [629-96-9] BTFJIXJJCSYFAL-UHFFFAOYSA-N	4.7×10^{-1}		HSDB (2015)	Q	100
	5.5×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.8×10^{-2}		Yaws et al. (1997)	Q	
1-docosanol $C_{22}H_{46}O$ (behenic alcohol) [661-19-8] NOPFSRXAKWQILS-UHFFFAOYSA-N	6.2×10^{-3}		HSDB (2015)	Q	100

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-tetracosanol $C_{24}H_{50}O$ [506-51-4] TYWMIZZBOVGFOV-UHFFFAOYSA-N	3.4×10^{-3}		HSDB (2015)	Q	100
cyclopentanol	4.2	8200	Plyasunov and Shock (2000)	L	
C_5H_9OH	2.2	5900	Hovorka et al. (2002)	M	11
[96-41-3]	4.3	8000	Cabani et al. (1975b)	T	
XCIXKGXIYUWCLL-UHFFFAOYSA-N	3.8		HSDB (2015)	Q	100
	2.0		Hilal et al. (2008)	Q	
		7200	Kühne et al. (2005)	Q	
	4.4		Nirmalakhandan et al. (1997)	Q	
		7300	Kühne et al. (2005)	?	
	4.3		Abraham et al. (1990)	?	
cyclohexanol	4.3	7700	Brockbank (2013)	L	
$C_6H_{11}OH$	4.4	8500	Plyasunov and Shock (2000)	L	
[108-93-0]	2.5		Chao et al. (2017)	M	
HPXRVTGHNJAIIH-UHFFFAOYSA-N	4.3	7700	Hovorka et al. (2002)	M	11
	2.2		Altschuh et al. (1999)	M	
	2.7		Chao et al. (2017)	V	
	4.5		Mackay et al. (2006c)	V	
	4.5		Mackay et al. (1995)	V	
	3.5		Meylan and Howard (1991)	V	
	1.7		Hine and Mookerjee (1975)	V	
	4.1	8500	Cabani et al. (1975b)	T	
	3.9		Yaws (2003)	X	259
	3.6		Howard (1993)	X	414
	6.2		Dupeux et al. (2022)	Q	260
	1.1		Keshavarz et al. (2022)	Q	
	4.1		Duchowicz et al. (2020)	Q	
	4.5×10^{-1}		Wang et al. (2017)	Q	81, 239
	4.5		Wang et al. (2017)	Q	81, 240
	6.3		Wang et al. (2017)	Q	81, 241
	1.6		Li et al. (2014)	Q	242
	2.0		Raventos-Duran et al. (2010)	Q	243, 244
	2.5		Raventos-Duran et al. (2010)	Q	245
	2.0		Raventos-Duran et al. (2010)	Q	246
	3.3		Hilal et al. (2008)	Q	
	2.3		Modarresi et al. (2007)	Q	68
		7500	Kühne et al. (2005)	Q	
	3.8		Yaffe et al. (2003)	Q	249, 250
	1.3		Yao et al. (2002)	Q	230
	4.1		English and Carroll (2001)	Q	231, 232
	2.3		Katritzky et al. (1998)	Q	
	2.7		Nirmalakhandan et al. (1997)	Q	
	3.6		Russell et al. (1992)	Q	280
	2.0		Suzuki et al. (1992)	Q	233

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.0		Meylan and Howard (1991)	Q	
	3.4		Nirmalakhandan and Speece (1988)	Q	
	2.2		Duchowicz et al. (2020)	?	186, 21
		7500	Kühne et al. (2005)	?	
	3.9		Yaws (1999)	?	21
	4.1		Abraham et al. (1990)	?	
cycloheptanol	4.6	9000	Plyasunov and Shock (2000)	L	
$C_7H_{13}OH$	4.2	9000	Cabani et al. (1975b)	T	
[502-41-0]	1.0		Hilal et al. (2008)	Q	
QCRFMSUKWRQZEM-UHFFFAOYSA-N	3.7		English and Carroll (2001)	Q	231, 232
	4.2		Abraham et al. (1990)	?	
4-methylcyclohexanol	2.5		Ebert et al. (2023)	?	319
$C_7H_{13}OH$					
[589-91-3]					
MQWCXKGKQLNYQG-UHFFFAOYSA-N					
2-methylcyclohexanol	1.4		Chao et al. (2017)	M	
$C_7H_{14}O$	1.3		Altschuh et al. (1999)	M	
[583-59-5]	5.9		Keshavarz et al. (2022)	Q	
NDVWOBYBJYUSMF-UHFFFAOYSA-N	1.7		Duchowicz et al. (2020)	Q	185
	1.6		Raventos-Duran et al. (2010)	Q	243, 244
	1.6		Raventos-Duran et al. (2010)	Q	245
	1.6		Raventos-Duran et al. (2010)	Q	246
	1.3		Hilal et al. (2008)	Q	
	3.2		Modarresi et al. (2007)	Q	68
	1.3		Duchowicz et al. (2020)	?	186, 21
3-methylcyclohexanol	2.9		Chao et al. (2017)	M	
$C_7H_{14}O$	2.7		Altschuh et al. (1999)	M	
[591-23-1]	5.9		Keshavarz et al. (2022)	Q	
HTSABYAWKQAHBT-UHFFFAOYSA-N	1.7		Duchowicz et al. (2020)	Q	300
	1.6		Raventos-Duran et al. (2010)	Q	243, 244
	1.6		Raventos-Duran et al. (2010)	Q	245
	1.6		Raventos-Duran et al. (2010)	Q	246
	1.7		Modarresi et al. (2007)	Q	68
	2.7		Duchowicz et al. (2020)	?	186, 21
MCM:C8BCOH	8.7×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O$	2.4		Wang et al. (2017)	Q	81, 240
CEOBYJRLFASWKF-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	81, 241
(4-methylcyclohexyl)methanol	1.5		HSDB (2015)	Q	100
$C_8H_{16}O$					
[34885-03-5]					
OSINZLLLLCUKJH-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
borneol $C_{10}H_{18}O$ [507-70-0] DTGKSKDOIYIVQL-UHFFFAOYSA-N	4.4×10^{-1}		Ebert et al. (2023)	?	317
fenchol $C_{10}H_{18}O$ (fenchyl alcohol) [1632-73-1] IAIHUHQCLTYTSF-UHFFFAOYSA-N	3.5×10^{-1}		Ebert et al. (2023)	?	373
menthol $C_{10}H_{20}O$ [1490-04-6] NOOLISFMXDJSKH-UHFFFAOYSA-N	3.1×10^{-1}		Ebert et al. (2023)	?	319
2-methylisoborneol $C_{11}H_{20}O$ [2371-42-8] LFYXNXGVLGKVCJ-BOBPJJCASA-N	8.9×10^{-2} 1.6	9800	Ömür-Özbek and Dietrich (2005) Wu et al. (2022a)	M Q	 415
geosmin $C_{12}H_{22}O$ [19700-21-1] JLPUXFOGCDVKGO-GRYCIOLGSA-N	8.1×10^{-2} 4.1	9800	Ömür-Özbek and Dietrich (2005) Wu et al. (2022a)	M Q	 415
cyclododecanol $C_{12}H_{24}O$ [1724-39-6] SFVWPXMPRCIVOK-UHFFFAOYSA-N	3.4 6.8 4.5 3.7×10^{-1} 3.4 8.0 5.3×10^{-2} 1.6 2.5×10^{-1} 3.4		Altschuh et al. (1999) Keshavarz et al. (2022) Duchowicz et al. (2020) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Duchowicz et al. (2020)	M Q Q Q Q Q Q Q Q ?	 288, 289 288, 290 288, 291 288, 292 68 186, 21
cedrol $C_{15}H_{26}O$ [77-53-2] SVURIXNDRWRAFU-OGMFBOKVSA-N	6.7		Dupeux et al. (2022)	Q	260
patchoulol $C_{15}H_{26}O$ [5986-55-0] GGHMUJBZYLPWFD-CUZKYEQNSA-N	1.3×10^{1}		Dupeux et al. (2022)	Q	260

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
perhydrobisphenol a	9.7		Zhang et al. (2010)	Q	288, 289
$C_{15}H_{28}O_2$	6.1×10^{4}		Zhang et al. (2010)	Q	288, 290
[80-04-6]	3.4×10^{4}		Zhang et al. (2010)	Q	288, 291
CDBAMNGURPMUTG-UHFFFAOYSA-N	1.8×10^{2}		Zhang et al. (2010)	Q	288, 292
3-(5,5,6-trimethyl-2-norbornyl)cyclohexanol	6.1×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_{28}O$	1.6×10^{1}		Zhang et al. (2010)	Q	288, 290
[3407-42-9]	1.1×10^{1}		Zhang et al. (2010)	Q	288, 291
BWVZAZPLUTUBKD-UHFFFAOYSA-N	2.7×10^{-1}		Zhang et al. (2010)	Q	288, 292
4-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexan-1-ol	6.1×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_{28}O$	1.8×10^{1}		Zhang et al. (2010)	Q	288, 290
[66068-84-6]	4.4×10^{1}		Zhang et al. (2010)	Q	288, 291
PCFHYANYPQEMPU-UHFFFAOYSA-N	2.7×10^{-1}		Zhang et al. (2010)	Q	288, 292
4-((1R,2R,4R)-born-2-yl)cyclohexanol	6.1×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_{28}O$	9.9		Zhang et al. (2010)	Q	288, 290
[66072-32-0]	4.3×10^{1}		Zhang et al. (2010)	Q	288, 291
LFHQKYSBKVWWOS-UHFFFAOYSA-N	1.6×10^{-1}		Zhang et al. (2010)	Q	288, 292
ethenol	8.5×10^{-1}		Wang et al. (2017)	Q	81, 239
C_2H_4O	2.0		Wang et al. (2017)	Q	81, 240
(vinyl alcohol)	1.7		Wang et al. (2017)	Q	81, 241
[557-75-5]					
IMROMDMJAWUWLK-UHFFFAOYSA-N					
2-propen-1-ol		6500	Plyasunov and Shock (2000)	L	
C_3H_5OH	2.0		Lide and Frederikse (1995)	V	
(allyl alcohol)	1.6		Yaws (2003)	X	259
[107-18-6]	4.3	7200	Goldstein (1982)	X	299
XXROGKLTLUQVRX-UHFFFAOYSA-N	2.0		Pierotti et al. (1959)	X	416
	1.5		Dupeux et al. (2022)	Q	260
	9.0×10^{-1}		Keshavarz et al. (2022)	Q	
	4.0		Duchowicz et al. (2020)	Q	300
	6.9×10^{-1}		Wang et al. (2017)	Q	81, 239
	5.9		Wang et al. (2017)	Q	81, 240
	2.1		Wang et al. (2017)	Q	81, 241
	2.0		Li et al. (2014)	Q	242
	4.9		Raventos-Duran et al. (2010)	Q	243, 244
	3.9		Raventos-Duran et al. (2010)	Q	245
	1.6		Raventos-Duran et al. (2010)	Q	246
	2.8		Hilal et al. (2008)	Q	
	3.7		Modarresi et al. (2007)	Q	68
	2.0		Yaffe et al. (2003)	Q	249, 250
	3.8		Yao et al. (2002)	Q	230

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.1		English and Carroll (2001)	Q	231, 232
	4.4		Katritzky et al. (1998)	Q	
	3.5		Nirmalakhandan et al. (1997)	Q	
	4.4		Suzuki et al. (1992)	Q	233
	3.4		Nirmalakhandan and Speece (1988)	Q	
	2.0		Duchowicz et al. (2020)	?	186, 21
	1.6		Yaws (1999)	?	21
	1.8		Yaws and Yang (1992)	?	21
	2.0		Abraham et al. (1990)	?	
2-propyn-1-ol	3.8	7400	Hiatt (2013)	M	
C_3H_4O	8.6		Duchowicz et al. (2020)	V	187
(propargyl alcohol)	9.0		HSDB (2015)	V	
[107-19-7]	7.0		Duchowicz et al. (2020)	Q	
TVDSBUOJIPERQY-UHFFFAOYSA-N	5.4		Hilal et al. (2008)	Q	
	7.0		Modarresi et al. (2007)	Q	68
2-buten-1-ol		6900	Plyasunov and Shock (2000)	L	
$CH_3CHCHCH_2OH$	3.1		Raventos-Duran et al. (2010)	Q	243, 244
[6117-91-5]	3.9		Raventos-Duran et al. (2010)	Q	245
WCASXYBKJHWFMY-UHFFFAOYSA-N	1.2		Raventos-Duran et al. (2010)	Q	246
	2.7		Hilal et al. (2008)	Q	
	3.0		Saxena and Hildemann (1996)	E	403
3-buten-1-ol		7000	Plyasunov and Shock (2000)	L	
C_4H_8O					
[627-27-0]					
ZSPTYLOMNJNZNG-UHFFFAOYSA-N					
4-penten-1-ol		7300	Plyasunov and Shock (2000)	L	
$C_5H_{10}O$					
[821-09-0]					
LQAVWYMTUMSFBE-UHFFFAOYSA-N					
3-pentyn-1-ol		7800	Plyasunov and Shock (2000)	L	
C_5H_8O					
[10229-10-4]					
IDYNOORNKYEHHO-UHFFFAOYSA-N					
2-methyl-3-buten-2-ol	6.4×10^{-1}		Iraci et al. (1999)	M	38
C_5H_9O	4.7×10^{-1}		Altschuh et al. (1999)	M	
[115-18-4]	1.6		Keshavarz et al. (2022)	Q	
HNVRRHSXBLFLIG-UHFFFAOYSA-N	7.9×10^{-1}		Duchowicz et al. (2020)	Q	300
	3.6×10^{-1}		Wang et al. (2017)	Q	81, 239
	1.2		Wang et al. (2017)	Q	81, 240
	7.3×10^{-1}		Wang et al. (2017)	Q	81, 241
	2.5		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	6.0×10^{-1}		Hilal et al. (2008)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.6		Modarresi et al. (2007)	Q	68
	4.7×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2-methyl-3-butyn-2-ol	2.5		Altschuh et al. (1999)	M	
C_5H_8O	1.6		Keshavarz et al. (2022)	Q	
[115-19-5]	1.5		Duchowicz et al. (2020)	Q	
CEBKHWWANWSNTI-UHFFFAOYSA-N	1.0		Hilal et al. (2008)	Q	
	8.3		Modarresi et al. (2007)	Q	68
	2.5		Duchowicz et al. (2020)	?	186, 21
3-methyl-1-pentyn-3-ol	9.9×10^{-1}		Hilal et al. (2008)	Q	
$C_6H_{10}O$	7.0		Modarresi et al. (2007)	Q	68
(meparfynol; methyl pentynol)	4.3		Katritzky et al. (1998)	Q	
[77-75-8]					
QXLPXWSKPNOQLE-UHFFFAOYSA-N					
2-cyclohexen-1-ol		8500	Plyasunov and Shock (2000)	L	
$C_6H_{10}O$					
[822-67-3]					
PQANGXXSEABURG-UHFFFAOYSA-N					
bicyclo[2.2.1]heptan-2-ol	2.2	5000	van Roon et al. (2005)	V	
$C_7H_{12}O$					
(norborneol)					
[1632-68-4]					
ZQTYQMYDIHMKQB-UHFFFAOYSA-N					
2-octen-1-ol	7.7×10^{-1}		Wu et al. (2022a)	Q	415
$C_8H_{16}O$					
[22104-78-5]					
AYQPVPFZWIQERS-UHFFFAOYSA-N					
1-octen-3-ol	1.9×10^{-1}	7900	Wu et al. (2022a)	M	
$C_8H_{16}O$	2.5×10^{-1}		Druaux et al. (1998)	M	
[3391-86-4]	1.3×10^{-1}		Roberts and Pollien (1997)	M	
VSMOENVRRABVKN-UHFFFAOYSA-N					
3,7-dimethyl-6-octen-1-ol	5.2		Martins et al. (2017)	V	316
$C_{10}H_{20}O$	4.9×10^{-1}		Dupeux et al. (2022)	Q	260
(citronellol)					
[106-22-9]					
QMVPMAAFGQKVCJ-UHFFFAOYSA-N					
3,7-dimethyl-1,6-octadien-3-ol	2.0×10^{-1}	4400	Leng et al. (2013)	M	
$C_{10}H_{18}O$	3.8×10^{-1}		Copolovici and Niinemets (2007)	M	
(linalool)	4.6×10^{-1}		Altschuh et al. (1999)	M	
[78-70-6]	4.0×10^{-1}		Martins et al. (2017)	V	316
CDOSHBSSFJOMGT-UHFFFAOYSA-N	4.8×10^{-1}		Copolovici and Niinemets (2005)	V	
	4.8×10^{-1}		Niinemets and Reichstein (2002)	V	
	2.1×10^{-1}	14000	Li et al. (1998)	V	
	1.6		Dupeux et al. (2022)	Q	260

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.3×10^{-1}		Keshavarz et al. (2022)	Q	
	3.3×10^{-1}		Duchowicz et al. (2020)	Q	185
	2.5×10^{-1}		Savary et al. (2014)	Q	
	2.5		Raventos-Duran et al. (2010)	Q	272, 244
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	6.9×10^{-1}		Hilal et al. (2008)	Q	
	1.4		Modarresi et al. (2007)	Q	68
	1.5×10^{-2}		Hertel and Sommer (2006)	Q	417
	4.6×10^{-1}		Duchowicz et al. (2020)	?	186, 21
linalool oxide $C_{10}H_{18}O_2$ [1365-19-1] BXOURKNXQXLKRK-UHFFFAOYSA-N	3.0×10^{2}		Dupeux et al. (2022)	Q	260
(*E*)-3,7-dimethyl-2,6-octadien-1-ol $C_{10}H_{18}O$ (geraniol) [106-24-1] GLZPCOQZEFWAFX-JXMROGBWSA-N	3.1		Martins et al. (2017)	V	316
	1.6		Dupeux et al. (2022)	Q	260
	1.7×10^{-1}		HSDB (2015)	Q	100
(*Z*)-3,7-dimethyl-2,6-octadien-1-ol $C_{10}H_{18}O$ [106-25-2] GLZPCOQZEFWAFX-YFHOEESVSA-N	8.6×10^{-1}		Duchowicz et al. (2020)	V	187
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	
tricyclo[3.3.1.1(3,7)]decan-1-ol $C_{10}H_{16}O$ (1-adamantanol) [768-95-6] VLLNJDMHDJRNFK-UHFFFAOYSA-N	6.0	5300	van Roon et al. (2005)	V	
3,7,11-trimethyl-2,6,10-dodecatrien-1-ol $C_{15}H_{26}O$ (farnesol) [4602-84-0] CRDAMVZIKSXKFV-YFVJMOTDSA-N	3.9×10^{-2}		HSDB (2015)	Q	100
(*Z*)-9-octadecen-1-ol $C_{18}H_{36}O$ (oleyl alcohol) [143-28-2] ALSTYHKOOCGGFT-KTKRTIGZSA-N	2.1×10^{-2}		HSDB (2015)	Q	100
(3*E*,13*Z*)-octadeca-3,13-dien-1-ol $C_{18}H_{34}O$ [66410-28-4] QBNCGBJHGBGHLS-IYUNJCAYSA-N	2.4×10^{-1}		Ebert et al. (2023)	?	319

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dihydroabietyl alcohol	1.9×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{20}H_{34}O$	2.4×10^{1}		Zhang et al. (2010)	Q	288, 290
[26266-77-3]	2.6×10^{1}		Zhang et al. (2010)	Q	288, 291
FLMIYUXOBAUKJM-UHFFFAOYSA-N	2.0×10^{-1}		Zhang et al. (2010)	Q	288, 292
ethylestrenol	4.3×10^{-1}		HSDB (2015)	Q	100
$C_{20}H_{32}O$					
[965-90-2]					
AOXRBFRFYPMWLR-UHFFFAOYSA-N					
trans-phytol	1.0×10^{-2}		Ebert et al. (2023)	?	367
$C_{20}H_{40}O$					
[150-86-7]					
BOTWFXYSPFMFNR-PYDDKJGSSA-N					
hydroxybenzene	1.8×10^{1}	3000	Schwardt et al. (2021)	L	1
C_6H_5OH	2.2×10^{1}	8900	Brockbank (2013)	L	1
(phenol)	2.2×10^{1}	9800	Ji et al. (2008)	M	
[108-95-2]	2.8×10^{1}	2700	Guo and Brimblecombe (2007)	M	
ISWSIDIOOBJBQZ-UHFFFAOYSA-N	6.4	7700	Feigenbrugel et al. (2004b)	M	
	3.0×10^{1}	5900	Harrison et al. (2002)	M	
	1.9×10^{1}		Sheikheldin et al. (2001)	M	12
	>4.2		Altschuh et al. (1999)	M	
	8.1×10^{1}	7400	Tabai et al. (1997)	M	11
	4.2		Heal et al. (1995)	M	375
	1.6×10^{1}	6000	Dohnal and Fenclová (1995)	M	
	1.5×10^{1}		Tremp et al. (1993)	M	12
	1.7×10^{1}	6100	Abd-El-Bary et al. (1986)	M	
	7.6		Warner et al. (1980)	M	
	2.0×10^{1}		Mackay et al. (2006c)	V	
	2.5×10^{1}		Lide and Frederikse (1995)	V	
	1.9×10^{1}		Mackay et al. (1995)	V	
	1.9×10^{1}		Shiu et al. (1994)	V	
	3.4		Hwang et al. (1992)	V	
	1.1×10^{1}		Riederer (1990)	V	
	9.0×10^{1}		Leuenberger et al. (1985)	V	418
	4.8		Hine and Weimar (1965)	R	
	2.8×10^{1}	6800	Parsons et al. (1971)	T	419
	1.3×10^{1}		Yaws (2003)	X	259
	1.9	3600	Janini and Quaddora (1986)	X	299
	1.9×10^{1}	7300	Goldstein (1982)	X	299
	2.5×10^{1}		Howard (1989)	X	420
	3.0×10^{1}		Gaffney and Senum (1984)	X	391
	3.7×10^{1}		McCarty (1980)	X	370
	2.5×10^{1}		Schüürmann (2000)	C	21
	7.6		Shiu et al. (1994)	C	
	7.6		Smith et al. (1993)	C	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.1×10^{1}		Ryan et al. (1988)	C	
	7.6		Shen (1982)	C	
	1.8×10^{1}		Dupeux et al. (2022)	Q	260
	6.4×10^{1}		Keshavarz et al. (2022)	Q	
	4.2×10^{1}		Duchowicz et al. (2020)	Q	185
	6.3×10^{1}		Wang et al. (2017)	Q	81, 239
	1.1×10^{1}		Wang et al. (2017)	Q	81, 240
	3.6×10^{1}		Wang et al. (2017)	Q	81, 241
	2.5×10^{1}		Li et al. (2014)	Q	242
	9.9		Raventos-Duran et al. (2010)	Q	243, 244
	7.8		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	246
	4.4		Hilal et al. (2008)	Q	
	1.8×10^{1}		Modarresi et al. (2007)	Q	68
		6200	Kühne et al. (2005)	Q	
	3.0×10^{1}		Yaffe et al. (2003)	Q	249, 250
	2.9×10^{1}		English and Carroll (2001)	Q	231, 232
	6.9		Katritzky et al. (1998)	Q	
	2.0×10^{1}		Russell et al. (1992)	Q	280
	2.0×10^{1}		Suzuki et al. (1992)	Q	233
	9.9		Nirmalakhandan and Speece (1988)	Q	
	3.0×10^{1}		Duchowicz et al. (2020)	?	186, 21
		5400	Kühne et al. (2005)	?	
	1.3×10^{1}		Yaws (1999)	?	21
	1.6×10^{1}		Abraham et al. (1990)	?	
(hydroxymethyl)-benzene	1.7×10^{1}		Chao et al. (2017)	M	
$C_6H_5CH_2OH$	$>3.7\times10^{1}$		Altschuh et al. (1999)	M	
(benzyl alcohol)	2.5×10^{1}		Chao et al. (2017)	V	
[100-51-6]	6.2×10^{-2}		Mackay et al. (2006c)	V	
WVDDGKGOMKODPV-UHFFFAOYSA-N	6.2×10^{-2}		Mackay et al. (1995)	V	
	2.9×10^{1}		Abraham et al. (1994a)	R	
	3.8×10^{1}		Yaws (2003)	X	259
	3.8×10^{1}		Yaws (2003)	X	238
	2.5×10^{1}		Howard (1993)	X	414
	1.6×10^{1}		Dupeux et al. (2022)	Q	260
	2.3×10^{1}		Keshavarz et al. (2022)	Q	
	2.3×10^{1}		Duchowicz et al. (2020)	Q	300
	3.8×10^{1}		Wang et al. (2017)	Q	81, 239
	4.9×10^{1}		Wang et al. (2017)	Q	81, 240
	3.8×10^{1}		Wang et al. (2017)	Q	81, 241
	8.6×10^{1}		Gharagheizi et al. (2012)	Q	
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	246
	4.1×10^{1}		Gharagheizi et al. (2010)	Q	247

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{1}		Hilal et al. (2008)	Q	
	5.5×10^{1}		Modarresi et al. (2007)	Q	68
	1.1×10^{1}		Yao et al. (2002)	Q	230
	2.1×10^{1}		English and Carroll (2001)	Q	231, 232
	6.9×10^{1}		Nirmalakhandan et al. (1997)	Q	
	8.9×10^{1}		Saxena and Hildemann (1996)	E	403
	2.9×10^{1}		Duchowicz et al. (2020)	?	186, 21
	2.9×10^{1}		HSDB (2015)	?	421
	3.8×10^{1}		Yaws (1999)	?	21
	1.8×10^{1}		Abraham et al. (1990)	?	
1-hydroxy-2-methylbenzene	6.7	7400	Brockbank (2013)	L	1
$HOC_6H_4CH_3$	6.5		Chao et al. (2017)	M	
(2-cresol; *o*-cresol)	4.2	8500	Feigenbrugel et al. (2004b)	M	
[95-48-7]	1.1×10^{1}	6700	Harrison et al. (2002)	M	
QWVGKYWNOKOFNN-UHFFFAOYSA-N	6.3		Altschuh et al. (1999)	M	
	5.6	5800	Dohnal and Fenclová (1995)	M	
	7.1		Tremp et al. (1993)	M	12
	8.2	7300	Parsons et al. (1972)	M	419
	5.8		Chao et al. (2017)	V	
			Mackay et al. (2006c)	V	422
	6.2		Lide and Frederikse (1995)	V	
	6.4		Mackay et al. (1995)	V	
	3.5×10^{1}		Leuenberger et al. (1985)	V	418
	8.8		Yaws (2003)	X	259
	2.6	4600	Janini and Quaddora (1986)	X	299
	6.2		Howard (1989)	X	420
	8.2		Gaffney and Senum (1984)	X	391
	8.3		Schüürmann (2000)	C	21
	8.4		Dupeux et al. (2022)	Q	260
	5.9		Keshavarz et al. (2022)	Q	
	2.3×10^{1}		Duchowicz et al. (2020)	Q	
	3.9×10^{1}		Wang et al. (2017)	Q	81, 239
	1.2×10^{1}		Wang et al. (2017)	Q	81, 240
	1.1×10^{1}		Wang et al. (2017)	Q	81, 241
	8.0		Li et al. (2014)	Q	242
	1.2×10^{1}		Gharagheizi et al. (2012)	Q	
	5.3		Hilal et al. (2008)	Q	
	6.2		Modarresi et al. (2007)	Q	68
		6500	Kühne et al. (2005)	Q	
	8.8		Yaffe et al. (2003)	Q	249, 250
	9.9		Yao et al. (2002)	Q	230, 268
	9.5		English and Carroll (2001)	Q	231, 232
	4.6		Katritzky et al. (1998)	Q	
	1.5×10^{1}		Suzuki et al. (1992)	Q	233
	7.2		Nirmalakhandan and Speece (1988)	Q	
	8.2		Duchowicz et al. (2020)	?	186, 21

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		8100	Kühne et al. (2005)	?	
	5.8		Yaws (1999)	?	21, 12
	1.2×10^{1}		Yaws and Yang (1992)	?	21, 12
	8.0		Abraham et al. (1990)	?	
1-hydroxy-3-methylbenzene	1.2×10^{1}	6200	Brockbank (2013)	L	1
$HOC_6H_4CH_3$	7.9	9000	Feigenbrugel et al. (2004b)	M	
(3-cresol; *m*-cresol)	1.2×10^{1}		Altschuh et al. (1999)	M	
[108-39-4]	1.2×10^{1}	6000	Dohnal and Fenclová (1995)	M	
RLSSMJSEOOYNOY-UHFFFAOYSA-N	1.3×10^{1}		Mackay et al. (2006c)	V	
	1.2×10^{1}		Schüürmann (2000)	V	
	1.1×10^{1}		Lide and Frederikse (1995)	V	
	1.1×10^{1}		Mackay et al. (1995)	V	
	1.1×10^{1}		Meylan and Howard (1991)	V	
	4.9×10^{1}		Leuenberger et al. (1985)	V	418
	2.2×10^{1}		Yaws (2003)	X	259
	6.1	7700	Janini and Quaddora (1986)	X	299
	1.1×10^{1}		Howard (1989)	X	420
	1.8×10^{1}		Dupeux et al. (2022)	Q	260
	5.9		Keshavarz et al. (2022)	Q	
	2.3×10^{1}		Duchowicz et al. (2020)	Q	185
	1.2×10^{1}		Gharagheizi et al. (2012)	Q	
	3.9		Hilal et al. (2008)	Q	
	1.1×10^{1}		Modarresi et al. (2007)	Q	68
		6500	Kühne et al. (2005)	Q	
	1.2×10^{1}		Yaffe et al. (2003)	Q	249, 250
	1.0×10^{1}		Yao et al. (2002)	Q	230
	1.7×10^{1}		Katritzky et al. (1998)	Q	
	1.6×10^{1}		Meylan and Howard (1991)	Q	
	1.2×10^{1}		Duchowicz et al. (2020)	?	186, 21
		6500	Kühne et al. (2005)	?	
	1.4×10^{1}		Yaws (1999)	?	21, 12
	1.4×10^{1}		Yaws and Yang (1992)	?	21, 12
	4.3		Abraham et al. (1990)	?	
1-hydroxy-4-methylbenzene	1.3×10^{1}	6600	Brockbank (2013)	L	1
$HOC_6H_4CH_3$	1.0×10^{1}	9300	Feigenbrugel et al. (2004b)	M	
(4-cresol; *p*-cresol)	>2.9		Altschuh et al. (1999)	M	
[106-44-5]	1.3×10^{1}	6100	Dohnal and Fenclová (1995)	M	
IWDCLRJOBJJRNH-UHFFFAOYSA-N	1.3×10^{1}		Tremp et al. (1993)	M	12
	1.3×10^{1}	7200	Parsons et al. (1972)	M	419
	1.8×10^{1}		Mackay et al. (2006c)	V	
	1.0×10^{1}		Lide and Frederikse (1995)	V	
	1.5×10^{1}		Mackay et al. (1995)	V	
	4.5×10^{1}		Leuenberger et al. (1985)	V	418
	1.2		Smith and Bomberger (1980)	V	24
	2.2×10^{1}		Yaws (2003)	X	259

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.2	4600	Janini and Quaddora (1986)	X	299
	1.0×10^1		Howard (1989)	X	420
	9.9		Gaffney and Senum (1984)	X	391
	1.3×10^1		Schüürmann (2000)	C	21
	1.6×10^1		Dupeux et al. (2022)	Q	260
	5.9		Keshavarz et al. (2022)	Q	
	2.3×10^1		Duchowicz et al. (2020)	Q	185
	1.8×10^1		Gharagheizi et al. (2012)	Q	
	4.2		Hilal et al. (2008)	Q	
	1.7×10^1		Modarresi et al. (2007)	Q	68
		6500	Kühne et al. (2005)	Q	
	8.8		Yaffe et al. (2003)	Q	249, 273
	1.5×10^1		Yao et al. (2002)	Q	230
	1.7×10^1		English and Carroll (2001)	Q	231, 232
	1.5×10^1		Katritzky et al. (1998)	Q	
	1.4×10^1		Suzuki et al. (1992)	Q	233
	7.0		Nirmalakhandan and Speece (1988)	Q	
	9.9		Duchowicz et al. (2020)	?	186, 21
		6000	Kühne et al. (2005)	?	
	1.3×10^1		Yaws (1999)	?	21, 12
	2.5×10^1		Yaws and Yang (1992)	?	21, 12
	1.3×10^1		Abraham et al. (1990)	?	
1-hydroxy-2,3-dimethylbenzene	6.7	6100	Brockbank (2013)	L	
$C_8H_{10}O$	9.3		Sheikheldin et al. (2001)	M	12
(2,3-xylenol; 2,3-dimethylphenol)	1.0×10^1	6800	Dohnal and Fenclová (1995)	M	
[526-75-0]	3.2		HSDB (2015)	V	
QWBBPBRQALCEIZ-UHFFFAOYSA-N	1.8×10^1		Mackay et al. (2006c)	V	
	1.9×10^1		Mackay et al. (1995)	V	
	4.9×10^1		Leuenberger et al. (1985)	V	418
	1.3×10^1		Abraham et al. (1994a)	R	
	7.9		Keshavarz et al. (2022)	Q	
	1.2×10^1		Duchowicz et al. (2020)	Q	185
	2.2×10^1		Wang et al. (2017)	Q	81, 239
	1.4×10^1		Wang et al. (2017)	Q	81, 240
	9.6		Wang et al. (2017)	Q	81, 241
	6.2		Raventos-Duran et al. (2010)	Q	243, 244
	7.8		Raventos-Duran et al. (2010)	Q	245
	1.6×10^1		Raventos-Duran et al. (2010)	Q	246
	5.8		Hilal et al. (2008)	Q	
	5.2		Modarresi et al. (2007)	Q	68
	1.4×10^1		Yaffe et al. (2003)	Q	249, 250
	1.2×10^1		English and Carroll (2001)	Q	231, 232
	4.6×10^1		Nirmalakhandan et al. (1997)	Q	
	1.3×10^1		Duchowicz et al. (2020)	?	186, 21

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-hydroxy-2,4-dimethylbenzene	3.5	5500	Brockbank (2013)	L	
$C_8H_{10}O$	6.6		Sheikheldin et al. (2001)	M	12
(2,4-xylenol; 2,4-dimethylphenol)	4.9	6100	Dohnal and Fenclová (1995)	M	
[105-67-9]	1.9×10^{-3}	-3200	Ashworth et al. (1988)	M	33, 279
KUFFULVDNCHOFZ-UHFFFAOYSA-N	5.5		Mackay et al. (2006c)	V	
	1.6×10^{1}		Lide and Frederikse (1995)	V	
	5.5		Mackay et al. (1995)	V	
	5.5×10^{-1}		Hwang et al. (1992)	V	
	4.9		Meylan and Howard (1991)	V	
	1.6×10^{1}		Leuenberger et al. (1985)	V	418
	1.0×10^{1}		Abraham et al. (1994a)	R	
	4.7		Yaws (2003)	X	259
	4.1	6600	Goldstein (1982)	X	299
	1.6×10^{1}		Howard (1989)	X	420
	5.8×10^{-1}		Smith et al. (1993)	C	
	5.4×10^{-1}		Ryan et al. (1988)	C	
	1.7×10^{1}		Petrasek et al. (1983)	C	
	6.7		Dupeux et al. (2022)	Q	260
	7.9		Keshavarz et al. (2022)	Q	
	1.2×10^{1}		Duchowicz et al. (2020)	Q	300
	2.2×10^{1}		Wang et al. (2017)	Q	81, 239
	1.2×10^{1}		Wang et al. (2017)	Q	81, 240
	8.7		Wang et al. (2017)	Q	81, 241
	4.6		Gharagheizi et al. (2012)	Q	
	6.2		Raventos-Duran et al. (2010)	Q	243, 244
	6.2		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	246
	5.1		Hilal et al. (2008)	Q	
	4.3		Modarresi et al. (2007)	Q	68
	1.1×10^{1}		Yaffe et al. (2003)	Q	249, 250
	1.6×10^{1}		English and Carroll (2001)	Q	231, 232
	6.7		Katritzky et al. (1998)	Q	
	4.6×10^{1}		Nirmalakhandan et al. (1997)	Q	
	1.4×10^{1}		Meylan and Howard (1991)	Q	
	1.0×10^{1}		Duchowicz et al. (2020)	?	186, 21
1-hydroxy-2,5-dimethylbenzene	8.2	8700	Brockbank (2013)	L	1
$C_8H_{10}O$	7.5	6800	Dohnal and Fenclová (1995)	M	
(2,5-xylenol; 2,5-dimethylphenol)	1.4		HSDB (2015)	V	
[95-87-4]	7.5		Mackay et al. (2006c)	V	
NKTOLZVEWDHZMU-UHFFFAOYSA-N	7.4		Mackay et al. (1995)	V	
	3.8×10^{1}		Leuenberger et al. (1985)	V	418
	8.8		Abraham et al. (1994a)	R	
	1.9		Yaws (2003)	X	259
	5.7		Dupeux et al. (2022)	Q	260
	7.9		Keshavarz et al. (2022)	Q	
	1.2×10^{1}		Duchowicz et al. (2020)	Q	300

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{1}		Wang et al. (2017)	Q	81, 239
	1.2×10^{1}		Wang et al. (2017)	Q	81, 240
	8.9		Wang et al. (2017)	Q	81, 241
	6.2		Raventos-Duran et al. (2010)	Q	243, 244
	6.2		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	246
	5.2		Hilal et al. (2008)	Q	
	4.8		Modarresi et al. (2007)	Q	68
	3.1		Yaffe et al. (2003)	Q	249, 273
	1.4×10^{1}		English and Carroll (2001)	Q	231, 275
	4.6×10^{1}		Nirmalakhandan et al. (1997)	Q	
	8.8		Duchowicz et al. (2020)	?	186, 21
1-hydroxy-2,6-dimethylbenzene	1.6	6300	Brockbank (2013)	L	1
$C_8H_{10}O$	2.3	6200	Dohnal and Fenclová (1995)	M	
(2,6-xylenol; 2,6-dimethylphenol)	1.3		Hawthorne et al. (1985)	M	
[576-26-1]	2.5		Mackay et al. (2006c)	V	
NXXYKOUNUYWIHA-UHFFFAOYSA-N	2.6		Mackay et al. (1995)	V	
	2.6		Shiu et al. (1994)	V	
	5.2		Leuenberger et al. (1985)	V	418
	2.9		Abraham et al. (1994a)	R	
	1.4		Yaws (2003)	X	259
	1.6		Dupeux et al. (2022)	Q	260
	7.9		Keshavarz et al. (2022)	Q	
	3.0		Duchowicz et al. (2020)	Q	300
	6.2		Raventos-Duran et al. (2010)	Q	243, 244
	3.9		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	246
	9.2		Hilal et al. (2008)	Q	
	1.8		Modarresi et al. (2007)	Q	68
	3.1		Yaffe et al. (2003)	Q	249, 250
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
	4.6×10^{1}		Nirmalakhandan et al. (1997)	Q	
	1.5		Duchowicz et al. (2020)	?	186, 21
	1.4		Yaws (1999)	?	21
1-hydroxy-3,4-dimethylbenzene	2.6×10^{1}	7200	Brockbank (2013)	L	
$C_8H_{10}O$	2.4×10^{1}	7100	Dohnal and Fenclová (1995)	M	
(3,4-xylenol; 3,4-dimethylphenol)	8.2		HSDB (2015)	V	
[95-65-8]	4.6×10^{1}		Mackay et al. (2006c)	V	
YCOXTKKNXUZSKD-UHFFFAOYSA-N	4.7×10^{1}		Mackay et al. (1995)	V	
	4.7×10^{1}		Shiu et al. (1994)	V	
	1.1×10^{2}		Leuenberger et al. (1985)	V	418
	2.4×10^{1}		Abraham et al. (1994a)	R	
	1.1×10^{1}		Yaws (2003)	X	259
	1.8×10^{1}		Dupeux et al. (2022)	Q	260
	7.9		Keshavarz et al. (2022)	Q	
	1.2×10^{1}		Duchowicz et al. (2020)	Q	300

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^{1}		Gharagheizi et al. (2012)	Q	
	6.2		Raventos-Duran et al. (2010)	Q	243, 244
	7.8		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	246
	4.4		Hilal et al. (2008)	Q	
	1.2×10^{1}		Modarresi et al. (2007)	Q	68
	2.4×10^{1}		Yaffe et al. (2003)	Q	249, 250
	2.1×10^{1}		English and Carroll (2001)	Q	231, 261
	4.6×10^{1}		Nirmalakhandan et al. (1997)	Q	
	2.4×10^{1}		Duchowicz et al. (2020)	?	186, 21
1-hydroxy-3,5-dimethylbenzene	1.5×10^{1}	7600	Brockbank (2013)	L	1
$C_8H_{10}O$	1.6×10^{1}	6900	Dohnal and Fenclová (1995)	M	
(3,5-xylenol; 3,5-dimethylphenol)	7.6		HSDB (2015)	V	
[108-68-9]	2.8×10^{1}		Mackay et al. (2006c)	V	
TUAMRELNJMMDMT-UHFFFAOYSA-N	3.1×10^{1}		Mackay et al. (1995)	V	
	2.5×10^{1}		Shiu et al. (1994)	V	
	6.2×10^{1}		Leuenberger et al. (1985)	V	418
	1.6×10^{1}		Abraham et al. (1994a)	R	
	7.3		Yaws (2003)	X	259
	1.2×10^{1}		Dupeux et al. (2022)	Q	260
	7.9		Keshavarz et al. (2022)	Q	
	1.2×10^{1}		Duchowicz et al. (2020)	Q	185
	6.2		Raventos-Duran et al. (2010)	Q	243, 244
	4.9		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	246
	3.2		Hilal et al. (2008)	Q	
	1.1×10^{1}		Modarresi et al. (2007)	Q	68
	1.6×10^{1}		Yaffe et al. (2003)	Q	249, 250
	1.7×10^{1}		English and Carroll (2001)	Q	231, 232
	4.6×10^{1}		Nirmalakhandan et al. (1997)	Q	
	1.6×10^{1}		Duchowicz et al. (2020)	?	186, 21
2-methylbenzenemethanol	2.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O$	5.6×10^{1}		Wang et al. (2017)	Q	81, 240
[89-95-2]	1.7×10^{1}		Wang et al. (2017)	Q	81, 241
XPNGNIFUDRPBFJ-UHFFFAOYSA-N					
3-methylbenzenemethanol	2.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O$	4.5×10^{1}		Wang et al. (2017)	Q	81, 240
[587-03-1]	3.4×10^{1}		Wang et al. (2017)	Q	81, 241
JJCKHVUTVOPLBV-UHFFFAOYSA-N					
4-methylbenzenemethanol	9.0		HSDB (2015)	V	
$C_8H_{10}O$	2.2×10^{1}		Wang et al. (2017)	Q	81, 239
[589-18-4]	5.3×10^{1}		Wang et al. (2017)	Q	81, 240
KMTDMTZBNYGUNX-UHFFFAOYSA-N	4.6×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
α-methylbenzyl alcohol $C_8H_{10}O$ [98-85-1] WAPNOHKVXSQRPX-UHFFFAOYSA-N	3.4×10^{1}		HSDB (2015)	Q	100
1-hydroxy-2-ethylbenzene	2.1		Duchowicz et al. (2020)	V	187
$C_8H_{10}O$	2.1		HSDB (2015)	V	
(2-ethylphenol)	5.6		Mackay et al. (2006c)	V	
[90-00-6]	2.4×10^{1}		Duchowicz et al. (2020)	Q	
IXQGCWUGDFDQMF-UHFFFAOYSA-N	3.0×10^{1}		Wang et al. (2017)	Q	81, 239
	8.1		Wang et al. (2017)	Q	81, 240
	7.3		Wang et al. (2017)	Q	81, 241
	6.2		Raventos-Duran et al. (2010)	Q	243, 244
	4.9		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	246
	1.6		Modarresi et al. (2007)	Q	68
	2.2		Yaffe et al. (2003)	Q	249, 250
	3.1		Katritzky et al. (1998)	Q	
1-hydroxy-3-ethylbenzene	4.9		Karl et al. (2003)	M	
$C_8H_{10}O$	1.6×10^{1}		Abraham et al. (1994a)	R	
(3-ethylphenol)	7.9		Keshavarz et al. (2022)	Q	
[620-17-7]	2.4×10^{1}		Duchowicz et al. (2020)	Q	185
HMNKTRSOROOSPP-UHFFFAOYSA-N	9.0		HSDB (2015)	Q	100
	6.2		Raventos-Duran et al. (2010)	Q	243, 244
	4.9		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	246
	3.4		Hilal et al. (2008)	Q	
	2.1×10^{1}		Modarresi et al. (2007)	Q	68
	1.5×10^{1}		Yaffe et al. (2003)	Q	249, 250
	1.8×10^{1}		English and Carroll (2001)	Q	231, 232
	5.4×10^{1}		Nirmalakhandan et al. (1997)	Q	
	1.6×10^{1}		Duchowicz et al. (2020)	?	186, 21
1-hydroxy-4-ethylbenzene	8.2		HSDB (2015)	V	
$C_8H_{10}O$	2.1×10^{1}		Mackay et al. (2006c)	V	
(4-ethylphenol)	1.3×10^{1}		Abraham et al. (1994a)	R	
[123-07-9]	7.9		Keshavarz et al. (2022)	Q	
HXDOZKJGKXYMEW-UHFFFAOYSA-N	2.4×10^{1}		Duchowicz et al. (2020)	Q	300
	6.2		Raventos-Duran et al. (2010)	Q	272, 244
	6.2		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	246
	3.8		Hilal et al. (2008)	Q	
	9.4		Modarresi et al. (2007)	Q	68
	1.6×10^{1}		English and Carroll (2001)	Q	231, 232
	5.4×10^{1}		Nirmalakhandan et al. (1997)	Q	
	1.3×10^{1}		Duchowicz et al. (2020)	?	186, 21

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4-trimethylphenol	1.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O$	1.8×10^{1}		Wang et al. (2017)	Q	81, 240
[526-85-2]	8.9		Wang et al. (2017)	Q	81, 241
XRUGBBIQLIVCSI-UHFFFAOYSA-N					
2,3,5-trimethylphenol	1.2×10^{1}		Mackay et al. (2006c)	V	
$C_9H_{12}O$	1.2×10^{1}		Mackay et al. (1995)	V	
[697-82-5]					
OGRAOKJKVGDSFR-UHFFFAOYSA-N					
2,3,6-trimethylphenol	2.5		Duchowicz et al. (2020)	V	187
$C_9H_{12}O$	2.5		HSDB (2015)	V	
[2416-94-6]	1.6		Duchowicz et al. (2020)	Q	
QQOMQLYQAXGHSU-UHFFFAOYSA-N	2.5		Wang et al. (2017)	Q	81, 239
	1.1×10^{1}		Wang et al. (2017)	Q	81, 240
	1.3		Wang et al. (2017)	Q	81, 241
	1.1×10^{1}		Hilal et al. (2008)	Q	
	4.1×10^{-1}		Modarresi et al. (2007)	Q	68
2,4,6-trimethylphenol	3.8		Duchowicz et al. (2020)	V	187
$C_9H_{12}O$	3.2		HSDB (2015)	V	
[527-60-6]	1.3		Mackay et al. (2006c)	V	
BPRYUXCVCCNUFE-UHFFFAOYSA-N	1.4		Mackay et al. (1995)	V	
	1.6		Duchowicz et al. (2020)	Q	
	2.5		Wang et al. (2017)	Q	81, 239
	8.9		Wang et al. (2017)	Q	81, 240
	1.2		Wang et al. (2017)	Q	81, 241
	4.9		Raventos-Duran et al. (2010)	Q	243, 244
	3.1		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	246
	9.2		Hilal et al. (2008)	Q	
	1.2		Modarresi et al. (2007)	Q	68
3,4,5-trimethylphenol	3.4×10^{1}		Mackay et al. (2006c)	V	
$C_9H_{12}O$	3.8×10^{1}		Mackay et al. (1995)	V	
[527-54-8]					
FDQQNNZKEJIHMS-UHFFFAOYSA-N					
1-hydroxy-4-propylbenzene	1.7		Mackay et al. (2006c)	V	
$C_9H_{12}O$	8.6		Abraham et al. (1994a)	R	
(4-propylphenol)	1.1×10^{1}		Keshavarz et al. (2022)	Q	
[645-56-7]	2.5×10^{1}		Duchowicz et al. (2020)	Q	
KLSLBUSXWBJMEC-UHFFFAOYSA-N	4.9		Raventos-Duran et al. (2010)	Q	272, 244
	3.9		Raventos-Duran et al. (2010)	Q	245
	9.9		Raventos-Duran et al. (2010)	Q	246
	3.1		Hilal et al. (2008)	Q	
	1.0×10^{1}		Modarresi et al. (2007)	Q	68
	8.8		Yaffe et al. (2003)	Q	249, 250
	1.2×10^{1}		English and Carroll (2001)	Q	231, 261

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.3×10^{1}		Nirmalakhandan et al. (1997)	Q	
	8.7		Duchowicz et al. (2020)	?	186, 21
2-(1-methylethyl)-phenol	2.6		Mackay et al. (2006c)	V	
$C_9H_{12}O$	2.8×10^{1}		Wang et al. (2017)	Q	81, 239
[88-69-7]	3.9		Wang et al. (2017)	Q	81, 240
CRBJBYGJVIBWIY-UHFFFAOYSA-N	4.5		Wang et al. (2017)	Q	81, 241
	2.8		Hilal et al. (2008)	Q	
2-phenylisopropanol	2.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O$	1.4×10^{1}		Wang et al. (2017)	Q	81, 240
[617-94-7]	1.2×10^{1}		Wang et al. (2017)	Q	81, 241
BDCFWIDZNLCTMF-UHFFFAOYSA-N	2.6×10^{1}		HSDB (2015)	Q	100
2-ethyl-3-methylphenol	1.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O$	8.9		Wang et al. (2017)	Q	81, 240
[6161-62-2]	5.8		Wang et al. (2017)	Q	81, 241
OCKYMBMCPOAFLL-UHFFFAOYSA-N					
2-ethyl-5-methylphenol	1.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O$	8.0		Wang et al. (2017)	Q	81, 240
[1687-61-2]	4.9		Wang et al. (2017)	Q	81, 241
LTRVUFFOMIUCPJ-UHFFFAOYSA-N					
2-ethyl-6-methylphenol	3.3		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O$	6.2		Wang et al. (2017)	Q	81, 240
[1687-64-5]	6.9×10^{-1}		Wang et al. (2017)	Q	81, 241
CIRRFAQIWQFQSS-UHFFFAOYSA-N					
5-ethyl-3-methylphenol	1.5×10^{1}		Duchowicz et al. (2020)	V	187
$C_9H_{12}O$	1.3×10^{1}		Duchowicz et al. (2020)	Q	
[698-71-5]	4.9		Raventos-Duran et al. (2010)	Q	243, 244
XTCHLXABLZQNNN-UHFFFAOYSA-N	3.9		Raventos-Duran et al. (2010)	Q	245
	9.9		Raventos-Duran et al. (2010)	Q	246
	2.9		Hilal et al. (2008)	Q	
	1.8×10^{1}		Modarresi et al. (2007)	Q	68
1-(2-methylphenyl)ethanol	2.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O$	2.9×10^{1}		Wang et al. (2017)	Q	81, 240
[7287-82-3]	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
SDCBYRLJYGORNK-UHFFFAOYSA-N					
2-propylphenol	2.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O$	5.6		Wang et al. (2017)	Q	81, 240
[644-35-9]	5.0		Wang et al. (2017)	Q	81, 241
LCHYEKKJCUJAKN-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-phenyl-1-propanol	2.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O$	2.3×10^{1}		Wang et al. (2017)	Q	81, 240
[93-54-9]	9.8		Wang et al. (2017)	Q	81, 241
DYUQAZSOFZSPHD-UHFFFAOYSA-N					
2,3-dimethylbenzyl alcohol	1.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O$	7.4×10^{1}		Wang et al. (2017)	Q	81, 240
[13651-14-4]	2.3×10^{1}		Wang et al. (2017)	Q	81, 241
ZQQIVMXQYUZKIQ-UHFFFAOYSA-N					
3,4-dimethylbenzyl alcohol	1.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O$	6.2×10^{1}		Wang et al. (2017)	Q	81, 240
[6966-10-5]	5.5×10^{1}		Wang et al. (2017)	Q	81, 241
OKGZCXPDJKKZAP-UHFFFAOYSA-N					
3,5-dimethylbenzyl alcohol	1.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O$	3.7×10^{1}		Wang et al. (2017)	Q	81, 240
[27129-87-9]	4.0×10^{1}		Wang et al. (2017)	Q	81, 241
IQWWTJDRVBWBEL-UHFFFAOYSA-N					
2-(1,1-dimethylethyl)-phenol	3.9×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{10}H_{14}O$	4.4		Duchowicz et al. (2020)	Q	
[88-18-6]	7.0		HSDB (2015)	Q	100
WJQOZHYUIDYNHM-UHFFFAOYSA-N					
3-(1,1-dimethylethyl)-phenol	5.1		Duchowicz et al. (2020)	V	187
$C_{10}H_{14}O$	4.4		Duchowicz et al. (2020)	Q	
[585-34-2]					
CYEKUDPFXBLGHH-UHFFFAOYSA-N					
2-(1-methylpropyl)phenol	4.7		HSDB (2015)	Q	100
$C_{10}H_{14}O$					
[89-72-5]					
NGFPWHGISWUQOI-UHFFFAOYSA-N					
4-(1-methylpropyl)-phenol	3.6		Mackay et al. (2006c)	V	
$C_{10}H_{14}O$	4.3		Mackay et al. (1995)	V	
(4-*sec*-butylphenol)					
[99-71-8]					
ZUTYZAFDFLLILI-UHFFFAOYSA-N					
4-*tert*-butylphenol	8.9	7700	Parsons et al. (1972)	M	419
$C_{10}H_{14}O$	1.6×10^{1}		Mackay et al. (2006c)	V	
[98-54-4]	2.1×10^{1}		Mackay et al. (1995)	V	
QHPQWRBYOIRBIT-UHFFFAOYSA-N	1.4×10^{1}		Keshavarz et al. (2022)	Q	
	4.4		Duchowicz et al. (2020)	Q	
	2.1		Hilal et al. (2008)	Q	
	4.8		Modarresi et al. (2007)	Q	68
	8.8		Yaffe et al. (2003)	Q	249, 250
	6.7		English and Carroll (2001)	Q	231, 232
	2.5×10^{1}		Katritzky et al. (1998)	Q	

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.4×10^{1}		Nirmalakhandan et al. (1997)	Q	
	5.2		Suzuki et al. (1992)	Q	233
	2.7		Nirmalakhandan and Speece (1988)	Q	
	8.3		Duchowicz et al. (2020)	?	186, 21
	1.5×10^{-1}		Betterton (1992)	?	423
	8.8		Abraham et al. (1990)	?	
2-methyl-5-(1-methylethyl)-phenol	1.5		Martins et al. (2017)	V	316
$C_{10}H_{14}O$	2.4	9300	van Roon et al. (2005)	V	
(carvacrol)					
[499-75-2]					
RECUKUPTGUEGMW-UHFFFAOYSA-N					
5-methyl-2-(1-methylethyl)-phenol	2.0×10^{1}		Duchowicz et al. (2020)	V	187
$C_{10}H_{14}O$	1.5		Martins et al. (2017)	V	316
(thymol)	3.0	9300	van Roon et al. (2005)	V	
[89-83-8]	5.1		Duchowicz et al. (2020)	Q	
MGSRCZKZVOBKFT-UHFFFAOYSA-N	3.1		Raventos-Duran et al. (2010)	Q	243, 244
	2.0		Raventos-Duran et al. (2010)	Q	245
	7.8		Raventos-Duran et al. (2010)	Q	246
	2.8		Hilal et al. (2008)	Q	
	7.1×10^{-1}		Modarresi et al. (2007)	Q	68
1-(3,5-dimethylphenyl)ethanol	1.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{14}O$	1.8×10^{1}		Wang et al. (2017)	Q	81, 240
[5379-18-0]	1.4×10^{1}		Wang et al. (2017)	Q	81, 241
RHBAJFPGUNNLFA-UHFFFAOYSA-N					
6-ethyl-2,4-xylenol	2.0		Wang et al. (2017)	Q	81, 239
$C_{10}H_{14}O$	5.8		Wang et al. (2017)	Q	81, 240
[2219-79-6]	6.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MXHAHSBTOVFDBK-UHFFFAOYSA-N					
2-(1,1-dimethylethyl)-4-methylphenol	6.6		HSDB (2015)	Q	100
$C_{11}H_{16}O$					
[2409-55-4]					
IKEHOXWJQXIQAG-UHFFFAOYSA-N					
4-(1,1-dimethylpropyl)phenol	4.9		HSDB (2015)	V	
$C_{11}H_{16}O$					
[80-46-6]					
NRZWYNLTFLDQQX-UHFFFAOYSA-N					
MCM:DE35TOH	1.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{16}O$	1.6×10^{1}		Wang et al. (2017)	Q	81, 240
OZZOZHVUMWFILP-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DEMPHOH	1.8		Wang et al. (2017)	Q	81, 239
$C_{11}H_{16}O$	3.8		Wang et al. (2017)	Q	81, 240
VUDWBUZLGAXSDX-UHFFFAOYSA-N	6.3×10^{-1}		Wang et al. (2017)	Q	81, 241
josenol	4.5×10^{1}		Dupeux et al. (2022)	Q	260
$C_{11}H_{14}O$					
(2-methyl-3-(4-methylphenyl)-2-propen-1-ol)					
[56138-10-4]					
WWHATUWNHYNMNW-UHFFFAOYSA-N					
lilyflore	1.3×10^{1}		Dupeux et al. (2022)	Q	260
$C_{12}H_{16}O$					
[285977-85-7]					
UWSPWQQZFOSTHS-UHFFFAOYSA-N					
benzhydrol	3.8×10^{2}		Ebert et al. (2023)	?	319
$C_{13}H_{12}O$					
[91-01-0]					
QILSFLSDHQAZET-UHFFFAOYSA-N					
1-hydroxy-4-octylbenzene	1.3		Mackay et al. (2006c)	V	
$C_{14}H_{22}O$	2.0		Mackay et al. (1995)	V	
(4-octylphenol)					
[1806-26-4]					
NTDQQZYCCIDJRK-UHFFFAOYSA-N					
4-(1,1,3,3-tetramethylbutyl)-phenol	2.3	9000	Xie et al. (2004)	M	
$C_{14}H_{22}O$	1.4		HSDB (2015)	Q	100
(*p-tert*-octylphenol)	2.2		Zhang et al. (2010)	Q	288, 289
[140-66-9]	2.3		Zhang et al. (2010)	Q	288, 290
ISAVYTVYFVQUDY-UHFFFAOYSA-N	1.0×10^{1}		Zhang et al. (2010)	Q	288, 291
	1.8		Zhang et al. (2010)	Q	288, 292
1-hydroxy-4-nonylbenzene	2.9×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{15}H_{24}O$	2.9×10^{-1}		HSDB (2015)	V	
(4-nonylphenol)	3.6×10^{-1}		Mackay et al. (2006c)	V	
[104-40-5]	6.4×10^{-1}		Mackay et al. (1995)	V	
IGFHQQFPSIBGKE-UHFFFAOYSA-N	2.8×10^{1}		Duchowicz et al. (2020)	Q	
2,6-bis(1,1-dimethylethyl)-4-methylphenol	2.9×10^{-3}		Yoshida et al. (1983)	V	
$C_{15}H_{24}O$					
(butylated hydroxytoluene; BHT)					
[128-37-0]					
NLZUEZXRPGMBCV-UHFFFAOYSA-N					

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-(3',5'-dimethyl-3'-heptyl)-phenol(+) $C_{15}H_{24}O$ RYIHVIPUIXFRNI-IUODEOHRSA-N	2.9	8700	Xie et al. (2004)	M	
4-(3',5'-dimethyl-3'-heptyl)-phenol(-) $C_{15}H_{24}O$ RYIHVIPUIXFRNI-SWLSCSKDSA-N	3.3	8600	Xie et al. (2004)	M	
2-phenylethanol	1.7×10^{1}	7200	Brockbank (2013)	L	1
$C_8H_{10}O$	$>3.7\times10^{1}$		Altschuh et al. (1999)	M	
[60-12-8]	6.6×10^{1}		HSDB (2015)	V	
WRMNZCZEMHIOCP-UHFFFAOYSA-N	3.9×10^{1}		Abraham et al. (1994a)	R	
	3.5		Yaws (2003)	X	259
	1.6×10^{1}		Dupeux et al. (2022)	Q	260
	3.0×10^{1}		Keshavarz et al. (2022)	Q	
	2.0×10^{-3}		Abney (2021)	Q	401
	8.5		Duchowicz et al. (2020)	Q	185
	8.5		Wang et al. (2017)	Q	81, 239
	3.9×10^{1}		Wang et al. (2017)	Q	81, 240
	3.9×10^{1}		Wang et al. (2017)	Q	81, 241
	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	246
	1.9×10^{1}		Hilal et al. (2008)	Q	
	3.2×10^{1}		Modarresi et al. (2007)	Q	68
	2.4×10^{-1}		Emel'yanenko et al. (2007)	Q	417
	2.4×10^{-1}		Hertel and Sommer (2005)	Q	417
	3.9×10^{1}		Yaffe et al. (2003)	Q	249, 250
	1.0×10^{1}		Yao et al. (2002)	Q	230
	2.8×10^{1}		English and Carroll (2001)	Q	231, 275
	5.4×10^{1}		Katritzky et al. (1998)	Q	
	5.3×10^{1}		Nirmalakhandan et al. (1997)	Q	
	3.9×10^{1}		Duchowicz et al. (2020)	?	186, 21
	3.5		Yaws (1999)	?	21
3-phenyl-1-propanol	$>1.8\times10^{2}$		Altschuh et al. (1999)	M	
$C_9H_{12}O$	4.8×10^{1}		Abraham et al. (1994a)	R	
[122-97-4]	4.1×10^{1}		Keshavarz et al. (2022)	Q	
VAJVDSVGBWFCLW-UHFFFAOYSA-N	8.8		Duchowicz et al. (2020)	Q	300
	1.4×10^{1}		Hilal et al. (2008)	Q	
	2.0×10^{1}		Modarresi et al. (2007)	Q	68
	3.4×10^{1}		English and Carroll (2001)	Q	231, 232
	4.2×10^{1}		Nirmalakhandan et al. (1997)	Q	
	4.9×10^{1}		Duchowicz et al. (2020)	?	186, 21

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-phenyl-1-butanol	>6.7		Altschuh et al. (1999)	M	
$C_{10}H_{14}O$	1.2×10^{1}		Hilal et al. (2008)	Q	
[3360-41-6]					
LDZLXQFDGRCELX-UHFFFAOYSA-N					
1-naphthalenol	1.6×10^{2}		HSDB (2015)	V	
$C_{10}H_8O$	2.9×10^{1}		Mackay et al. (2006c)	V	
(1-naphthol)	1.7×10^{2}		Abraham et al. (1994a)	R	
[90-15-3]	2.1×10^{2}		Keshavarz et al. (2022)	Q	
KJCVRFUGPWSIIH-UHFFFAOYSA-N	1.7×10^{2}		Duchowicz et al. (2020)	Q	
	6.9×10^{1}		Hilal et al. (2008)	Q	
	8.4×10^{1}		Modarresi et al. (2007)	Q	68
	4.5×10^{2}		English and Carroll (2001)	Q	231, 232
	1.5×10^{3}		Nirmalakhandan et al. (1997)	Q	
	1.6×10^{2}		Duchowicz et al. (2020)	?	186, 21
2-naphthalenol	1.1×10^{2}		Mackay et al. (2006c)	V	
$C_{10}H_8O$	3.6×10^{2}		Abraham et al. (1994a)	R	
(2-naphthol)	2.1×10^{2}		Keshavarz et al. (2022)	Q	
[135-19-3]	1.7×10^{2}		Duchowicz et al. (2020)	Q	
JWAZRIHNYRIHIV-UHFFFAOYSA-N	2.1×10^{2}		HSDB (2015)	Q	100
	7.0×10^{1}		Hilal et al. (2008)	Q	
	2.7×10^{2}		Modarresi et al. (2007)	Q	68
		7400	Kühne et al. (2005)	Q	
	5.8×10^{2}		English and Carroll (2001)	Q	231, 232
	1.7×10^{3}		Nirmalakhandan et al. (1997)	Q	
	3.6×10^{2}		Duchowicz et al. (2020)	?	186, 21
		7200	Kühne et al. (2005)	?	
o-hydroxybiphenyl	9.4		Duchowicz et al. (2020)	V	187
$C_{12}H_{10}O$	9.4		HSDB (2015)	V	
[90-43-7]	2.9×10^{-1}		Mackay et al. (2006c)	V	
LLEMOWNGBBNAJR-UHFFFAOYSA-N	2.1×10^{2}		Duchowicz et al. (2020)	Q	
	3.1×10^{1}		Hilal et al. (2008)	Q	
	1.1×10^{1}		Modarresi et al. (2007)	Q	68
p-hydroxybiphenyl	1.6×10^{-1}		Mackay et al. (2006c)	V	
$C_{12}H_{10}O$	1.9×10^{2}		HSDB (2015)	Q	100
[92-69-3]					
YXVFYQXJAXKLAK-UHFFFAOYSA-N					
2,4,6-tris(1,1-dimethylethyl)phenol	1.0		Zhang et al. (2010)	Q	288, 289
$C_{18}H_{30}O$	5.6×10^{-2}		Zhang et al. (2010)	Q	288, 290
[732-26-3]	3.3×10^{-2}		Zhang et al. (2010)	Q	288, 291
PFEFOYRSMXVNEL-UHFFFAOYSA-N	5.3×10^{-2}		Zhang et al. (2010)	Q	288, 292

Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dehydroabietol	8.4		Zhang et al. (2010)	Q	288, 289
$C_{20}H_{30}O$	1.8×10^{2}		Zhang et al. (2010)	Q	288, 290
[3772-55-2]	2.4×10^{1}		Zhang et al. (2010)	Q	288, 291
WSKGRAGZAQRSED-IOJLRTSASA-N	7.2×10^{-1}		Zhang et al. (2010)	Q	288, 292
2,2'-methylenebis(6-(1,1-dimethylethyl)-4-methylphenol)	1.2×10^{6}		HSDB (2015)	Q	100
$C_{23}H_{32}O_2$					
[119-47-1]					
KGRVJHAUYBGFFP-UHFFFAOYSA-N					
2,4-dinonylphenol	1.5×10^{-1}		HSDB (2015)	Q	100
$C_{24}H_{42}O$	1.6×10^{-1}		Zhang et al. (2010)	Q	288, 289
[137-99-5]	3.8×10^{-1}		Zhang et al. (2010)	Q	288, 290
FDAJTLLBHNHECW-UHFFFAOYSA-N	7.0×10^{-1}		Zhang et al. (2010)	Q	288, 291
	2.5×10^{-1}		Zhang et al. (2010)	Q	288, 292

A3.3 Polyols ($R(OH)_n$)

Table A3.3: Polyols ($R(OH)_n$)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
methanediol	9.9×10^{1}		Franco et al. (2021)	R	424
$HOCH_2OH$	4.0×10^{3}		Mansfield (2020)	T	425
[463-57-0]	7.1×10^{2}		Mansfield (2020)	T	425
CKFGINPQOCXMAZ-UHFFFAOYSA-N					
1,1-ethanediol	4.0×10^{1}		Mansfield (2020)	T	425
$CH_3CH_2(OH)_2$	1.4×10^{1}		Mansfield (2020)	T	425
[4433-56-1]					
AZHSSKPUVBVXLK-UHFFFAOYSA-N					
1,2-ethanediol	6.5×10^{3}		Burkholder et al. (2019)	L	
$HO(CH_2)_2OH$	6.5×10^{3}		Burkholder et al. (2015)	L	
(ethylene glycol)	4.0×10^{3}		Bone et al. (1983)	M	12
[107-21-1]	1.6×10^{2}		Butler and Ramchandani (1935)	M	426
LYCAIKOWRPUZTN-UHFFFAOYSA-N	4.7		HSDB (2015)	V	
	6.5×10^{3}	8800	Compernolle and Müller (2014b)	V	
	5.0×10^{3}		Hwang et al. (1992)	V	
	7.0×10^{3}		Yaws (2003)	X	259
	7.0×10^{3}		Yaws (2003)	X	238
	4.8×10^{3}		Dupeux et al. (2022)	Q	260
	2.9×10^{2}		Keshavarz et al. (2022)	Q	
	6.4×10^{2}		Duchowicz et al. (2020)	Q	185
	3.3×10^{2}		Wang et al. (2017)	Q	81, 239
	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
	6.3×10^{3}		Wang et al. (2017)	Q	81, 241
	5.6×10^{2}		Olsen et al. (2016)	Q	427
	4.0×10^{2}		Olsen et al. (2016)	Q	428
	4.3×10^{2}		Olsen et al. (2016)	Q	429
	1.3×10^{4}		Gharagheizi et al. (2012)	Q	
	7.8×10^{3}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{2}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	246
	2.5×10^{3}		Gharagheizi et al. (2010)	Q	247
	7.2×10^{2}		Hilal et al. (2008)	Q	
	3.1×10^{3}		Modarresi et al. (2007)	Q	68
	6.9×10^{3}		Yao et al. (2002)	Q	230
	8.6×10^{2}		Katritzky et al. (1998)	Q	
	1.6×10^{2}		Duchowicz et al. (2020)	?	186, 21
	5.2×10^{3}		Yaws (1999)	?	21

Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1,2-propanediol	2.7×10^3		Burkholder et al. (2019)	L	
$C_3H_8O_2$	2.7×10^3		Burkholder et al. (2015)	L	
(propylene glycol)	7.7×10^2		Duchowicz et al. (2020)	V	187
[57-55-6]	7.6×10^2		HSDB (2015)	V	
DNIAPMSPPWPWGF-UHFFFAOYSA-N	2.7×10^3	9500	Compernolle and Müller (2014b)	V	
	2.7×10^3		Yaws (2003)	X	259
	2.7×10^3		Yaws (2003)	X	238
	1.9×10^3		Dupeux et al. (2022)	Q	260
	3.5×10^2		Duchowicz et al. (2020)	Q	
	3.1×10^2		Wang et al. (2017)	Q	81, 239
	1.0×10^3		Wang et al. (2017)	Q	81, 240
	1.3×10^3		Wang et al. (2017)	Q	81, 241
	3.9×10^3		Gharagheizi et al. (2012)	Q	
	2.7×10^3		Gharagheizi et al. (2010)	Q	247
			Saxena and Hildemann (1996)	E	403, 430
1,3-propanediol	1.6×10^4		Burkholder et al. (2019)	L	
$C_3H_8O_2$	1.6×10^4		Burkholder et al. (2015)	L	
[504-63-2]	9.1×10^3		Bone et al. (1983)	M	12
YPFDHNVEDLHUCE-UHFFFAOYSA-N	1.6×10^4	9500	Compernolle and Müller (2014b)	V	
	7.4×10^2		Wang et al. (2017)	Q	81, 239
	6.3×10^3		Wang et al. (2017)	Q	81, 240
	4.8×10^3		Wang et al. (2017)	Q	81, 241
	3.1×10^3		Raventos-Duran et al. (2010)	Q	272, 244
	2.5×10^3		Raventos-Duran et al. (2010)	Q	245
	6.2×10^1		Raventos-Duran et al. (2010)	Q	246
	4.0×10^2		Hilal et al. (2008)	Q	
	2.0×10^3		Modarresi et al. (2007)	Q	68
1,2,3-propanetriol	4.7×10^6		Burkholder et al. (2019)	L	
$C_3H_8O_3$	4.7×10^6		Burkholder et al. (2015)	L	
(glycerol)	5.8×10^2		Butler and Ramchandani (1935)	M	426
[56-81-5]	4.7×10^6	11000	Compernolle and Müller (2014b)	V	
PEDCQBHIVMGVHV-UHFFFAOYSA-N	5.0×10^6		Hwang et al. (1992)	V	
	3.8×10^2		Keshavarz et al. (2022)	Q	
	1.7×10^5		Duchowicz et al. (2020)	Q	
			Saxena and Hildemann (1996)	E	403, 431
	5.7×10^2		Duchowicz et al. (2020)	?	186, 21
1,2-butanediol	2.1×10^3		Burkholder et al. (2019)	L	432
$C_4H_{10}O_2$	2.1×10^3		Burkholder et al. (2015)	L	433
[584-03-2]	$>3.4\times10^2$		Altschuh et al. (1999)	M	
BMRWNKZVCUKKSR-UHFFFAOYSA-N	1.7×10^3		Duchowicz et al. (2020)	V	187
	2.1×10^3	9900	Compernolle and Müller (2014b)	V	
	4.4×10^2		Duchowicz et al. (2020)	Q	
	2.9×10^2		Wang et al. (2017)	Q	81, 239
	7.6×10^2		Wang et al. (2017)	Q	81, 240

Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	4.8×10^{2}		Wang et al. (2017)	Q	81, 241
1,3-butanediol	7.0×10^{3}		Burkholder et al. (2019)	L	
$C_4H_{10}O_2$	7.0×10^{3}		Burkholder et al. (2015)	L	
[107-88-0]	4.1×10^{3}		Duchowicz et al. (2020)	V	187
PUPZLCDOIYMWBV-UHFFFAOYSA-N	7.0×10^{3}	10000	Compernolle and Müller (2014b)	V	
	9.5×10^{2}		Duchowicz et al. (2020)	Q	
	6.9×10^{2}		Wang et al. (2017)	Q	81, 239
	4.0×10^{3}		Wang et al. (2017)	Q	81, 240
	2.5×10^{3}		Wang et al. (2017)	Q	81, 241
	4.9×10^{4}		Saxena and Hildemann (1996)	E	403
1,4-butanediol	3.5×10^{4}		Burkholder et al. (2019)	L	
$C_4H_{10}O_2$	3.5×10^{4}		Burkholder et al. (2015)	L	
[110-63-4]	$>9.0\times10^{2}$		Altschuh et al. (1999)	M	
WERYXYBDKMZEQL-UHFFFAOYSA-N	7.6×10^{3}		Duchowicz et al. (2020)	V	187
	7.6×10^{3}		HSDB (2015)	V	
	3.5×10^{4}	11000	Compernolle and Müller (2014b)	V	
	2.4×10^{3}		Duchowicz et al. (2020)	Q	
	6.0×10^{2}		Wang et al. (2017)	Q	81, 239
	7.6×10^{3}		Wang et al. (2017)	Q	81, 240
	9.6×10^{3}		Wang et al. (2017)	Q	81, 241
	3.1×10^{4}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{3}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	246
	8.0×10^{3}		Hilal et al. (2008)	Q	
	1.6×10^{3}		Modarresi et al. (2007)	Q	68
			Saxena and Hildemann (1996)	E	403, 434
	1.9×10^{4}		Yaws (1999)	?	21, 12
2,3-butanediol	1.1×10^{3}		Burkholder et al. (2019)	L	
$C_4H_{10}O_2$	1.1×10^{3}		Burkholder et al. (2015)	L	
[513-85-9]	3.4×10^{2}		Duchowicz et al. (2020)	V	187
OWBTYPJTUOEWEK-UHFFFAOYSA-N	3.4×10^{2}		HSDB (2015)	V	
	1.1×10^{3}	9900	Compernolle and Müller (2014b)	V	
	9.7×10^{2}		Yaws (2003)	X	238, 12
	1.7×10^{2}		Duchowicz et al. (2020)	Q	
	3.3×10^{2}		Wang et al. (2017)	Q	81, 239
	1.2×10^{3}		Wang et al. (2017)	Q	81, 240
	4.1×10^{2}		Wang et al. (2017)	Q	81, 241
	1.7×10^{3}		Gharagheizi et al. (2012)	Q	
	7.8×10^{2}		Gharagheizi et al. (2010)	Q	247
			Saxena and Hildemann (1996)	E	403, 435

Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
meso-2,3-butanediol	2.2×10^{2}		Duchowicz et al. (2020)	V	187
$C_4H_{10}O_2$	6.8×10^{2}		Yaws (2003)	X	238, 12
[5341-95-7]	1.7×10^{2}		Duchowicz et al. (2020)	Q	
OWBTYPJTUOEWEK-ZXZARUISSA-N	1.6×10^{3}		Gharagheizi et al. (2012)	Q	
	7.8×10^{2}		Gharagheizi et al. (2010)	Q	247
2-methylpropane-1,2-diol	1.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_2$	5.1×10^{2}		Wang et al. (2017)	Q	81, 240
[558-43-0]	3.2×10^{2}		Wang et al. (2017)	Q	81, 241
BTVWZWFKMIUSGS-UHFFFAOYSA-N					
2-methylpropane-1,3-diol	6.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_2$	5.0×10^{3}		Wang et al. (2017)	Q	81, 240
[2163-42-0]	2.6×10^{3}		Wang et al. (2017)	Q	81, 241
QWGRWMMWNDWRQN-UHFFFAOYSA-N	4.3×10^{1}		HSDB (2015)	Q	100
1,2,3-butanetriol $C_4H_{10}O_3$ [4435-50-1] YAXKTBLXMTYWDQ-UHFFFAOYSA-N	3.0×10^{9}		Saxena and Hildemann (1996)	E	403
1,2,4-butanetriol	7.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	1.9×10^{6}		Wang et al. (2017)	Q	81, 240
[3068-00-6]	3.2×10^{5}		Wang et al. (2017)	Q	81, 241
ARXKVVRQIIOZGF-UHFFFAOYSA-N	3.0×10^{9}		Saxena and Hildemann (1996)	E	403
1,2,3,4-butanetetrol $C_4H_{10}O_4$ (1,2,3,4-tetrahydroxybutane; tetritol) [7541-59-5] UNXHWFMMPAWVPI-UHFFFAOYSA-N	2.0×10^{14}		Saxena and Hildemann (1996)	E	403
2(*R*),3(*S*)-1,2,3,4-butanetetrol	1.1×10^{10}		Burkholder et al. (2019)	L	
$C_4H_{10}O_4$	1.1×10^{10}		Burkholder et al. (2015)	L	
(erythritol)	2.5×10^{9}		Qin et al. (2021)	M	436
[149-32-6]	1.1×10^{10}	16000	Compernolle and Müller (2014b)	V	
UNXHWFMMPAWVPI-ZXZARUISSA-N	3.2×10^{4}		Qin et al. (2021)	Q	437
	4.1×10^{8}		Qin et al. (2021)	Q	438
	3.2×10^{4}		HSDB (2015)	Q	100
1,2-pentanediol	1.4×10^{3}		Compernolle and Müller (2014b)	V	
$C_5H_{12}O_2$	2.2×10^{2}		Wang et al. (2017)	Q	81, 239
[5343-92-0]	5.9×10^{2}		Wang et al. (2017)	Q	81, 240
WCVRQHFDJLLWFE-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	81, 241
1,3-pentanediol	5.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	3.1×10^{3}		Wang et al. (2017)	Q	81, 240
[3174-67-2]	1.5×10^{3}		Wang et al. (2017)	Q	81, 241
RUOPINZRYMFPBF-UHFFFAOYSA-N					

Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\ Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1,4-pentanediol	2.3×10^4		Compernolle and Müller (2014b)	V	
$C_5H_{12}O_2$	5.6×10^2		Wang et al. (2017)	Q	81, 239
[626-95-9]	3.9×10^3		Wang et al. (2017)	Q	81, 240
GLOBUAZSRIOKLN-UHFFFAOYSA-N	4.8×10^3		Wang et al. (2017)	Q	81, 241
1,5-pentanediol	7.0×10^4	12000	Compernolle and Müller (2014b)	V	
$C_5H_{12}O_2$	2.0×10^4		Raventos-Duran et al. (2010)	Q	243, 244
[111-29-5]	1.6×10^4		Raventos-Duran et al. (2010)	Q	245
ALQSHHUCVQOPAS-UHFFFAOYSA-N	3.1×10^1		Raventos-Duran et al. (2010)	Q	246
	7.7×10^3		Hilal et al. (2008)	Q	
	3.9×10^4		Saxena and Hildemann (1996)	E	403
2,3-pentanediol	2.6×10^2		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	1.2×10^3		Wang et al. (2017)	Q	81, 240
[42027-23-6]	1.7×10^2		Wang et al. (2017)	Q	81, 241
XLMFDCKSFJWJTP-UHFFFAOYSA-N	3.0×10^4		Saxena and Hildemann (1996)	E	403
2,4-pentanediol	3.8×10^3		Compernolle and Müller (2014b)	V	
$C_5H_{12}O_2$	6.5×10^2		Wang et al. (2017)	Q	81, 239
[625-69-4]	5.4×10^3		Wang et al. (2017)	Q	81, 240
GTCCGKPBSJZVRZ-UHFFFAOYSA-N	2.3×10^3		Wang et al. (2017)	Q	81, 241
	3.0×10^4		Saxena and Hildemann (1996)	E	403
3-methylbutane-1,2-diol	2.6×10^2		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	8.5×10^2		Wang et al. (2017)	Q	81, 240
[50468-22-9]	3.3×10^2		Wang et al. (2017)	Q	81, 241
HJJZIMFAIMUSBW-UHFFFAOYSA-N					
3-methylbutane-1,3-diol	4.0×10^2		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	2.6×10^3		Wang et al. (2017)	Q	81, 240
[2568-33-4]	2.1×10^3		Wang et al. (2017)	Q	81, 241
XPFCZYUVICHKDS-UHFFFAOYSA-N					
2-methylbutane-1,2-diol	1.6×10^2		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	4.3×10^2		Wang et al. (2017)	Q	81, 240
[41051-72-3]	1.1×10^2		Wang et al. (2017)	Q	81, 241
DOPZLYNWNJHAOS-UHFFFAOYSA-N					
2-methylbutane-1,3-diol	6.5×10^2		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	4.7×10^3		Wang et al. (2017)	Q	81, 240
[684-84-4]	2.0×10^3		Wang et al. (2017)	Q	81, 241
GNBPEYCZELNJMS-UHFFFAOYSA-N					
2-methylbutane-1,4-diol	5.6×10^2		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	6.0×10^3		Wang et al. (2017)	Q	81, 240
[2938-98-9]	6.2×10^3		Wang et al. (2017)	Q	81, 241
MWCBGWLCXSUTHK-UHFFFAOYSA-N					

Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
2-methylbutane-2,3-diol	1.8×10^2		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	7.3×10^2		Wang et al. (2017)	Q	81, 240
[5396-58-7]	2.0×10^2		Wang et al. (2017)	Q	81, 241
IDEOPBXRUBNYBN-UHFFFAOYSA-N					
2,2-dimethylpropane-1,3-diol	4.0×10^2		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	3.1×10^3		Wang et al. (2017)	Q	81, 240
[126-30-7]	6.8×10^2		Wang et al. (2017)	Q	81, 241
SLCVBVWXLSEKPL-UHFFFAOYSA-N					
2-(hydroxymethyl)-2-methyl-1,3-propanediol $C_5H_{12}O_3$ [77-85-0] QXJQHYBHAIHNGG-UHFFFAOYSA-N	9.0×10^2		HSDB (2015)	Q	100
2-methylbutane-1,2,4-triol	3.9×10^5		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	1.0×10^6		Wang et al. (2017)	Q	81, 240
[62875-07-4]	1.7×10^5		Wang et al. (2017)	Q	81, 241
XYHGSPUTABMVOC-UHFFFAOYSA-N					
MCM:C56OH	6.6×10^5		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	2.0×10^6		Wang et al. (2017)	Q	81, 240
RXEJCNRKXVSXDJ-UHFFFAOYSA-N	8.1×10^4		Wang et al. (2017)	Q	81, 241
MCM:HO124C5	6.6×10^5		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	1.3×10^6		Wang et al. (2017)	Q	81, 240
MOIOWCZVZKHQIC-UHFFFAOYSA-N	1.5×10^5		Wang et al. (2017)	Q	81, 241
MCM:HO134C5	6.6×10^5		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	3.2×10^6		Wang et al. (2017)	Q	81, 240
ANUUQAHHEZMTAS-UHFFFAOYSA-N	1.4×10^5		Wang et al. (2017)	Q	81, 241
MCM:MBOAOH	3.0×10^5		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	1.1×10^6		Wang et al. (2017)	Q	81, 240
QFZITDCVRJQLMZ-UHFFFAOYSA-N	5.4×10^3		Wang et al. (2017)	Q	81, 241
2-pentene-2,4,5-triol $C_5H_{10}O_3$ (ME1TRIOL) MTMASQITBHTGFW-UHFFFAOYSA-N	4.8×10^7	11000	Wieser et al. (2023)	Q	439
2-methyl-3-butene-1,2,3-triol	3.9×10^8		Qin et al. (2021)	M	436
$C_5H_{10}O_3$	1.5×10^2		Qin et al. (2021)	Q	437
YXPJRFSYSVRDQI-UHFFFAOYSA-N	3.1×10^2		Qin et al. (2021)	Q	438
(E)-2-methyl-1-butene-1,3,4-triol	6.2×10^8		Qin et al. (2021)	M	436
$C_5H_{10}O_3$	1.3×10^2		Qin et al. (2021)	Q	437
FVYHKVMWBMOFGS-DUXPYHPUSA-N	3.7×10^6		Qin et al. (2021)	Q	438

Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
(Z)-2-methyl-1-butene-1,3,4-triol	7.8×10^{8}		Qin et al. (2021)	M	436
$C_5H_{10}O_3$	1.3×10^{2}		Qin et al. (2021)	Q	437
FVYHKVMWBMOFGS-RQOWECAXSA-N	3.7×10^{6}		Qin et al. (2021)	Q	438
2-methylthreitol	2.0×10^{8}		Qin et al. (2021)	M	436
$C_5H_{12}O_4$	2.4×10^{4}		Qin et al. (2021)	Q	437
HGVJFBSSLICXEM-WHFBIAKZSA-N	3.3×10^{8}		Qin et al. (2021)	Q	438
2-methylerythritol	3.1×10^{8}		Qin et al. (2021)	M	436
$C_5H_{12}O_4$	2.4×10^{4}		Qin et al. (2021)	Q	437
[93921-83-6]	3.3×10^{8}		Qin et al. (2021)	Q	438
HGVJFBSSLICXEM-CRCLSJGQSA-N	6.2×10^{10}		Isaacman-VanWertz et al. (2016)	Q	440, 441
	3.1×10^{8}		Isaacman-VanWertz et al. (2016)	Q	442, 443
	3.1×10^{4}		Isaacman-VanWertz et al. (2016)	Q	444
2-Methylbutane-1,2,3,4-tetrol	6.1×10^{10}	14000	Wieser et al. (2023)	Q	439
$C_5H_{12}O_4$					
(MeBuTETROL)					
[42933-13-1]					
HGVJFBSSLICXEM-UHFFFAOYSA-N					
2,2-bis(hydroxymethyl)1,3-propanediol	7.3×10^{10}		Burkholder et al. (2019)	L	
$C_5H_{12}O_4$	7.3×10^{10}		Burkholder et al. (2015)	L	
(pentaerythritol)	7.3×10^{10}	16000	Compernolle and Müller (2014b)	V	
[115-77-5]	1.5×10^{9}		Yaws (2003)	X	238, 12
WXZMFSXDPGVJKK-UHFFFAOYSA-N	2.4×10^{4}		HSDB (2015)	Q	100
	1.2×10^{8}		Gharagheizi et al. (2012)	Q	
	2.4×10^{9}		Gharagheizi et al. (2010)	Q	247
1,2,3,4,5-pentanepentol	8.9×10^{18}		Saxena and Hildemann (1996)	E	403
$C_5H_{12}O_5$					
[7643-75-6]					
HEBKCHPVOIAQTA-UHFFFAOYSA-N					
(2R,3R,4S)-pentane-1,2,3,4,5-pentol	4.9×10^{8}		Qin et al. (2021)	M	436
$C_5H_{12}O_5$	3.9×10^{11}	17000	Compernolle and Müller (2014b)	V	
(xylitol)	6.6×10^{5}		Qin et al. (2021)	Q	437
[87-99-0]	7.3×10^{11}		Qin et al. (2021)	Q	438
HEBKCHPVOIAQTA-SCDXWVJYSA-N	6.6×10^{5}		HSDB (2015)	Q	100
(2R,3S,4S)-pentane-1,2,3,4,5-pentol	4.6×10^{11}	18000	Compernolle and Müller (2014b)	V	
$C_5H_{12}O_5$					
(adonitol; ribitol)					
[488-81-3]					
HEBKCHPVOIAQTA-ZXFHETKHSA-N					

Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
(2R,4R)-pentane-1,2,3,4,5-pentol	9.9×10^{9}		Qin et al. (2021)	M	436
$C_5H_{12}O_5$	6.7×10^{11}	18000	Compernolle and Müller (2014b)	V	
(arabitol; arabinitol)	6.6×10^{5}		Qin et al. (2021)	Q	437
[2152-56-9]	7.3×10^{11}		Qin et al. (2021)	Q	438
HEBKCHPVOIAQTA-QWWZWVQMSA-N					
levoglucosan	4.9×10^{10}		Qin et al. (2021)	M	436
$C_6H_{10}O_5$	6.9×10^{7}		Qin et al. (2021)	Q	437
[498-07-7]	4.3×10^{10}		Qin et al. (2021)	Q	438
TWNIBLMWSKIRAT-VFUOTHLCSA-N					
fructose	1.2×10^{9}		Qin et al. (2021)	M	436
$C_6H_{12}O_6$	1.0×10^{9}		Qin et al. (2021)	Q	437
[30237-26-4]	1.6×10^{14}		Qin et al. (2021)	Q	438
BJHIKXHVCXFQLS-UYFOZJQFSA-N					
mannose	1.2×10^{9}		Qin et al. (2021)	M	436
$C_6H_{12}O_6$	1.7×10^{5}		Qin et al. (2021)	Q	437
[3458-28-4]	1.4×10^{13}		Qin et al. (2021)	Q	438
GZCGUPFRVQAUEE-KVTDHHQDSA-N					
glucose	7.8×10^{8}		Qin et al. (2021)	M	436
$C_6H_{12}O_6$	1.0×10^{9}		Qin et al. (2021)	Q	437
[50-99-7]	1.8×10^{15}		Qin et al. (2021)	Q	438
GZCGUPFRVQAUEE-SLPGGIOYSA-N					
1,2-hexanediol	1.7×10^{3}		Compernolle and Müller (2014b)	V	
$C_6H_{14}O_2$	1.9×10^{2}		Wang et al. (2017)	Q	81, 239
[6920-22-5]	4.4×10^{2}		Wang et al. (2017)	Q	81, 240
FHKSXSQHXQEMOK-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	81, 241
1,4-hexanediol	4.5×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	3.3×10^{3}		Wang et al. (2017)	Q	81, 240
[16432-53-4]	1.6×10^{3}		Wang et al. (2017)	Q	81, 241
QVTWBMUAJHVAIJ-UHFFFAOYSA-N					
1,6-hexanediol	4.5×10^{4}		HSDB (2015)	Q	100
$C_6H_{14}O_2$	3.0×10^{4}		Saxena and Hildemann (1996)	E	403
[629-11-8]					
XXMIOPMDWAUFGU-UHFFFAOYSA-N					
2,3-hexanediol	2.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	8.7×10^{2}		Wang et al. (2017)	Q	81, 240
[617-30-1]	1.3×10^{2}		Wang et al. (2017)	Q	81, 241
QCIYAEYRVFUFAP-UHFFFAOYSA-N					

Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\ Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
2,5-hexanediol	1.4×10^{4}		Compernolle and Müller (2014b)	V	
$C_6H_{14}O_2$	5.1×10^{2}		Wang et al. (2017)	Q	81, 239
[2935-44-6]	5.9×10^{3}		Wang et al. (2017)	Q	81, 240
OHMBHFSEKCCCBW-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241
	2.0×10^{4}		Saxena and Hildemann (1996)	E	403
1,2-cyclohexanediol	6.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
[931-17-9]	1.3×10^{3}		Wang et al. (2017)	Q	81, 241
PFURGBBHAOXLIO-UHFFFAOYSA-N					
2-methyl-1,3-pentanediol	3.0×10^{4}		Saxena and Hildemann (1996)	E	403
$C_6H_{14}O_2$					
[149-31-5]					
SPXWGAHNKXLXAP-UHFFFAOYSA-N					
2-methyl-1,4-pentanediol	5.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	4.0×10^{3}		Wang et al. (2017)	Q	81, 240
[6287-17-8]	4.1×10^{3}		Wang et al. (2017)	Q	81, 241
PNJNLCNHYSWUPT-UHFFFAOYSA-N					
2-methyl-2,4-pentanediol	2.5×10^{1}		HSDB (2015)	Q	100
$C_6H_{14}O_2$	2.0×10^{4}		Saxena and Hildemann (1996)	E	403
[107-41-5]					
SVTBMSDMJJWYQN-UHFFFAOYSA-N					
3-methyl-1,3-pentanediol	3.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	2.3×10^{3}		Wang et al. (2017)	Q	81, 240
[33879-72-0]	8.9×10^{2}		Wang et al. (2017)	Q	81, 241
HIYKOZFIVZIBFO-UHFFFAOYSA-N					
3-methyl-1,4-pentanediol	5.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	5.8×10^{3}		Wang et al. (2017)	Q	81, 240
[26787-63-3]	2.6×10^{3}		Wang et al. (2017)	Q	81, 241
WOHXXIWTEHLCQK-UHFFFAOYSA-N					
4-methyl-1,4-pentanediol	3.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	2.9×10^{3}		Wang et al. (2017)	Q	81, 240
[1462-10-8]	2.5×10^{3}		Wang et al. (2017)	Q	81, 241
HAIVWDGLCRYQMC-UHFFFAOYSA-N					
2,3-dimethyl-2,3-butanediol	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	8.7×10^{2}		Wang et al. (2017)	Q	81, 240
[76-09-5]	6.9×10^{1}		Wang et al. (2017)	Q	81, 241
IVDFJHOHABJVEH-UHFFFAOYSA-N					
2,3-dimethyl-1,4-butanediol	5.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	8.1×10^{3}		Wang et al. (2017)	Q	81, 240
[57716-80-0]	2.8×10^{3}		Wang et al. (2017)	Q	81, 241
SKQUTIPQJKQFRA-UHFFFAOYSA-N					

Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\ Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
2,2-dimethyl-1,4-butanediol $C_6H_{14}O_2$ [32812-23-0] GQSZUUPRBBBHRI-UHFFFAOYSA-N	3.1×10^{2} 4.5×10^{3} 2.5×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
1,2,6-hexanetriol $C_6H_{14}O_3$ [106-69-4] ZWVMLYRJXORSEP-UHFFFAOYSA-N	2.0×10^{9}		Saxena and Hildemann (1996)	E	403
MCM:H134M3C5 $C_6H_{14}O_3$ XPUHQLFLUQJINS-UHFFFAOYSA-N	3.6×10^{5} 2.4×10^{6} 8.3×10^{4}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
1,2,3,4,5,6-hexahydroxy hexane $C_6H_{14}O_6$ [45007-61-2] FBPFZTCFMRRESA-UHFFFAOYSA-N	3.9×10^{23}		Saxena and Hildemann (1996)	E	403
(2S,3R,4R,5R)-hexane-1,2,3,4,5,6-hexol $C_6H_{14}O_6$ (sorbitol) [50-70-4] FBPFZTCFMRRESA-JGWLITMVSA-N	6.6×10^{14} 1.4×10^{7}	22000	Compernolle and Müller (2014b) HSDB (2015)	V Q	 100
(2R,3R,4R,5R)-hexane-1,2,3,4,5,6-hexol $C_6H_{14}O_6$ (mannitol) [69-65-8] FBPFZTCFMRRESA-KVTDHHQDSA-N	3.1×10^{9} 1.8×10^{15} 1.4×10^{7} 1.0×10^{15} 1.4×10^{7}	 22000	Qin et al. (2021) Compernolle and Müller (2014b) Qin et al. (2021) Qin et al. (2021) HSDB (2015)	M V Q Q Q	436 437 438 100
(2R,3S,4R,5S)-hexane-1,2,3,4,5,6-hexol $C_6H_{14}O_6$ (dulcitol; galactitol) [608-66-2] FBPFZTCFMRRESA-GUCUJZIJSA-N	9.0×10^{14}	22000	Compernolle and Müller (2014b)	V	
1,2,4,5-cyclohexanetetrol $C_6H_{12}O_4$ (1,2,4,5-tetrahydroxycyclohexane) [35652-37-0] RDIDGZFQASQXBU-UHFFFAOYSA-N	3.9×10^{14}		Saxena and Hildemann (1996)	E	403

Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1,2,3,4,5,6-hexahydroxycyclohexane $C_6H_{12}O_6$ [87-89-8] CDAISMWEOUEBRE-UHFFFAOYSA-N	9.9×10^{23}		Saxena and Hildemann (1996)	E	403
1,7-heptanediol $C_7H_{16}O_2$ [629-30-1] SXCBDZAEHILGLM-UHFFFAOYSA-N	2.0×10^{4}		Compernolle and Müller (2014b) Saxena and Hildemann (1996)	V E	445 403
2,4-heptanediol $C_7H_{16}O_2$ [20748-86-1] XVEOUOTUJBYHNL-UHFFFAOYSA-N	2.0×10^{4}		Saxena and Hildemann (1996)	E	403
2,5-heptanediol $C_7H_{16}O_2$ [70444-25-6] XTVHTJKQKUOEQA-UHFFFAOYSA-N	4.2×10^{2} 4.7×10^{3} 7.3×10^{2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
4-methyl-1,4-hexanediol $C_7H_{16}O_2$ [40646-08-0] ZRCYHJNCCBSTSZ-UHFFFAOYSA-N	2.5×10^{2} 2.6×10^{3} 1.2×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
2-methyl-2,5-hexanediol $C_7H_{16}O_2$ [29044-06-2] KZWQVDXGMOSSNY-UHFFFAOYSA-N	2.9×10^{2} 4.1×10^{3} 1.2×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
3-methyl-2,5-hexanediol $C_7H_{16}O_2$ PMORVUNYTOZCSE-UHFFFAOYSA-N	4.8×10^{2} 7.6×10^{3} 2.2×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
2,2-diethyl-1,3-propanediol $C_7H_{16}O_2$ [115-76-4] XRVCFZPJAHWYTB-UHFFFAOYSA-N	2.0×10^{4}		Saxena and Hildemann (1996)	E	403
1,2,3,4,5-pentahydroxyheptane $C_7H_{16}O_5$ HUYORHVLGRMTGF-UHFFFAOYSA-N	4.9×10^{18}		Saxena and Hildemann (1996)	E	403
1,2,3,4,6-pentahydroxyheptane $C_7H_{16}O_5$ HBKKLPCMKBGRJH-UHFFFAOYSA-N	3.9×10^{18}		Saxena and Hildemann (1996)	E	403
1,2,3,5,7-pentahydroxyheptane $C_7H_{16}O_5$ NSOOVWLSFZLKQX-UHFFFAOYSA-N	4.9×10^{18}		Saxena and Hildemann (1996)	E	403

Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1,2,3,4,5,6-hexahydroxyheptane $C_7H_{16}O_6$ (1-deoxy-heptitol) [688007-16-1] YMEXGEAJNZRQEH-VIFPVBQESA-N	3.0×10^{23}		Saxena and Hildemann (1996)	E	403
3,6-octanediol	3.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_{18}O_2$	4.1×10^{3}		Wang et al. (2017)	Q	81, 240
[24434-09-1]	2.1×10^{2}		Wang et al. (2017)	Q	81, 241
BCKOQWWRTRBSGR-UHFFFAOYSA-N					
1,4-cyclohexanedimethanol $C_8H_{16}O_2$ [105-08-8] YIMQCDZDWXUDCA-UHFFFAOYSA-N	1.5×10^{5}		HSDB (2015)	V	
2-ethyl-1,3-hexanediol	7.2×10^{2}		Duchowicz et al. (2020)	V	187
$C_8H_{18}O_2$	5.4×10^{2}		Duchowicz et al. (2020)	Q	
[94-96-2]	7.8×10^{2}		Raventos-Duran et al. (2010)	Q	243, 244
RWLALWYNXFYRGW-UHFFFAOYSA-N	7.8×10^{2}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	246
	1.1×10^{2}		Hilal et al. (2008)	Q	
	7.5×10^{2}		Modarresi et al. (2007)	Q	68
	2.0×10^{4}		Saxena and Hildemann (1996)	E	403
2,2,4-trimethyl-1,3-pentanediol	2.2×10^{2}		Duchowicz et al. (2020)	V	187
$C_8H_{18}O_2$	9.2×10^{1}		Duchowicz et al. (2020)	Q	
[144-19-4]	1.4×10^{1}		HSDB (2015)	Q	100
JCTXKRPTIMZBJT-UHFFFAOYSA-N					
2,5-dimethyl-2,5-hexanediol	1.4×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_8H_{18}O_2$	1.9×10^{3}		Zhang et al. (2010)	Q	288, 290
[110-03-2]	7.9×10^{2}		Zhang et al. (2010)	Q	288, 291
ZWNMRZQYWRLGMM-UHFFFAOYSA-N	4.7×10^{1}		Zhang et al. (2010)	Q	288, 292
1,9-nonanediol $C_9H_{20}O_2$ [3937-56-2] ALVZNPYWJMLXKV-UHFFFAOYSA-N			Compernolle and Müller (2014b)	V	446
3,6-nonanediol	3.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{20}O_2$	3.2×10^{3}		Wang et al. (2017)	Q	81, 240
[4469-85-6]	1.8×10^{2}		Wang et al. (2017)	Q	81, 241
YKEWIFGQPMVBEF-UHFFFAOYSA-N					
1,10-decanediol $C_{10}H_{22}O_2$ [112-47-0] FOTKYAAJKYLFFN-UHFFFAOYSA-N			Compernolle and Müller (2014b)	V	447

Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
3,6-decanediol	2.4×10^2		Wang et al. (2017)	Q	81, 239
$C_{10}H_{22}O_2$	2.6×10^3		Wang et al. (2017)	Q	81, 240
RBFBEPALGOYNGK-UHFFFAOYSA-N	2.8×10^2		Wang et al. (2017)	Q	81, 241
MCM:APINBOH	5.5×10^2		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_2$	3.2×10^3		Wang et al. (2017)	Q	81, 240
MOILFCKRQFQVFS-UHFFFAOYSA-N	6.5×10^3		Wang et al. (2017)	Q	81, 241
MCM:APINCOH	1.8×10^3		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_2$	2.0×10^5		Wang et al. (2017)	Q	81, 240
OMDMTHRBGUBUCO-UHFFFAOYSA-N	3.0×10^4		Wang et al. (2017)	Q	81, 241
MCM:BPINAOH	5.5×10^2		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_2$	7.4×10^2		Wang et al. (2017)	Q	81, 240
VXXAKGMRLUXFQH-UHFFFAOYSA-N	1.0×10^3		Wang et al. (2017)	Q	81, 241
MCM:BPINCOH	1.6×10^3		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_2$	3.5×10^5		Wang et al. (2017)	Q	81, 240
XYKGEKWHBMLSGS-UHFFFAOYSA-N	5.5×10^4		Wang et al. (2017)	Q	81, 241
MCM:HO36C11	2.2×10^2		Wang et al. (2017)	Q	81, 239
$C_{11}H_{24}O_2$	2.0×10^3		Wang et al. (2017)	Q	81, 240
VCLRIEYYOZNUNU-UHFFFAOYSA-N	2.2×10^2		Wang et al. (2017)	Q	81, 241
MCM:HO36C12	1.7×10^2		Wang et al. (2017)	Q	81, 239
$C_{12}H_{26}O_2$	1.6×10^3		Wang et al. (2017)	Q	81, 240
CLQOYXKLYNGAHW-UHFFFAOYSA-N	1.5×10^2		Wang et al. (2017)	Q	81, 241
2-butene-1,4-diol	$>3.4\times10^2$		Altschuh et al. (1999)	M	
$C_4H_8O_2$	2.5×10^3		Wang et al. (2017)	Q	81, 239
[110-64-5]	1.2×10^5		Wang et al. (2017)	Q	81, 240
ORTVZLZNOYNASJ-UHFFFAOYSA-N	3.4×10^4		Wang et al. (2017)	Q	81, 241
3-butene-1,2-diol	7.8×10^2		Wang et al. (2017)	Q	81, 239
$C_4H_8O_2$	8.5×10^2		Wang et al. (2017)	Q	81, 240
[497-06-3]	3.0×10^2		Wang et al. (2017)	Q	81, 241
ITMIAZBRRZANGB-UHFFFAOYSA-N					
2-butyne-1,4-diol	$>2.0\times10^3$		Altschuh et al. (1999)	M	
$C_4H_6O_2$	5.8×10^5		HSDB (2015)	V	
(1,4-dihydroxy-2-butyne)					
[110-65-6]					
DLDJFQGPPSQZKI-UHFFFAOYSA-N					
MCM:C524OH	1.3×10^6		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	6.5×10^4		Wang et al. (2017)	Q	81, 240
PGARYUHLQUORKU-UHFFFAOYSA-N	6.0×10^4		Wang et al. (2017)	Q	81, 241
MCM:ISOPAOH	1.6×10^3		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	7.4×10^4		Wang et al. (2017)	Q	81, 240
FLXLJBCLEUWWCG-UHFFFAOYSA-N	3.4×10^4		Wang et al. (2017)	Q	81, 241

Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:ISOPBOH	4.5×10^2		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	5.4×10^2		Wang et al. (2017)	Q	81, 240
XZRGYMKUQMPDQH-UHFFFAOYSA-N	7.1×10^1		Wang et al. (2017)	Q	81, 241
MCM:ISOPDOH	5.3×10^2		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	7.4×10^2		Wang et al. (2017)	Q	81, 240
HBHXLSPUXXXICF-UHFFFAOYSA-N	2.1×10^2		Wang et al. (2017)	Q	81, 241
MCM:C622OH	1.0×10^3		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	4.3×10^3		Wang et al. (2017)	Q	81, 240
VCGCHTQYUUAIGQ-UHFFFAOYSA-N	7.6×10^2		Wang et al. (2017)	Q	81, 241
MCM:C624OH	1.0×10^3		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	3.6×10^3		Wang et al. (2017)	Q	81, 240
BZQZWOYZOVQJLT-UHFFFAOYSA-N	8.7×10^2		Wang et al. (2017)	Q	81, 241
MCM:C720OH	4.5×10^3		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_2$	8.7×10^4		Wang et al. (2017)	Q	81, 240
JRLLENLHZCUEBJ-UHFFFAOYSA-N	7.6×10^4		Wang et al. (2017)	Q	81, 241
MCM:LIMAOH	5.1×10^2		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_2$	5.5×10^3		Wang et al. (2017)	Q	81, 240
WKZWTZTZWGWEGE-UHFFFAOYSA-N	1.9×10^3		Wang et al. (2017)	Q	81, 241
MCM:LIMCOH	6.9×10^2		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_2$	4.3×10^3		Wang et al. (2017)	Q	81, 240
ZJALAEQNHJQSTN-UHFFFAOYSA-N	1.2×10^3		Wang et al. (2017)	Q	81, 241
(*E*,*E*)-8,10-dodecadien-1-ol $C_{12}H_{22}O$ (codlemone) [33956-49-9] CSWBSLXBXRFNST-MQQKCMAXSA-N	1.7		Ebert et al. (2023)	?	317
MCM:BCAOH	5.4×10^2		Wang et al. (2017)	Q	81, 239
$C_{15}H_{26}O_2$	1.2×10^4		Wang et al. (2017)	Q	81, 240
XZTGVWRBZDBQLP-UHFFFAOYSA-N	1.1×10^4		Wang et al. (2017)	Q	81, 241
MCM:BCCOH	6.8×10^2		Wang et al. (2017)	Q	81, 239
$C_{15}H_{26}O_2$	1.8×10^4		Wang et al. (2017)	Q	81, 240
ALNVAIGKARRJOT-UHFFFAOYSA-N	5.9×10^3		Wang et al. (2017)	Q	81, 241
1,2-dihydroxybenzene	8.2×10^3		Duchowicz et al. (2020)	V	187
$C_6H_4(OH)_2$	8.2×10^3		HSDB (2015)	V	
(pyrocatechol)	1.8×10^3		Mackay et al. (2006c)	V	
[120-80-9]	1.6×10^2		Schüürmann (2000)	V	
YCIMNLLNPGFGHC-UHFFFAOYSA-N	4.5×10^1		Mackay et al. (1995)	V	
	2.6×10^3		Duchowicz et al. (2020)	Q	
	1.4×10^4		Wang et al. (2017)	Q	81, 239
	5.4×10^3		Wang et al. (2017)	Q	81, 240
	4.4×10^3		Wang et al. (2017)	Q	81, 241

Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	7.8×10^3		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^3		Raventos-Duran et al. (2010)	Q	245
	1.6×10^5		Raventos-Duran et al. (2010)	Q	246
	1.2×10^3		Hilal et al. (2008)	Q	
	7.9×10^2		Modarresi et al. (2007)	Q	68
		8300	Kühne et al. (2005)	Q	
		7400	Kühne et al. (2005)	?	
1,3-dihydroxybenzene	1.0×10^5		Duchowicz et al. (2020)	V	187
$C_6H_4(OH)_2$	1.0×10^5		HSDB (2015)	V	
(resorcinol)	8.5×10^4		Mackay et al. (2006c)	V	
[108-46-3]	5.0×10^3		Schüürmann (2000)	V	
GHMLBKRAJCXXBS-UHFFFAOYSA-N	6.4×10^4		Goldstein (1982)	X	448
	8.1×10^4	6300	Goldstein (1982)	X	299
	1.4×10^5		Duchowicz et al. (2020)	Q	
	2.4×10^4		Gharagheizi et al. (2012)	Q	
	5.3×10^4		Hilal et al. (2008)	Q	
1,4-dihydroxybenzene	2.1×10^5		Duchowicz et al. (2020)	V	187
$C_6H_4(OH)_2$	2.6×10^5		HSDB (2015)	V	
(hydroquinone)	2.5×10^5		Mackay et al. (2006c)	V	
[123-31-9]	3.2×10^4		Schüürmann (2000)	V	
QIGBRXMKCJKVMJ-UHFFFAOYSA-N	2.5×10^5		Mackay et al. (1995)	V	
	2.6×10^5		Meylan and Howard (1991)	V	
	7.6×10^3		Yaws (2003)	X	259
	2.3×10^5		Dupeux et al. (2022)	Q	260
	1.3×10^5		Duchowicz et al. (2020)	Q	
	3.1×10^4		Raventos-Duran et al. (2010)	Q	272, 244
	1.2×10^5		Raventos-Duran et al. (2010)	Q	245
	1.6×10^5		Raventos-Duran et al. (2010)	Q	246
	3.7×10^4		Hilal et al. (2008)	Q	
		8300	Kühne et al. (2005)	Q	
	1.7×10^5		Meylan and Howard (1991)	Q	
		7700	Kühne et al. (2005)	?	
1,2,3-benzenetriol	6.3×10^4		HSDB (2015)	V	
$C_6H_6O_3$	5.1×10^6		Gharagheizi et al. (2012)	Q	
(pyrogallic acid)					
[87-66-1]					
WQGWDDDVZFFDIG-UHFFFAOYSA-N					
1,2-dihydroxy-3-methylbenzene	8.1×10^3		Wang et al. (2017)	Q	81, 239
$C_7H_8O_2$	3.7×10^3		Wang et al. (2017)	Q	81, 240
[488-17-5]	7.4×10^2		Wang et al. (2017)	Q	81, 241
PGSWEKYNAOWQDF-UHFFFAOYSA-N					

Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:ECATECHOL	7.4×10^3		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_2$	2.3×10^3		Wang et al. (2017)	Q	81, 240
UUCQGNWZASKXNN-UHFFFAOYSA-N	3.8×10^2		Wang et al. (2017)	Q	81, 241
MCM:MXYCATECH	4.8×10^3		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_2$	2.9×10^3		Wang et al. (2017)	Q	81, 240
YGLVLWAMIJMBPF-UHFFFAOYSA-N	6.0×10^2		Wang et al. (2017)	Q	81, 241
MCM:OXYCATECH	4.8×10^3		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_2$	3.6×10^3		Wang et al. (2017)	Q	81, 240
RYHGQTREHREIBC-UHFFFAOYSA-N	3.1×10^2		Wang et al. (2017)	Q	81, 241
MCM:PXYCATECH	4.8×10^3		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_2$	3.9×10^3		Wang et al. (2017)	Q	81, 240
RGUZWBOJHNWZOK-UHFFFAOYSA-N	7.8×10^1		Wang et al. (2017)	Q	81, 241
MCM:IPCATECHOL	6.8×10^3		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	1.1×10^3		Wang et al. (2017)	Q	81, 240
XLZHGKDRKSKCAU-UHFFFAOYSA-N	2.9×10^2		Wang et al. (2017)	Q	81, 241
MCM:METCATECH	4.4×10^3		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	1.9×10^3		Wang et al. (2017)	Q	81, 240
IFERDVOUSBGAOD-UHFFFAOYSA-N	3.3×10^2		Wang et al. (2017)	Q	81, 241
MCM:OETCATECH	4.4×10^3		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	2.2×10^3		Wang et al. (2017)	Q	81, 240
QTXIMHKRKLVXRS-UHFFFAOYSA-N	3.4×10^2		Wang et al. (2017)	Q	81, 241
MCM:PCATECHOL	5.9×10^3		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	1.5×10^3		Wang et al. (2017)	Q	81, 240
GOZVFLWHGAXTPA-UHFFFAOYSA-N	3.6×10^2		Wang et al. (2017)	Q	81, 241
MCM:PETCATECH	4.4×10^3		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	2.5×10^3		Wang et al. (2017)	Q	81, 240
WVRWBYUJPWRFQO-UHFFFAOYSA-N	4.3×10^1		Wang et al. (2017)	Q	81, 241
MCM:T123CATECH	2.9×10^3		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	4.6×10^3		Wang et al. (2017)	Q	81, 240
DEIKGXRMQUHZJD-UHFFFAOYSA-N	5.1×10^2		Wang et al. (2017)	Q	81, 241
MCM:T124CATECH	2.9×10^3		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	4.9×10^3		Wang et al. (2017)	Q	81, 240
NZEZVJPYSAXNTR-UHFFFAOYSA-N	4.8×10^1		Wang et al. (2017)	Q	81, 241
2,3-dihydroxynaphthalene $C_{10}H_8O_2$ [92-44-4] JRNGUTKWMSBIBF-UHFFFAOYSA-N	2.0×10^5		Ebert et al. (2023)	?	317

Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
hexylresorcinol $C_{12}H_{18}O_2$ [136-77-6] WFJIVOKAWHGMBH-UHFFFAOYSA-N	3.8×10^{4}		HSDB (2015)	Q	100
2,6-bis(1,1-dimethylethyl)phenol $C_{14}H_{22}O$ [128-39-2] DKCPKDPYUFEZCP-UHFFFAOYSA-N	3.1		HSDB (2015)	Q	100
4-(1-methyl-1-phenylethyl)phenol $C_{15}H_{16}O$ [599-64-4] QBDSZLJBMIMQRS-UHFFFAOYSA-N	1.1×10^{2}		HSDB (2015)	Q	449
2,2',3,3'-tetrahydro-3,3,3',3'-tetramethyl-1,1'-spirobi(1H-indene)-6,6'-diol	1.5×10^{6}		Zhang et al. (2010)	Q	288, 289
$C_{21}H_{24}O_2$	1.0×10^{6}		Zhang et al. (2010)	Q	288, 290
[1568-80-5]	2.2×10^{6}		Zhang et al. (2010)	Q	288, 291
SICLLPHPVFCNTJ-UHFFFAOYSA-N	8.2×10^{5}		Zhang et al. (2010)	Q	288, 292
4,4'-(3,3,5-trimethylcyclohexane-1,1-diyl)diphenol	4.4×10^{5}		Zhang et al. (2010)	Q	288, 289
$C_{21}H_{26}O_2$	3.2×10^{5}		Zhang et al. (2010)	Q	288, 290
[129188-99-4]	2.7×10^{6}		Zhang et al. (2010)	Q	288, 291
UMPGNGRIGSEMTC-UHFFFAOYSA-N	7.9×10^{5}		Zhang et al. (2010)	Q	288, 292
3,3,3',3'-tetramethyl-1,1'-spirobi(indan)-5,5',6,6'-tetrol	1.4×10^{14}		Zhang et al. (2010)	Q	288, 289
$C_{21}H_{24}O_4$	1.6×10^{10}		Zhang et al. (2010)	Q	288, 290
[77-08-7]	2.0×10^{11}		Zhang et al. (2010)	Q	288, 291
POFMQEVZKZVAPQ-UHFFFAOYSA-N	2.7×10^{10}		Zhang et al. (2010)	Q	288, 292
9,9-bis(4-hydroxyphenyl)fluorene	8.4×10^{8}		Zhang et al. (2010)	Q	288, 289
$C_{25}H_{18}O_2$	6.2×10^{7}		Zhang et al. (2010)	Q	288, 290
[3236-71-3]	2.1×10^{8}		Zhang et al. (2010)	Q	288, 291
YWFPGFJLYRKYJZ-UHFFFAOYSA-N	3.1×10^{9}		Zhang et al. (2010)	Q	288, 292

A3.4 Peroxides (ROOH) and peroxy radicals (ROO)

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl hydroperoxide	3.0	5300	Burkholder et al. (2019)	L	
CH_3OOH	3.0	5300	Burkholder et al. (2015)	L	
(methyl peroxide)	3.0	5200	Brockbank (2013)	L	
[3031-73-0]	2.9	5200	Warneck and Williams (2012)	L	
MEUKEBNAABNAEX-UHFFFAOYSA-N	3.0	5300	Sander et al. (2011)	L	
	3.0	5300	Sander et al. (2006)	L	
	3.1	5300	Staudinger and Roberts (2001)	L	
	2.5	4400	Li et al. (2004)	M	
	>6.9		Magi et al. (1997)	M	450
	1.2×10^{1}		Sauer (1997)	M	451
	3.1	5200	O'Sullivan et al. (1996)	M	
	3.0	5300	Lind and Kok (1994)	M	53
	1.0×10^{1}		Wang et al. (2017)	Q	81, 239
	1.0×10^{1}		Wang et al. (2017)	Q	81, 240
	6.2		Wang et al. (2017)	Q	81, 241
	4.9		Raventos-Duran et al. (2010)	Q	272, 244
	1.2		Raventos-Duran et al. (2010)	Q	245
	1.6		Raventos-Duran et al. (2010)	Q	246
	9.0×10^{-1}		Hilal et al. (2008)	Q	
	1.3×10^{1}		Modarresi et al. (2007)	Q	68
		6200	Kühne et al. (2005)	Q	
		5200	Kühne et al. (2005)	?	
ethyl hydroperoxide	3.3	6000	Burkholder et al. (2019)	L	
C_2H_5OOH	3.3	6000	Burkholder et al. (2015)	L	
(ethyl peroxide)	3.3	6000	Brockbank (2013)	L	
[3031-74-1]	3.3	6000	Sander et al. (2011)	L	
ILHIHKRJJMKBEE-UHFFFAOYSA-N	1.1×10^{1}		Sauer (1997)	M	451
	3.3	6000	O'Sullivan et al. (1996)	M	
	5.0		Keshavarz et al. (2022)	Q	
	1.0×10^{1}		Duchowicz et al. (2020)	Q	185
	8.1		Wang et al. (2017)	Q	81, 239
	8.0		Wang et al. (2017)	Q	81, 240
	5.5		Wang et al. (2017)	Q	81, 241
	3.9		Raventos-Duran et al. (2010)	Q	272, 244
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	5.8×10^{-1}		Hilal et al. (2008)	Q	
		6600	Kühne et al. (2005)	Q	
	3.4		Duchowicz et al. (2020)	?	186, 21
		6000	Kühne et al. (2005)	?	

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hydroxymethyl hydroperoxide	1.7×10^{4}	9900	Burkholder et al. (2019)	L	
$HOCH_2OOH$	1.7×10^{4}	9900	Burkholder et al. (2015)	L	
(HMHP; HMP)	1.7×10^{4}	9900	Sander et al. (2011)	L	
[15932-89-5]	1.7×10^{4}	9900	Sander et al. (2006)	L	
NEZWFWIACBUQMN-UHFFFAOYSA-N	1.6×10^{4}	10000	Staudinger and Roberts (2001)	L	
	1.6×10^{4}	9700	O'Sullivan et al. (1996)	M	
	1.6×10^{4}	10000	Staffelbach and Kok (1993)	M	
	4.7×10^{3}	1500	Zhou and Lee (1992)	M	
	1.6×10^{4}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{4}		Raventos-Duran et al. (2010)	Q	246
		8600	Kühne et al. (2005)	Q	
		10000	Kühne et al. (2005)	?	
bis-(hydroxymethyl)-peroxide	$>9.9\times10^{4}$		Staffelbach and Kok (1993)	M	
$HOCH_2OOCH_2OH$	4.4×10^{3}	8400	Zhou and Lee (1992)	M	
(BHMP)		9400	Kühne et al. (2005)	Q	
[17088-73-2]		8500	Kühne et al. (2005)	?	
JLJXMZMKMRQOLN-UHFFFAOYSA-N					
tert-butyl hydroperoxide	4.2		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_2$	1.4		Wang et al. (2017)	Q	81, 240
[75-91-2]	3.6		Wang et al. (2017)	Q	81, 241
CIHOLLKRGTVIJN-UHFFFAOYSA-N	6.2×10^{-1}		HSDB (2015)	Q	100
di-*tert*-butylperoxide	8.2×10^{-4}		HSDB (2015)	Q	100
$C_8H_{18}O_2$	1.2×10^{-4}		Hilal et al. (2008)	Q	
[110-05-4]	1.6×10^{-2}		Modarresi et al. (2007)	Q	68
LSXWFXONGKSEMY-UHFFFAOYSA-N					
1-methyl-1- phenylethylhydroperoxide	2.1×10^{2}		Duchowicz et al. (2020)	V	187
$C_9H_{12}O_2$	2.1×10^{2}		HSDB (2015)	V	
[80-15-9]	2.3×10^{1}		Duchowicz et al. (2020)	Q	
YQHLDYVWEZKEOX-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	81, 239
	2.3×10^{1}		Wang et al. (2017)	Q	81, 240
	2.3×10^{1}		Wang et al. (2017)	Q	81, 241
	2.3		Hilal et al. (2008)	Q	
	7.3×10^{1}		Modarresi et al. (2007)	Q	68
dicumyl peroxide	2.2×10^{-1}		HSDB (2015)	Q	100
$C_{18}H_{22}O_2$					
[80-43-3]					
XMNIXWIUMCBBBL-UHFFFAOYSA-N					
methylperoxy radical	1.5×10^{-1}	3700	Leriche et al. (2000)	E	452
CH_3OO			Lelieveld and Crutzen (1991)	E	453
[2143-58-0]	5.9×10^{-2}	5600	Jacob (1986)	E	454
WTFNSXYULBQCQV-UHFFFAOYSA-N					

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hydroxymethylperoxy radical $HOCH_2OO$ [27828-51-9] OLHGCLQZCFQBGO-UHFFFAOYSA-N	7.9×10^{2}	8200	Leriche et al. (2000)	E	452
peroxyacetyl radical $CH_3C(O)O_2$ [36709-10-1] ZBQKPDHUDKSCRS-UHFFFAOYSA-N	$<9.9\times10^{-4}$ $<9.9\times10^{-4}$ $<9.9\times10^{-4}$ $<9.9\times10^{-4}$ $<9.9\times10^{-4}$		Burkholder et al. (2019) Burkholder et al. (2015) Sander et al. (2011) Sander et al. (2006) Villalta et al. (1996)	L L L L M	
MCM:ACO3H $C_3H_4O_3$ AZIQALWHRUQPHV-UHFFFAOYSA-N	2.7×10^{2} 1.4×10^{1} 2.0×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:IC3H7OOH $C_3H_8O_2$ SGJUFIMCHSLMRJ-UHFFFAOYSA-N	7.6 3.9 4.4		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:NC3H7OOH $C_3H_8O_2$ TURGQPDWYFJEDY-UHFFFAOYSA-N	6.8 4.7 3.0		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:PERPROACID $C_3H_6O_3$ CZPZWMPYEINMCF-UHFFFAOYSA-N	9.8×10^{1} 5.3 6.3×10^{-2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:C3DBCO3H $C_4H_6O_3$ TXNBRZBEFMJQMW-UHFFFAOYSA-N	3.2×10^{2} 1.0×10^{1} 5.4×10^{-2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:IC4H9OOH $C_4H_{10}O_2$ FUHWWEDRJKHMKK-UHFFFAOYSA-N	6.0 3.6 2.2		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:MACO3H $C_4H_6O_3$ OELQSSWXRGADDE-UHFFFAOYSA-N	1.8×10^{2} 8.7 1.6×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
IEPOX1CO3H $C_4H_6O_5$ DJPWYFXNRMHUNU-UHFFFAOYSA-N	9.0×10^{2}	14000	Wieser et al. (2023)	Q	439
MCM:NC4H9OOH $C_4H_{10}O_2$ AKUNSTOMHUXJOZ-UHFFFAOYSA-N	5.3 3.4 3.2		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:PERBUACID $C_4H_8O_3$ LBAYFEDWGHXMSM-UHFFFAOYSA-N	7.8×10^{1} 2.8 4.1×10^{-2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PERIBUACID	8.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	3.2		Wang et al. (2017)	Q	81, 240
LVQKOPBJHBWELS-UHFFFAOYSA-N	2.4×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:SC4H9OOH	6.0		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_2$	2.4		Wang et al. (2017)	Q	81, 240
SPQMVUPFYWDFCB-UHFFFAOYSA-N	2.4		Wang et al. (2017)	Q	81, 241
MCM:BUT2CO3H	7.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	2.0		Wang et al. (2017)	Q	81, 240
LWBFPIVRZGBOFS-UHFFFAOYSA-N	1.8×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C3ME3CO3H	7.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	2.3		Wang et al. (2017)	Q	81, 240
GTLLKMCVRPVGBK-UHFFFAOYSA-N	2.8×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:IPEAOOH	5.5		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	2.6		Wang et al. (2017)	Q	81, 240
HIHRAMNMOMKJDG-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	81, 241
MCM:IPEBOOH	5.6		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	2.1		Wang et al. (2017)	Q	81, 240
VIUWCQFVAFABHL-UHFFFAOYSA-N	2.1		Wang et al. (2017)	Q	81, 241
MCM:IPECOOH	3.4		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	9.8×10^{-1}		Wang et al. (2017)	Q	81, 240
XRXANEMIFVRKLN-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	81, 241
MCM:NEOPOOH	3.4		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	2.1		Wang et al. (2017)	Q	81, 240
UEQURRFROJBOLG-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	81, 241
MCM:PEAOOH	4.7		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	2.6		Wang et al. (2017)	Q	81, 240
KCHNMIKAMRQBHD-UHFFFAOYSA-N	2.3		Wang et al. (2017)	Q	81, 241
MCM:PEBOOH	5.5		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	1.8		Wang et al. (2017)	Q	81, 240
XRIRVAYMWUMXBR-UHFFFAOYSA-N	2.4		Wang et al. (2017)	Q	81, 241
MCM:PECOOH	5.5		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	1.7		Wang et al. (2017)	Q	81, 240
RLBQWRSRDVXRTJ-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	81, 241
MCM:PERPENACID	6.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	1.9		Wang et al. (2017)	Q	81, 240
UQGPCEVQKLOLLM-UHFFFAOYSA-N	2.8×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:TBUTCO3H	5.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	1.8		Wang et al. (2017)	Q	81, 240
YVAACGXAZGGQSM-UHFFFAOYSA-N	1.6×10^{-2}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
C520OOH $C_5H_{10}O_7$ GRPDYNZWDDUILX-UHFFFAOYSA-N	5.3×10^{11}	22000	Wieser et al. (2023)	Q	439
C518OOH $C_5H_8O_4$ PQEISBQMLHJHJQ-UHFFFAOYSA-N	4.1×10^{4}	14000	Wieser et al. (2023)	Q	439
MCM:C54CO3H $C_6H_{12}O_3$ JTSRVXQXWWOTER-UHFFFAOYSA-N	5.6×10^{1} 1.4 1.4×10^{-2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:C5H11CO3H $C_6H_{12}O_3$ NQUPKCJGWCPODR-UHFFFAOYSA-N	5.6×10^{1} 1.4 2.5×10^{-2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
ROO6R7OOH $C_6H_{12}O_4$ UPAWKBDHGPWUCG-UHFFFAOYSA-N	3.3×10^{7}	14000	Wieser et al. (2023)	Q	439
ROO6R6OOH $C_6H_{12}O_5$ QZPUZDFJKAEVLL-UHFFFAOYSA-N	2.6×10^{8}	14000	Wieser et al. (2023)	Q	439
C624OOH $C_6H_{12}O_6$ FUTSLQULSAKEJA-UHFFFAOYSA-N	1.2×10^{13}	20000	Wieser et al. (2023)	Q	439
MCM:CHEXOOH $C_6H_{12}O_2$ FGGJBCRKSVGDPO-UHFFFAOYSA-N	1.2×10^{1} 1.4×10^{1} 3.0×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:HEXAOOH $C_6H_{14}O_2$ RZICEOJUAFHYFO-UHFFFAOYSA-N	3.8 2.1 2.2		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:HEXBOOH $C_6H_{14}O_2$ XWXUHAUZCICPHE-UHFFFAOYSA-N	9.9×10^{-1} 4.4 1.4 1.8	7300	Wieser et al. (2023) Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q Q	439 81, 239 81, 240 81, 241
MCM:HEXCOOH $C_6H_{14}O_2$ NMNOLZYZNVYLRJ-UHFFFAOYSA-N	4.4 1.4 1.1		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:M22C3CO3H $C_6H_{12}O_3$ RQLGMECUXRQENU-UHFFFAOYSA-N	4.0×10^{1} 1.5 2.1×10^{-2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:M22C43OOH $C_6H_{14}O_2$ XDWQBMWWYOVNSC-UHFFFAOYSA-N	3.2 1.4 1.4		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:M22C4OOH	3.0		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	2.0		Wang et al. (2017)	Q	81, 240
VWOCCXGIWJLCIT-UHFFFAOYSA-N	3.6		Wang et al. (2017)	Q	81, 241
MCM:M23C43OOH	3.2		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	1.1		Wang et al. (2017)	Q	81, 240
UPTQBPSUWRBZRD-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	81, 241
MCM:M23C4OOH	5.1		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	2.6		Wang et al. (2017)	Q	81, 240
MCTQHWIBGOKRHO-UHFFFAOYSA-N	1.6		Wang et al. (2017)	Q	81, 241
MCM:M2C43CO3H	6.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.8		Wang et al. (2017)	Q	81, 240
KGAQRBNLHLEGET-UHFFFAOYSA-N	1.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:M2PEAOOH	4.4		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	2.1		Wang et al. (2017)	Q	81, 240
OTKKOLXSCMINFN-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	81, 241
MCM:M2PEBOOH	5.1		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	1.4		Wang et al. (2017)	Q	81, 240
XHHITPKXZQXJIC-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	81, 241
MCM:M2PECOOH	5.1		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	1.5		Wang et al. (2017)	Q	81, 240
JBJSMFBSVBRLAK-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	81, 241
MCM:M2PEDOOH	3.0		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	8.0×10^{-1}		Wang et al. (2017)	Q	81, 240
BZGMEGUFFDTCNP-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	81, 241
MCM:M33C3CO3H	4.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.2		Wang et al. (2017)	Q	81, 240
IHLWWYDUPGXTHJ-UHFFFAOYSA-N	8.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:M33C4OOH	3.0		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	1.7		Wang et al. (2017)	Q	81, 240
OUMLJDCULPJYHU-UHFFFAOYSA-N	1.8		Wang et al. (2017)	Q	81, 241
MCM:M3C4CO3H	5.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.7		Wang et al. (2017)	Q	81, 240
CHSVHHKRTQKZCN-UHFFFAOYSA-N	2.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:M3PEAOOH	4.4		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	2.5		Wang et al. (2017)	Q	81, 240
AOZFMIRWQXSLHO-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	81, 241
MCM:M3PEBOOH	5.1		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	1.9		Wang et al. (2017)	Q	81, 240
XCSSHHOKPSJZJS-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:M3PECOOH	3.0		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	7.8×10^{-1}		Wang et al. (2017)	Q	81, 240
BWMWVYKKWYNWMF-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
ROO6R5OOH	4.6×10^{7}	16000	Wieser et al. (2023)	Q	439
$C_7H_{12}O_6$					
RAASFOSVQCCDRJ-UHFFFAOYSA-N					
MCM:C6H13CO3H	4.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_3$	1.1		Wang et al. (2017)	Q	81, 240
GLAYRDYYNSCSPO-UHFFFAOYSA-N	2.2×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:HEPTOOH	3.6		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O_2$	1.1		Wang et al. (2017)	Q	81, 240
RCPMMXGHMBPBLI-UHFFFAOYSA-N	9.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:M2HEXAOOH	4.1		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O_2$	1.2		Wang et al. (2017)	Q	81, 240
MZRXBNCEXTUOSL-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	81, 241
MCM:M2HEXBOOH	2.5		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O_2$	6.6×10^{-1}		Wang et al. (2017)	Q	81, 240
VERXWMXNIBWXFV-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
MCM:M3HEXAOOH	4.1		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O_2$	1.4		Wang et al. (2017)	Q	81, 240
SLXXGGKZGKGOKQ-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	81, 241
MCM:M3HEXBOOH	2.5		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O_2$	6.8×10^{-1}		Wang et al. (2017)	Q	81, 240
YDBMAIVJCSJSKQ-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
1-methylhexyl hydroperoxide	7.7×10^{-1}	7600	Wieser et al. (2023)	Q	439
$C_7H_{16}O_2$					
(C7H15O2H)					
[762-46-9]					
FWELUXZVATZEMI-UHFFFAOYSA-N					
C7OHOOH	4.1×10^{3}	12000	Wieser et al. (2023)	Q	439
$C_7H_{16}O_3$					
KHWIBANUCNWWGW-UHFFFAOYSA-N					
MCM:C8BCOOH	2.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_2$	7.4		Wang et al. (2017)	Q	81, 240
TWXDGALDAWYAQL-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:OCTOOH	2.8		Wang et al. (2017)	Q	81, 239
$C_8H_{18}O_2$	9.8×10^{-1}		Wang et al. (2017)	Q	81, 240
PXUMFRDGKQLDGL-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methylheptl hydroperoxide $C_8H_{18}O_2$ (C8H17O2H) NAXZMRYIZGEALQ-UHFFFAOYSA-N	5.8×10^{-1}	8000	Wieser et al. (2023)	Q	439
C8OHOOH $C_8H_{18}O_3$ QQTSMKQYSKGCOU-UHFFFAOYSA-N	3.2×10^{3}	12000	Wieser et al. (2023)	Q	439
MCM:NONOOH $C_9H_{20}O_2$ BXPIMWLPPYUCSQ-UHFFFAOYSA-N	2.6 8.3×10^{-1} 9.6×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:DECOOH $C_{10}H_{22}O_2$ MPMVWDJTKHXCAN-UHFFFAOYSA-N	2.0 7.3×10^{-1} 1.2		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
C5H11O2H $C_{10}H_{22}O_4$ AXIHYONNAPPFSO-UHFFFAOYSA-N	1.4	7000	Wieser et al. (2023)	Q	439
LIMAB15OOH2 $C_{10}H_{20}O_6$ IRUZCTPAAZATQM-UHFFFAOYSA-N	2.3×10^{12}	20000	Wieser et al. (2023)	Q	439
RO5R1O2H $C_{10}H_{18}O_4$ NSOHXIGSWKLSHV-UHFFFAOYSA-N	9.9×10^{5}	17000	Wieser et al. (2023)	Q	439
RO5R2O2H $C_{10}H_{18}O_5$ MFXJOKCSTDMZRM-UHFFFAOYSA-N	1.8×10^{7}	19000	Wieser et al. (2023)	Q	439
ROO6R1OOH $C_{10}H_{18}O_5$ GBBPAXKBVMQHIG-UHFFFAOYSA-N	6.8×10^{4}	16000	Wieser et al. (2023)	Q	439
RO5R3O2H $C_{10}H_{18}O_6$ IEPFJXDIWPQIRC-UHFFFAOYSA-N	7.7×10^{7}	22000	Wieser et al. (2023)	Q	439
MCM:UDECOOH $C_{11}H_{24}O_2$ PPEGYVQDERYKNI-UHFFFAOYSA-N	1.6 6.5×10^{-1} 9.6×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:DDECOOH $C_{12}H_{26}O_2$ ONWAGJMEBPWHEG-UHFFFAOYSA-N	1.5 5.8×10^{-1} 8.3×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:C6H5OOH $C_6H_6O_2$ JYINMLPNDRBKKZ-UHFFFAOYSA-N	3.2×10^{2} 8.9×10^{1} 3.0×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C6H5CH2OOH	2.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_2$	9.1×10^{1}		Wang et al. (2017)	Q	81, 240
YVJRCWCFDJYONJ-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C6H5CO3H	3.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_6O_3$	6.2×10^{1}		Wang et al. (2017)	Q	81, 240
XCRBXWCUXJNEFX-UHFFFAOYSA-N	2.4		Wang et al. (2017)	Q	81, 241
MCM:MXYL1OOH	1.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_2$	7.8×10^{1}		Wang et al. (2017)	Q	81, 240
VCTGBWYTEXZDNM-UHFFFAOYSA-N	3.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:OXYL1OOH	1.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_2$	1.0×10^{2}		Wang et al. (2017)	Q	81, 240
OCSKWYCRTWOMLG-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PXYL1OOH	1.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_2$	9.1×10^{1}		Wang et al. (2017)	Q	81, 240
ZCUUEQJCOSBJOR-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C6H5C2CO3H	3.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_8O_3$	6.3×10^{1}		Wang et al. (2017)	Q	81, 240
BXGXGTXWGGOFSP-UHFFFAOYSA-N	2.7		Wang et al. (2017)	Q	81, 241
MCM:C6H5C2OOH	2.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_2$	6.9×10^{1}		Wang et al. (2017)	Q	81, 240
VZQOBPXGQJXYGY-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DM123OOH	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_2$	1.3×10^{2}		Wang et al. (2017)	Q	81, 240
FPXURWFXMHYDGM-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DM124OOH	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_2$	1.0×10^{2}		Wang et al. (2017)	Q	81, 240
UQJVEYMRRMOLPI-UHFFFAOYSA-N	3.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DMPHOOH	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_2$	6.5×10^{1}		Wang et al. (2017)	Q	81, 240
AGQLZSPEKWKXRP-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:EBENZOOH	1.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_2$	6.3×10^{1}		Wang et al. (2017)	Q	81, 240
SULLUHFYVRLICT-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MXY1OOH	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_2$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
LDNGPDBEDBLXJS-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MXYLCO3H	2.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_8O_3$	5.0×10^{1}		Wang et al. (2017)	Q	81, 240
INFFZTZRGNVBOC-UHFFFAOYSA-N	2.7×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MXYLOOH	1.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_2$	8.3×10^{1}		Wang et al. (2017)	Q	81, 240
UTKFWOZXPFIBPQ-UHFFFAOYSA-N	7.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:OXYLCO3H	2.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_8O_3$	6.2×10^{1}		Wang et al. (2017)	Q	81, 240
DNEXRQSSNZPAJJ-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:OXYLOOH	1.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_2$	9.3×10^{1}		Wang et al. (2017)	Q	81, 240
JTJQZHCBMBJJMV-UHFFFAOYSA-N	6.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PXY1OOH	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_2$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
QBGYVNGBYXOUAG-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PXYLCO3H	2.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_8O_3$	5.6×10^{1}		Wang et al. (2017)	Q	81, 240
IFDPVSBDNAQBRQ-UHFFFAOYSA-N	7.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:PXYLOOH	1.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_2$	9.8×10^{1}		Wang et al. (2017)	Q	81, 240
VCEHMDXCOGIOJJ-UHFFFAOYSA-N	8.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:EMPHOOH	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	4.0×10^{1}		Wang et al. (2017)	Q	81, 240
MKWUSWBHCPKVBI-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ETOLOOH	1.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	5.0×10^{1}		Wang et al. (2017)	Q	81, 240
DWPOLKIWKCGPAM-UHFFFAOYSA-N	4.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:IPBENZOOH	1.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	5.0×10^{1}		Wang et al. (2017)	Q	81, 240
CZNJIWCDRJWKLG-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MET1OOH	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	6.5×10^{1}		Wang et al. (2017)	Q	81, 240
HUAUUZDXRNWOSS-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:OET1OOH	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	7.4×10^{1}		Wang et al. (2017)	Q	81, 240
KVZSMDLRNLVTLK-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PBENZOOH	1.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	4.9×10^{1}		Wang et al. (2017)	Q	81, 240
BFUPNGCSYHWOOH-UHFFFAOYSA-N	1.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PET1OOH	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	6.6×10^{1}		Wang et al. (2017)	Q	81, 240
IKLGQZOVXYBNEV-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PHC3OOH	2.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	3.6×10^{1}		Wang et al. (2017)	Q	81, 240
JYLUDNGUBXOJPX-UHFFFAOYSA-N	5.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:TM123BCO3H	1.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_3$	7.3×10^{1}		Wang et al. (2017)	Q	81, 240
NQSDUJYDMWXHMR-UHFFFAOYSA-N	3.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:TM123BOOH	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	1.2×10^{2}		Wang et al. (2017)	Q	81, 240
HSKYDUVZGAHSEO-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:TM123OOH	6.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	1.6×10^{2}		Wang et al. (2017)	Q	81, 240
QIIZMGNSXSJCNA-UHFFFAOYSA-N	5.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:TM124BCO3H	1.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_3$	6.0×10^{1}		Wang et al. (2017)	Q	81, 240
HPLBJCPAWPQKDU-UHFFFAOYSA-N	4.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:TM124BOOH	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
ZUEBLWOBXMLPMV-UHFFFAOYSA-N	7.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:TM124OOH	6.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	1.3×10^{2}		Wang et al. (2017)	Q	81, 240
DSGKIBNJTLHQCN-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:TMBCO3H	1.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_3$	3.9×10^{1}		Wang et al. (2017)	Q	81, 240
APDYULOMODUXLL-UHFFFAOYSA-N	2.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:TMBOOH	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	6.9×10^{1}		Wang et al. (2017)	Q	81, 240
GOKTXPLVCSLYGI-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DM35EBOOH	9.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{14}O_2$	3.6×10^{1}		Wang et al. (2017)	Q	81, 240
NSJZLSFVHPJVDL-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:EMPHCO3H	1.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{12}O_3$	2.3×10^{1}		Wang et al. (2017)	Q	81, 240
GYXFVTDASBFNQD-UHFFFAOYSA-N	2.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:DE35TOOH	7.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{16}O_2$	2.4×10^{1}		Wang et al. (2017)	Q	81, 240
HPTJZRKCFIXEOP-UHFFFAOYSA-N	3.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HOCH2CO3H	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_2H_4O_4$	1.9×10^{2}		Wang et al. (2017)	Q	81, 240
IUEZWLCUORJBDZ-UHFFFAOYSA-N	8.5×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HYETHO2H	2.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_2H_6O_3$	2.9×10^{3}		Wang et al. (2017)	Q	81, 240
FKPAKAOEHCFKLE-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C2OHOCOOH	1.8×10^{7}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_5$	2.2×10^{5}		Wang et al. (2017)	Q	81, 240
GTTVGDRVLZEEEW-UHFFFAOYSA-N	3.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C3DIOLOOH	2.8×10^{7}		Wang et al. (2017)	Q	81, 239
$C_3H_8O_4$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
XSLBWJPPWWFTQY-UHFFFAOYSA-N	3.5×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:HO1C3OOH	2.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_3H_8O_3$	2.1×10^{3}		Wang et al. (2017)	Q	81, 240
LTKFKDLZMYUGKU-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HOC2H4CO3H	2.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_4$	8.9×10^{4}		Wang et al. (2017)	Q	81, 240
HPIZQAHZLDXVRM-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HYPROPO2H	2.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_3H_8O_3$	3.0×10^{3}		Wang et al. (2017)	Q	81, 240
CGHALRGHFXEMJB-UHFFFAOYSA-N	4.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:IPROPOLO2H	2.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_3H_8O_3$	2.1×10^{3}		Wang et al. (2017)	Q	81, 240
LGTUXDWECPSIQO-UHFFFAOYSA-N	4.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:IPROPOLPER	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_4$	1.5×10^{2}		Wang et al. (2017)	Q	81, 240
LLWVBKQQPPRNEX-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:BUT2OLOOH	2.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	1.5×10^{3}		Wang et al. (2017)	Q	81, 240
VRQPOZSYDWHVQK-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:BUTDAOOH	6.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	2.5×10^{5}		Wang et al. (2017)	Q	81, 240
ATNKTSDVMCPWQK-UHFFFAOYSA-N	1.6×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:BUTDBOOH	5.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	2.3×10^{3}		Wang et al. (2017)	Q	81, 240
VQGAWAMXUXLZCZ-UHFFFAOYSA-N	2.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:BUTDCOOH	5.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	1.9×10^{3}		Wang et al. (2017)	Q	81, 240
TVUDLONEIXNOQY-UHFFFAOYSA-N	3.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HC3CCO3H	3.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_4$	2.2×10^{2}		Wang et al. (2017)	Q	81, 240
ZSVMRAYUVFDTKB-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HC3CO3H	9.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_4$	1.9×10^{5}		Wang et al. (2017)	Q	81, 240
AVWVUWGQXKTDKD-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HMACO3H	4.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_4$	2.0×10^{4}		Wang et al. (2017)	Q	81, 240
IZGOVIKWSGSSGB-UHFFFAOYSA-N	9.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO13C3CO3H	3.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_5$	9.8×10^{5}		Wang et al. (2017)	Q	81, 240
SAVJJQFYFPVKTL-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HO13C4OOH	5.9×10^{7}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_4$	7.3×10^{6}		Wang et al. (2017)	Q	81, 240
WTIWPVYZJGYFOG-UHFFFAOYSA-N	1.2×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:HO1C4OOH	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	6.9×10^{4}		Wang et al. (2017)	Q	81, 240
RCPPCOTVBKCJGX-UHFFFAOYSA-N	3.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO2C3CO3H	2.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	1.0×10^{5}		Wang et al. (2017)	Q	81, 240
WSXMRWGMMYXEOT-UHFFFAOYSA-N	4.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO2C4OOH	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	9.1×10^{2}		Wang et al. (2017)	Q	81, 240
VJLLYXNZUMWUFH-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HO3C3CO3H	1.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	8.9×10^{1}		Wang et al. (2017)	Q	81, 240
BPXTXQLLUZFFNC-UHFFFAOYSA-N	1.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO3C4OOH	2.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
RMYCTZOJULYKEL-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HOC3H6CO3H	2.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	8.9×10^{4}		Wang et al. (2017)	Q	81, 240
CAGKPIQTEWLESW-UHFFFAOYSA-N	3.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HOIPRCO3H	2.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	9.8×10^{4}		Wang et al. (2017)	Q	81, 240
XMJMNOOOSJCSST-UHFFFAOYSA-N	6.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:IBUTOLBO2H	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
NCECNUIKMRTTTQ-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:IBUTOLCO2H	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	1.5×10^{3}		Wang et al. (2017)	Q	81, 240
IYIYQILWOLBTBM-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:IPRHOCO3H	8.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	3.2×10^{1}		Wang et al. (2017)	Q	81, 240
VAHIZEUROSIQMC-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	81, 241
MCM:NBUTOLAOOH	2.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	2.1×10^{3}		Wang et al. (2017)	Q	81, 240
KPUCJKMFRKKADT-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NBUTOLBOOH	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
UKXKMFPUVLQYHV-UHFFFAOYSA-N	2.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:TBUTOLOOH	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	8.0×10^{2}		Wang et al. (2017)	Q	81, 240
OLMJQPVPWWPTBW-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C3M3OHCO3H	1.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	7.6×10^{1}		Wang et al. (2017)	Q	81, 240
OPXDDGDNASPZKO-UHFFFAOYSA-N	8.1		Wang et al. (2017)	Q	81, 241
MCM:C42CO3H	3.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_5$	1.2×10^{6}		Wang et al. (2017)	Q	81, 240
ZMIMRJOKAFWNST-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C46CO3H	4.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	1.4×10^{5}		Wang et al. (2017)	Q	81, 240
VWNMYJVYTYSNQP-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C4OH2CO3H	9.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_5$	2.0×10^{5}		Wang et al. (2017)	Q	81, 240
WQUIEUVQOLAPHC-UHFFFAOYSA-N	9.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C4OHCO3H	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	5.5×10^{1}		Wang et al. (2017)	Q	81, 240
OQVSVCDIVLTQNI-UHFFFAOYSA-N	6.8		Wang et al. (2017)	Q	81, 241
MCM:C51OH2OOH	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	1.7×10^{3}		Wang et al. (2017)	Q	81, 240
YEVLRKKUVOPQLT-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C524OOH	1.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	1.2×10^{7}		Wang et al. (2017)	Q	81, 240
CMYVSBWTXHBCDK-UHFFFAOYSA-N	8.5×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C52OH1OOH	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	1.0×10^{3}		Wang et al. (2017)	Q	81, 240
UCQFCLCUMHUGLJ-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C52OH3OOH	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	1.7×10^{3}		Wang et al. (2017)	Q	81, 240
HJJMDLGJAJYCSL-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C52OOH	1.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	5.1×10^{4}		Wang et al. (2017)	Q	81, 240
ZPHQYWRKWRKGNS-UHFFFAOYSA-N	3.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C53OH2OOH	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	1.0×10^{3}		Wang et al. (2017)	Q	81, 240
AJVYEIIRONFKES-UHFFFAOYSA-N	8.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C54OOH	3.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_4$	5.9×10^{6}		Wang et al. (2017)	Q	81, 240
YUSGXJKDHCBGQE-UHFFFAOYSA-N	6.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C56OOH	5.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_4$	7.6×10^{6}		Wang et al. (2017)	Q	81, 240
ZJCLGCDNIIJGCW-UHFFFAOYSA-N	7.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:H13C43CO3H	1.9×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_5$	4.1×10^{5}		Wang et al. (2017)	Q	81, 240
AHAADFOLDXPWKJ-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:H2M2C3CO3H	1.4×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	5.9×10^{4}		Wang et al. (2017)	Q	81, 240
WNBRWGLXVYJADJ-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:H2M3C4OOH	1.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	8.5×10^{2}		Wang et al. (2017)	Q	81, 240
ZUPZYIDTDVLJQO-UHFFFAOYSA-N	6.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HC4ACO3H	6.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	2.0×10^{5}		Wang et al. (2017)	Q	81, 240
RKJIARBOZVRICG-UHFFFAOYSA-N	8.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HC4CCO3H	6.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	1.9×10^{5}		Wang et al. (2017)	Q	81, 240
BKBSBVFBLVOVGK-UHFFFAOYSA-N	7.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HM22C3OOH	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	9.8×10^{2}		Wang et al. (2017)	Q	81, 240
YTVLHPDOOITGNI-UHFFFAOYSA-N	2.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HM22CO3H	1.4×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	5.4×10^{4}		Wang et al. (2017)	Q	81, 240
JLDURWTXWMLEQQ-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HM2C43OOH	1.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
HSLVQIVCJSWUOZ-UHFFFAOYSA-N	8.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HM33C3OOH	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	7.3×10^{2}		Wang et al. (2017)	Q	81, 240
WHBWUNCJQHRHKD-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HO13C5OOH	5.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_4$	7.6×10^{6}		Wang et al. (2017)	Q	81, 240
MPQCFHWMMIVYQV-UHFFFAOYSA-N	1.3×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:HO1C5OOH	1.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	4.8×10^{4}		Wang et al. (2017)	Q	81, 240
NOIFGIIKGVCIDM-UHFFFAOYSA-N	2.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO24C4CO3H	3.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_5$	7.6×10^{5}		Wang et al. (2017)	Q	81, 240
BPXJXZFDALRNCD-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HO24C5OOH	5.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_4$	3.4×10^{6}		Wang et al. (2017)	Q	81, 240
LXCUFKDAZLTFBK-UHFFFAOYSA-N	7.6×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:HO2C43CO3H	2.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	7.3×10^{4}		Wang et al. (2017)	Q	81, 240
JJSNUFSNLCXQDD-UHFFFAOYSA-N	3.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO2C4CO3H	2.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	6.3×10^{4}		Wang et al. (2017)	Q	81, 240
WEYKGJBTAJHRDZ-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO2C54OOH	1.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	5.4×10^{2}		Wang et al. (2017)	Q	81, 240
NQEGDBNDYHCERX-UHFFFAOYSA-N	6.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO2C5OOH	7.1×10^{3}	11000	Wieser et al. (2023)	Q	439
$C_5H_{12}O_3$	1.5×10^{4}		Wang et al. (2017)	Q	81, 239
GSRFGQMXWRCOMF-UHFFFAOYSA-N	5.4×10^{4}		Wang et al. (2017)	Q	81, 240
	1.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO2M2C4OOH	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	5.4×10^{2}		Wang et al. (2017)	Q	81, 240
BPHNXEOBBWBBGO-UHFFFAOYSA-N	4.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO3C4CO3H	2.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	5.6×10^{4}		Wang et al. (2017)	Q	81, 240
OFXAQZFPCOWEPU-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO3C5OOH	1.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	6.9×10^{2}		Wang et al. (2017)	Q	81, 240
AMTQAQGRUCFWLQ-UHFFFAOYSA-N	5.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HOBUT2CO3H	2.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	5.8×10^{4}		Wang et al. (2017)	Q	81, 240
HHXRGEGWJUDFIW-UHFFFAOYSA-N	1.9×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HOIBUTCO3H	2.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	5.6×10^{4}		Wang et al. (2017)	Q	81, 240
JVGUWDNKCJEDLO-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:ISOPAOOH	4.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	1.7×10^{5}		Wang et al. (2017)	Q	81, 240
PEJOQVDRQFVMLE-UHFFFAOYSA-N	8.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:ISOPBOOH	1.2×10^{3}	9900	Rivera-Rios (2018)	M	
$C_5H_{10}O_3$	9.9×10^{2}		Rivera-Rios (2018)	Q	455
QTGGFXPTAQEODO-UHFFFAOYSA-N	1.3×10^{4}		Rivera-Rios (2018)	Q	456
	3.3×10^{4}		Wang et al. (2017)	Q	81, 239
	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
	4.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:ISOPCOOH	4.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	2.0×10^{5}		Wang et al. (2017)	Q	81, 240
FCLDANRCFPUKED-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:ISOPDOOH	1.2×10^{2}	7500	Rivera-Rios (2018)	M	
$C_5H_{10}O_3$	2.6×10^{4}		Rivera-Rios (2018)	Q	455
HYHMYONEYJINON-UHFFFAOYSA-N	1.3×10^{4}		Rivera-Rios (2018)	Q	456
	4.0×10^{4}		Wang et al. (2017)	Q	81, 239
	1.8×10^{3}		Wang et al. (2017)	Q	81, 240
	8.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:M2BU2OLOOH	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	1.1×10^{3}		Wang et al. (2017)	Q	81, 240
YWZMEYHQKKHRJF-UHFFFAOYSA-N	2.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:M2BUOL2OOH	1.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	1.1×10^{3}		Wang et al. (2017)	Q	81, 240
KLOVYRXVQOACLZ-UHFFFAOYSA-N	6.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:M3BU2OLOOH	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	1.1×10^{3}		Wang et al. (2017)	Q	81, 240
AFEDOYRLNKBWPZ-UHFFFAOYSA-N	8.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MBOAOOH	4.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_4$	4.5×10^{6}		Wang et al. (2017)	Q	81, 240
VJEOLZUQMDEVMO-UHFFFAOYSA-N	6.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:MBOBOOH	1.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_4$	6.3×10^{5}		Wang et al. (2017)	Q	81, 240
GXJWPCHTRDIVHR-UHFFFAOYSA-N	5.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:ME2BUOLOOH	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	6.9×10^{2}		Wang et al. (2017)	Q	81, 240
SAXHQAUHEBEDAO-UHFFFAOYSA-N	9.3×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:ME3BUOLOOH	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	2.3×10^{3}		Wang et al. (2017)	Q	81, 240
MUYQYONVNPPJGI-UHFFFAOYSA-N	9.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PROL11MOOH	1.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	5.6×10^{2}		Wang et al. (2017)	Q	81, 240
UVDGWSPEOVCOFS-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:PROL1MCO3H	6.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	2.1×10^{1}		Wang et al. (2017)	Q	81, 240
KTQROZYFUGXCGA-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	81, 241
MCM:BZBIPER2OH	3.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	1.9×10^{6}		Wang et al. (2017)	Q	81, 240
BVNIDXNYDXJAFS-UHFFFAOYSA-N	8.5×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:BZBIPEROOH	7.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	9.3×10^{6}		Wang et al. (2017)	Q	81, 240
MXPMOVDECINDPN-UHFFFAOYSA-N	2.3×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C4ME2OHOOH	7.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	3.8×10^{2}		Wang et al. (2017)	Q	81, 240
HOGFDWYRBLIMGM-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C518CO3H	4.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	5.6×10^{4}		Wang et al. (2017)	Q	81, 240
HLKDNTMYLJJNIF-UHFFFAOYSA-N	5.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C622OOH	1.3×10^{4}	12000	Wieser et al. (2023)	Q	439
$C_6H_{12}O_3$	2.9×10^{4}		Wang et al. (2017)	Q	81, 239
GWTGWFHICNOSTQ-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
	1.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C624OOH	2.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
DDEGWHJCSBWJSM-UHFFFAOYSA-N	8.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C64OH5OOH	1.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	7.8×10^{2}		Wang et al. (2017)	Q	81, 240
ZEOCDIHFKNFYIT-UHFFFAOYSA-N	6.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C65OH4OOH	1.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
PVVIDEIOKNUTFV-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C6OH5OOH	1.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
HRDCBAWVKIWIOZ-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CYHXOLAOOH	5.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	8.5×10^{4}		Wang et al. (2017)	Q	81, 240
UBIBQRDHLFTCKX-UHFFFAOYSA-N	6.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:H13M3C5OOH	3.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_4$	7.3×10^{6}		Wang et al. (2017)	Q	81, 240
KEIPMCKLLYLETP-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:H1MC5OOH	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	5.5×10^{4}		Wang et al. (2017)	Q	81, 240
NRUVZELSEXXOEO-UHFFFAOYSA-N	2.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:H2M2C4CO3H	1.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	4.6×10^{4}		Wang et al. (2017)	Q	81, 240
NRXKHRBCIJLLIW-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:H2M3C4CO3H	2.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	5.0×10^{4}		Wang et al. (2017)	Q	81, 240
BSSSRXSGDLZQTD-UHFFFAOYSA-N	6.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:H2MC5OOH	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	4.9×10^{4}		Wang et al. (2017)	Q	81, 240
VFABJBQUVDJTMS-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:H3M2C4CO3H	2.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	4.6×10^{4}		Wang et al. (2017)	Q	81, 240
BXUACBWFNFVFRM-UHFFFAOYSA-N	8.0		Wang et al. (2017)	Q	81, 241
MCM:H3M3C4CO3H	1.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	4.1×10^{4}		Wang et al. (2017)	Q	81, 240
QREFYDOYYWEEBY-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	81, 241
MCM:H3M3C5OOH	8.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	4.6×10^{2}		Wang et al. (2017)	Q	81, 240
SFWIETIRFCEPBV-UHFFFAOYSA-N	2.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HM22C3CO3H	1.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	3.5×10^{4}		Wang et al. (2017)	Q	81, 240
CFTUKLJUHGJIMT-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HM22C4OOH	8.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	3.2×10^{4}		Wang et al. (2017)	Q	81, 240
RBKQZGUZSABUAQ-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HM23C4OOH	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	6.9×10^{4}		Wang et al. (2017)	Q	81, 240
OEDZXCCMDSIVQE-UHFFFAOYSA-N	1.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HM2C43CO3H	2.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	5.5×10^{4}		Wang et al. (2017)	Q	81, 240
AAGQWOGOWVBCOC-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HM33C3CO3H	1.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	3.8×10^{4}		Wang et al. (2017)	Q	81, 240
CJLFHOYFCBYSAF-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HM33C4OOH	8.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	4.5×10^{4}		Wang et al. (2017)	Q	81, 240
IRDKGYBPQHNNSI-UHFFFAOYSA-N	6.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO1C6OOH	1.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	3.7×10^{4}		Wang et al. (2017)	Q	81, 240
AODLLEVTDATZKZ-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO1MC5OOH	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	2.5×10^{4}		Wang et al. (2017)	Q	81, 240
XFJAYUAZOYAZNW-UHFFFAOYSA-N	2.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO2C54CO3H	2.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	4.3×10^{4}		Wang et al. (2017)	Q	81, 240
HFXNQHIGYFOTHL-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO2C6OOH	5.4×10^{3}	11000	Wieser et al. (2023)	Q	439
$C_6H_{14}O_3$	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
BVOYWPYSMMRYPX-UHFFFAOYSA-N	2.4×10^{4}		Wang et al. (2017)	Q	81, 240
	1.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO2M2C5OOH	8.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	4.1×10^{4}		Wang et al. (2017)	Q	81, 240
XDJWSJNLVSIJHD-UHFFFAOYSA-N	5.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO2MC5OOH	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	4.8×10^{4}		Wang et al. (2017)	Q	81, 240
AGNBGPUCVJMPGZ-UHFFFAOYSA-N	4.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO3C5CO3H	1.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	4.5×10^{4}		Wang et al. (2017)	Q	81, 240
NIDIDJCFEJYKBD-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO3C6OOH	1.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	4.0×10^{4}		Wang et al. (2017)	Q	81, 240
WSWZWPBQPMRENX-UHFFFAOYSA-N	8.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO4C5CO3H	1.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	4.2×10^{4}		Wang et al. (2017)	Q	81, 240
YRMQNGAQYQCFSB-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO5C5CO3H	8.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	4.0×10^{1}		Wang et al. (2017)	Q	81, 240
ZOLITBGWKBFVQG-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HO5C6OOH	1.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	7.6×10^{2}		Wang et al. (2017)	Q	81, 240
VKWHJFIJUJODAG-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:PHENOH	5.5×10^{10}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	4.5×10^{8}		Wang et al. (2017)	Q	81, 240
JRROYJLQPIXCRD-UHFFFAOYSA-N	1.2×10^{8}		Wang et al. (2017)	Q	81, 241
MCM:PHENOOH	1.4×10^{12}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_6$	2.0×10^{8}		Wang et al. (2017)	Q	81, 240
WQYYYMQUZFKHHO-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C622CO3H	3.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	3.5×10^{4}		Wang et al. (2017)	Q	81, 240
JSEAPEOJJJOJEL-UHFFFAOYSA-N	9.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C624CO3H	3.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	3.9×10^{4}		Wang et al. (2017)	Q	81, 240
VELNAHZLHYPPOS-UHFFFAOYSA-N	2.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C720OOH	1.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_3$	2.9×10^{5}		Wang et al. (2017)	Q	81, 240
LPMHECUYQWFTDP-UHFFFAOYSA-N	2.4×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:CRESOH	3.0×10^{10}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	1.7×10^{8}		Wang et al. (2017)	Q	81, 240
UMHUAUCNJCQCRC-UHFFFAOYSA-N	1.6×10^{9}		Wang et al. (2017)	Q	81, 241
MCM:CRESOOH	7.8×10^{11}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_6$	7.6×10^{7}		Wang et al. (2017)	Q	81, 240
POYQJFWARUGMBT-UHFFFAOYSA-N	2.5×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:H2M2C65OOH	7.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O_3$	2.9×10^{4}		Wang et al. (2017)	Q	81, 240
MDRLNEUVCFZYIZ-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:H2M4C65OOH	1.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O_3$	3.9×10^{4}		Wang et al. (2017)	Q	81, 240
HGFYTCXFDJYCQF-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:H2M5C65OOH	7.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O_3$	1.0×10^{4}		Wang et al. (2017)	Q	81, 240
NIKXNAUPHRWTEG-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:H3M3C5CO3H	9.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_4$	3.8×10^{4}		Wang et al. (2017)	Q	81, 240
DTTYYTHTMWEWDN-UHFFFAOYSA-N	4.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:H3M3C6OOH	6.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O_3$	3.3×10^{4}		Wang et al. (2017)	Q	81, 240
IWLJNMJTDMGLQI-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HO3C76OOH	1.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O_3$	2.0×10^{4}		Wang et al. (2017)	Q	81, 240
YDKPOQVDDHNRNK-UHFFFAOYSA-N	9.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO5C6CO3H	1.4×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_4$	3.3×10^{4}		Wang et al. (2017)	Q	81, 240
KSOZMYOJLUVTBJ-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO6C7OOH	1.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O_3$	5.9×10^{2}		Wang et al. (2017)	Q	81, 240
YGTQIECBHSKCOV-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:TLBIPER2OH	1.7×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	9.6×10^{5}		Wang et al. (2017)	Q	81, 240
CXEVRKZODGVABW-UHFFFAOYSA-N	2.6×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:TLBIPEROOH	3.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	3.8×10^{6}		Wang et al. (2017)	Q	81, 240
JAKOWCUSWIMTAF-UHFFFAOYSA-N	9.8×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:EBENZOLOH	2.5×10^{10}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	1.0×10^{8}		Wang et al. (2017)	Q	81, 240
BUWSXDLGJSAPEF-UHFFFAOYSA-N	6.0×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:EBENZOLOOH	6.3×10^{11}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_6$	4.8×10^{7}		Wang et al. (2017)	Q	81, 240
RHHRSXIXEXUGSZ-UHFFFAOYSA-N	3.9×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:EBZBPER2OH	1.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	6.3×10^{5}		Wang et al. (2017)	Q	81, 240
AUMASFBINMOOAH-UHFFFAOYSA-N	3.8×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:EBZBPEROOH	3.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	2.5×10^{6}		Wang et al. (2017)	Q	81, 240
SCDRKAWXSVOIOT-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:HO3C86OOH	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{18}O_3$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
SPJZDLLIJATZHB-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO6C7CO3H	1.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_{16}O_4$	2.9×10^{4}		Wang et al. (2017)	Q	81, 240
UKHVIUJOBBSNIJ-UHFFFAOYSA-N	9.1		Wang et al. (2017)	Q	81, 241
MCM:HO7C8OOH	1.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{18}O_3$	4.7×10^{2}		Wang et al. (2017)	Q	81, 240
NDXYTTLTSMWWGD-UHFFFAOYSA-N	7.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MXYBPER2OH	9.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	4.0×10^{5}		Wang et al. (2017)	Q	81, 240
HJWPGRMMUKJUOW-UHFFFAOYSA-N	1.5×10^{6}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MXYBPEROOH	2.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	1.5×10^{6}		Wang et al. (2017)	Q	81, 240
JLBHNTWNBASURB-UHFFFAOYSA-N	1.2×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:MXYOLOH	1.7×10^{10}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	7.4×10^{7}		Wang et al. (2017)	Q	81, 240
HYWULKMMJLAVGS-UHFFFAOYSA-N	1.5×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:MXYOLOOH	4.4×10^{11}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_6$	3.2×10^{7}		Wang et al. (2017)	Q	81, 240
GRFXDNYNQVBVKX-UHFFFAOYSA-N	3.2×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:OXYBPER2OH	9.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	5.0×10^{5}		Wang et al. (2017)	Q	81, 240
VCLGCGXZSIRZEA-UHFFFAOYSA-N	4.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:OXYBPEROOH	2.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	1.5×10^{6}		Wang et al. (2017)	Q	81, 240
AMPOFIFBYJNSOH-UHFFFAOYSA-N	2.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:OXYOLOH	2.0×10^{10}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	1.2×10^{8}		Wang et al. (2017)	Q	81, 240
CAIZPBLFMULAII-UHFFFAOYSA-N	4.0×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:OXYOLOOH	5.3×10^{11}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_6$	5.5×10^{7}		Wang et al. (2017)	Q	81, 240
QYYRJAPHRBSJOE-UHFFFAOYSA-N	8.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PXYBPER2OH	9.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	5.0×10^{5}		Wang et al. (2017)	Q	81, 240
IOEDFCIBQPWSMP-UHFFFAOYSA-N	4.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:PXYBPEROOH	2.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	1.6×10^{6}		Wang et al. (2017)	Q	81, 240
LZVOCZWDZPUJRQ-UHFFFAOYSA-N	5.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PXYOLOH	2.0×10^{10}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	1.6×10^{8}		Wang et al. (2017)	Q	81, 240
YSBIHFSZRPVTOU-UHFFFAOYSA-N	9.6×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:PXYOLOOH	5.3×10^{11}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_6$	6.8×10^{7}		Wang et al. (2017)	Q	81, 240
ROOFTVJQSDLVOJ-UHFFFAOYSA-N	4.4×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:HO3C96OOH	8.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{20}O_3$	1.9×10^{4}		Wang et al. (2017)	Q	81, 240
GGTTUTGCXALAOI-UHFFFAOYSA-N	8.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO7C8CO3H	1.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{18}O_4$	2.6×10^{4}		Wang et al. (2017)	Q	81, 240
LZPDGAGYXQEGIA-UHFFFAOYSA-N	9.6		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HO8C9OOH	8.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{20}O_3$	3.8×10^{2}		Wang et al. (2017)	Q	81, 240
DDKPTZKAQLYQQK-UHFFFAOYSA-N	6.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:IPBENZOLOH	2.6×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	1.0×10^{8}		Wang et al. (2017)	Q	81, 240
MXOPSFWTSRHQGT-UHFFFAOYSA-N	1.5×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:IPBZBPR2OH	1.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	6.8×10^{5}		Wang et al. (2017)	Q	81, 240
ZYFWWFFTFWUTQU-UHFFFAOYSA-N	8.9×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:IPBZBPROOH	2.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	2.6×10^{6}		Wang et al. (2017)	Q	81, 240
PFZQQVVUSVRBJH-UHFFFAOYSA-N	2.5×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:IPBZOLOOH	5.9×10^{11}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_6$	4.9×10^{7}		Wang et al. (2017)	Q	81, 240
CHCZSTHNGRHXBM-UHFFFAOYSA-N	3.6×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:METLBPR2OH	7.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	2.8×10^{5}		Wang et al. (2017)	Q	81, 240
WBMKIPDFTCRXQQ-UHFFFAOYSA-N	5.3×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:METLBPROOH	1.7×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	1.0×10^{6}		Wang et al. (2017)	Q	81, 240
JDOROKVPYHJTEM-UHFFFAOYSA-N	4.9×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:METOLOH	1.3×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	5.0×10^{7}		Wang et al. (2017)	Q	81, 240
JGSZPUTWQXTPGZ-UHFFFAOYSA-N	5.1×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:METOLOOH	3.5×10^{11}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_6$	2.3×10^{7}		Wang et al. (2017)	Q	81, 240
WHWNZVSDBMWGPT-UHFFFAOYSA-N	2.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:OETLBPR2OH	7.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	3.6×10^{5}		Wang et al. (2017)	Q	81, 240
HUTNYAIOWRBWAA-UHFFFAOYSA-N	7.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:OETLBPROOH	1.7×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
JWHYGBDQJAPXFD-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:OETOLOH	1.7×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	7.6×10^{7}		Wang et al. (2017)	Q	81, 240
RKSMHAQFVDQZCV-UHFFFAOYSA-N	5.1×10^{8}		Wang et al. (2017)	Q	81, 241
MCM:OETOLOOH	4.4×10^{11}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_6$	3.1×10^{7}		Wang et al. (2017)	Q	81, 240
HMIPOFAAVJMIHR-UHFFFAOYSA-N	4.5×10^{6}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PBENZOLOH	2.1×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	7.8×10^{7}		Wang et al. (2017)	Q	81, 240
PPOCUJCGHLIXAB-UHFFFAOYSA-N	2.8×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:PBENZOLOOH	5.6×10^{11}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_6$	3.7×10^{7}		Wang et al. (2017)	Q	81, 240
YYEAFIOCCPRRFC-UHFFFAOYSA-N	9.8×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PBZBPER2OH	1.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	5.0×10^{5}		Wang et al. (2017)	Q	81, 240
NXHGWQBANLWNAY-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:PBZBPEROOH	2.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	2.0×10^{6}		Wang et al. (2017)	Q	81, 240
BDTBCPZZIFVKES-UHFFFAOYSA-N	2.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:PETLBPR2OH	7.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	3.6×10^{5}		Wang et al. (2017)	Q	81, 240
ZJSMOJBPUXMKGO-UHFFFAOYSA-N	2.8×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PETLBPROOH	1.7×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
HYHORQQVDRWXSH-UHFFFAOYSA-N	8.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PETOLOH	1.7×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	8.5×10^{7}		Wang et al. (2017)	Q	81, 240
WWMQWQMHOYSCPT-UHFFFAOYSA-N	1.6×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:PETOLOOH	4.4×10^{11}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_6$	3.6×10^{7}		Wang et al. (2017)	Q	81, 240
NWKQTACFFZGFMV-UHFFFAOYSA-N	6.6×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:TM123BP2OH	4.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	2.3×10^{5}		Wang et al. (2017)	Q	81, 240
XELNTWYHIBVYRB-UHFFFAOYSA-N	1.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:TM123BPOOH	1.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	8.7×10^{5}		Wang et al. (2017)	Q	81, 240
VYRKWTIFXGFOKI-UHFFFAOYSA-N	1.6×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:TM123OLOH	1.4×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	8.5×10^{7}		Wang et al. (2017)	Q	81, 240
CUPCKHHMKYENPF-UHFFFAOYSA-N	7.8×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:TM123OLOOH	3.6×10^{11}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_6$	3.8×10^{7}		Wang et al. (2017)	Q	81, 240
QKUAZMPWBBDUFL-UHFFFAOYSA-N	3.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:TM124BP2OH	4.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	2.3×10^{5}		Wang et al. (2017)	Q	81, 240
ALTMQDHYGSUKTA-UHFFFAOYSA-N	1.5×10^{5}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:TM124BPOOH	1.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	7.1×10^{5}		Wang et al. (2017)	Q	81, 240
WAGRVRZIKOHUQN-UHFFFAOYSA-N	2.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:TM124OLOH	1.4×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	1.2×10^{8}		Wang et al. (2017)	Q	81, 240
BDZMWXRIFUJLAS-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:TM124OLOOH	3.6×10^{11}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_6$	5.4×10^{7}		Wang et al. (2017)	Q	81, 240
BWEFFYCDYKVJMY-UHFFFAOYSA-N	2.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:TM135BP2OH	5.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	2.8×10^{5}		Wang et al. (2017)	Q	81, 240
UOFFRVMQLZOQAS-UHFFFAOYSA-N	1.2×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:TM135BPOOH	1.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	7.3×10^{5}		Wang et al. (2017)	Q	81, 240
JMJJTOHEWPZJQK-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:TM135OLOH	1.1×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	5.4×10^{7}		Wang et al. (2017)	Q	81, 240
QLKJHZCZIQIKHZ-UHFFFAOYSA-N	2.1×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:TM135OLOOH	2.9×10^{11}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_6$	2.1×10^{7}		Wang et al. (2017)	Q	81, 240
BLJZZZVPECPSDH-UHFFFAOYSA-N	6.5×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:APINAOOH	4.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_3$	1.5×10^{4}		Wang et al. (2017)	Q	81, 240
RYIWEMFTAFVTLU-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:APINBOOH	4.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_3$	1.8×10^{4}		Wang et al. (2017)	Q	81, 240
USRGRUOHOYDFID-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:APINCOOH	4.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_3$	1.6×10^{5}		Wang et al. (2017)	Q	81, 240
PONCTWLYBMTTOF-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:BPINAOOH	4.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_3$	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
YIWAKBLZYMRLPO-UHFFFAOYSA-N	4.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:BPINBOOH	4.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_3$	1.2×10^{3}		Wang et al. (2017)	Q	81, 240
LNOABRBKZGHYLB-UHFFFAOYSA-N	5.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:BPINCOOH	4.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_3$	2.7×10^{5}		Wang et al. (2017)	Q	81, 240
ONJNLKNHLLSXIR-UHFFFAOYSA-N	3.0×10^{5}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C918CO3H	2.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_4$	5.9×10^{1}		Wang et al. (2017)	Q	81, 240
NCSYYALRPIRWRM-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DMEBPR2OH	5.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_4$	2.0×10^{5}		Wang et al. (2017)	Q	81, 240
JNPNKLHEXQFLDW-UHFFFAOYSA-N	4.4×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:DMEBPROOH	1.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_5$	7.4×10^{5}		Wang et al. (2017)	Q	81, 240
FGEXZPMCUOXGAY-UHFFFAOYSA-N	3.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:DMEPHOLOH	8.9×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_5$	3.7×10^{7}		Wang et al. (2017)	Q	81, 240
KIALIUKUKYONFN-UHFFFAOYSA-N	4.9×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:DMEPHOLOOH	2.3×10^{11}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_6$	1.4×10^{7}		Wang et al. (2017)	Q	81, 240
NQWKUASPEMANIL-UHFFFAOYSA-N	3.2×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:HO3C106OOH	6.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{22}O_3$	1.6×10^{4}		Wang et al. (2017)	Q	81, 240
FUGKCLXVXWNPCD-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO8C9CO3H	8.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{20}O_4$	2.5×10^{4}		Wang et al. (2017)	Q	81, 240
UIPJRQQFQSAZPI-UHFFFAOYSA-N	7.3		Wang et al. (2017)	Q	81, 241
MCM:LIMAOOH	3.6×10^{4}	13000	Wieser et al. (2023)	Q	439
$C_{10}H_{18}O_3$	4.4×10^{4}		Wang et al. (2017)	Q	81, 239
FPMDSGWWEURSNO-UHFFFAOYSA-N	2.7×10^{4}		Wang et al. (2017)	Q	81, 240
	7.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:LIMBOOH	4.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_3$	2.9×10^{4}		Wang et al. (2017)	Q	81, 240
KUZZIHAARVNWSI-UHFFFAOYSA-N	2.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:LIMCOOH	3.6×10^{4}	13000	Wieser et al. (2023)	Q	439
$C_{10}H_{18}O_3$	5.3×10^{4}		Wang et al. (2017)	Q	81, 239
VVHMRXSQYYKNLC-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	81, 240
	4.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:DEMPHOLOH	8.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_5$	2.3×10^{7}		Wang et al. (2017)	Q	81, 240
ZTCJTCVANLKQAR-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:DEMPHOLOOH	2.1×10^{11}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_6$	1.1×10^{7}		Wang et al. (2017)	Q	81, 240
MGZZNFCOXGVYJN-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DETLBPR2OH	4.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_4$	1.7×10^{5}		Wang et al. (2017)	Q	81, 240
DLRWBBGTDDBDMY-UHFFFAOYSA-N	8.5×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:DETLBPROOH	1.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_5$	4.2×10^{5}		Wang et al. (2017)	Q	81, 240
XWTOJCWARUYVPA-UHFFFAOYSA-N	1.1×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:HO3C116OOH	5.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{24}O_3$	1.3×10^{4}		Wang et al. (2017)	Q	81, 240
XCBVDNPGCYSIMS-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO3C126OOH	4.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{26}O_3$	1.0×10^{4}		Wang et al. (2017)	Q	81, 240
FENUAUYSPLOZDX-UHFFFAOYSA-N	4.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:BCAOOH	4.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{26}O_3$	3.6×10^{3}		Wang et al. (2017)	Q	81, 240
UHQMVBPMTRQRFN-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:BCBOOH	4.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{26}O_3$	1.0×10^{4}		Wang et al. (2017)	Q	81, 240
LZWWDZWHHIWFFS-UHFFFAOYSA-N	6.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:BCCOOH	5.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{26}O_3$	3.7×10^{4}		Wang et al. (2017)	Q	81, 240
LYZHLRDUTRINQK-UHFFFAOYSA-N	2.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:CATEC1OOH	7.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_3$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
GQLFYNLDVCYDKN-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MCATEC1OOH	4.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_3$	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
XVDDPRZRYAGIKB-UHFFFAOYSA-N	2.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:ECATEC1OOH	4.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_3$	8.3×10^{2}		Wang et al. (2017)	Q	81, 240
WXEIAPGLSOOSMJ-UHFFFAOYSA-N	5.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MXCTEC1OOH	3.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_3$	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
OTSRNDWSIFNBPX-UHFFFAOYSA-N	8.3×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:OCATEC1OOH	3.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_3$	1.7×10^{3}		Wang et al. (2017)	Q	81, 240
FFFASTPMSYAWLR-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:PCATEC1OOH	3.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_3$	3.1×10^{3}		Wang et al. (2017)	Q	81, 240
XEPXMQBYFZNYBF-UHFFFAOYSA-N	5.6×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:STYRENOOH	3.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_3$	2.1×10^{4}		Wang et al. (2017)	Q	81, 240
PRSNAZGJNCSLPW-UHFFFAOYSA-N	4.4×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:IPCATC1OOH	3.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	6.0×10^{2}		Wang et al. (2017)	Q	81, 240
LUGXJULPVOELPW-UHFFFAOYSA-N	5.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MTCTEC1OOH	2.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	7.6×10^{2}		Wang et al. (2017)	Q	81, 240
RXVYKZMASOKYNM-UHFFFAOYSA-N	6.5×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:OTCTEC1OOH	2.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	8.9×10^{2}		Wang et al. (2017)	Q	81, 240
BNYRTZAXTAHDLR-UHFFFAOYSA-N	8.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PRCATC1OOH	3.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	5.9×10^{2}		Wang et al. (2017)	Q	81, 240
WDHGVTVSFNORIO-UHFFFAOYSA-N	6.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PTCTEC1OOH	2.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
SXYSFXQBYZNKPP-UHFFFAOYSA-N	4.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:T123CT1OOH	1.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	2.0×10^{3}		Wang et al. (2017)	Q	81, 240
XFULZEJTRUOVEV-UHFFFAOYSA-N	7.3×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:T124CT1OOH	1.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	3.2×10^{3}		Wang et al. (2017)	Q	81, 240
XVSFIBYJDMNABQ-UHFFFAOYSA-N	2.7×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:HCOCH2OOH	7.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_2H_4O_3$	1.4×10^{2}		Wang et al. (2017)	Q	81, 240
TUJPSEFVDYHSJJ-UHFFFAOYSA-N	4.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HCOCO3H	9.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_2H_2O_4$	3.9×10^{2}		Wang et al. (2017)	Q	81, 240
JOALXJIWVKUVBR-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C3DIALOOH	5.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_3H_4O_4$	1.7×10^{4}		Wang et al. (2017)	Q	81, 240
VUPDPJIDXKCVGY-UHFFFAOYSA-N	4.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CHOC2H4OOH	5.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_3$	5.3×10^{3}		Wang et al. (2017)	Q	81, 240
XSASRUDTFFBDDK-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	81, 241

A3.5 Aldehydes (RCHO)

Table A3.5: Aldehydes (RCHO)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methanal	3.2×10^{1}	7100	Burkholder et al. (2019)	L	457
HCHO	3.2×10^{1}	7100	Burkholder et al. (2015)	L	457
(formaldehyde)	3.2×10^{1}	6800	Warneck and Williams (2012)	L	457
[50-00-0]	3.2×10^{1}	7100	Sander et al. (2011)	L	457
WSFSSNUMVMOOMR-UHFFFAOYSA-N	3.2×10^{1}	7100	Sander et al. (2006)	L	457
	3.2×10^{1}	6800	Staudinger and Roberts (2001)	L	457
	3.2×10^{1}	6800	Staudinger and Roberts (1996)	L	457
	3.5×10^{1}	5700	Liu et al. (2015)	M	457
	3.4×10^{1}	6400	Allou et al. (2011)	M	457
	5.3×10^{1}	1600	Seyfioglu and Odabasi (2007)	M	457
	9.9×10^{1}		Kim et al. (2000)	M	88, 457
	3.1×10^{1}	6500	Zhou and Mopper (1990)	M	458, 457
	3.1×10^{1}	7200	Betterton and Hoffmann (1988)	M	457
			Dong and Dasgupta (1986)	M	459
			Ledbury and Blair (1925)	M	460
			Blair and Ledbury (1925)	M	460
	3.0×10^{1}		Lide and Frederikse (1995)	V	457
	2.3		Hwang et al. (1992)	V	457
	6.9×10^{1}	6400	Chameides (1984)	T	457
	2.9×10^{1}	7200	Bell (1966)	X	461, 457
	5.9×10^{1}		Gaffney and Senum (1984)	X	457, 391
	4.5×10^{1}		Lee and Zhou (1993)	C	88, 457
			Hough (1991)	C	460
	1.4×10^{2}		Warneck (1988)	C	457
	7.8×10^{-2}		Wang et al. (2017)	Q	81, 239
	4.9×10^{-2}		Wang et al. (2017)	Q	81, 240
	1.0×10^{-2}		Wang et al. (2017)	Q	81, 241
	2.8×10^{-2}		Hilal et al. (2008)	Q	
	7.5×10^{-2}		Modarresi et al. (2007)	Q	68
	4.3×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	9.0×10^{-2}		English and Carroll (2001)	Q	231, 232
	6.2×10^{-2}		Katritzky et al. (1998)	Q	
	1.8×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.0×10^{2}		Meylan and Howard (1991)	Q	457
	4.2×10^{-2}		Abraham et al. (1990)	?	
	6.2×10^{1}		Seinfeld (1986)	?	21, 457
			Lelieveld and Crutzen (1991)	W	460
			Pandis and Seinfeld (1989)	W	460

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethanal	1.3×10^{-1}	5900	Burkholder et al. (2019)	L	462
CH_3CHO	1.3×10^{-1}	5900	Burkholder et al. (2015)	L	462
(acetaldehyde)	1.5×10^{-1}	5600	Brockbank (2013)	L	
[75-07-0]	1.3×10^{-1}	5900	Sander et al. (2011)	L	
IKHGUXGNUITLKF-UHFFFAOYSA-N	1.3×10^{-1}	5900	Sander et al. (2006)	L	
	1.3×10^{-1}	5700	Staudinger and Roberts (2001)	L	
	1.4×10^{-1}	5600	Staudinger and Roberts (1996)	L	
	1.7×10^{-1}	5600	Wieland et al. (2015)	M	463
	1.5×10^{-1}	6400	Ji and Evans (2007)	M	
	1.1×10^{-1}		Straver and de Loos (2005)	M	
	1.5×10^{-1}		Marin et al. (1999)	M	
	1.3×10^{-1}	5700	Benkelberg et al. (1995)	M	
	1.7×10^{-1}	5000	Zhou and Mopper (1990)	M	458
	7.1×10^{-2}		Guitart et al. (1989)	M	14
	1.2×10^{-1}	6300	Betterton and Hoffmann (1988)	M	462
	1.2×10^{-1}	5800	Snider and Dawson (1985)	M	
	8.3×10^{-2}		Richon et al. (1985)	M	38
	1.6×10^{-1}		Mazza (1980)	M	
	2.5×10^{-1}		Vitenberg et al. (1974)	M	375
	1.5×10^{-1}		Buttery et al. (1969)	M	
	1.2×10^{-1}		Marin et al. (1999)	V	
	1.2×10^{-1}		Hwang et al. (1992)	V	
	7.8×10^{-2}		Yaws (2003)	X	259
	1.7×10^{-2}	4500	Janini and Quaddora (1986)	X	299
	1.7×10^{-1}	4700	Goldstein (1982)	X	299
	1.5×10^{-1}		Gaffney and Senum (1984)	X	391
	1.5×10^{-1}		Pierotti et al. (1959)	X	464
	1.8×10^{-1}		Dupeux et al. (2022)	Q	260
	9.0×10^{-2}		Keshavarz et al. (2022)	Q	
	9.8×10^{-2}		Duchowicz et al. (2020)	Q	
	9.8×10^{-2}		Wang et al. (2017)	Q	81, 239
	3.4×10^{-1}		Wang et al. (2017)	Q	81, 240
	1.3×10^{-1}		Wang et al. (2017)	Q	81, 241
	1.5×10^{-1}		Li et al. (2014)	Q	242
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	1.1×10^{-1}		Hilal et al. (2008)	Q	
	1.0×10^{-1}		Modarresi et al. (2007)	Q	68
		5200	Kühne et al. (2005)	Q	
	1.5×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	6.6×10^{-2}		Yao et al. (2002)	Q	230
	1.4×10^{-1}		English and Carroll (2001)	Q	231, 232
	1.4×10^{-1}		Marin et al. (1999)	Q	
	7.7×10^{-2}		Katritzky et al. (1998)	Q	
	1.5×10^{-1}		Nirmalakhandan et al. (1997)	Q	

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.3×10^{-1}		Suzuki et al. (1992)	Q	233
	1.5×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	1.5×10^{-1}		Mackay et al. (2006c)	?	21
		5800	Kühne et al. (2005)	?	
	1.0×10^{-1}		Yaws (1999)	?	21
	9.8×10^{-2}		Yaws and Yang (1992)	?	21
	1.5×10^{-1}		Abraham et al. (1990)	?	
ethanedial	4.1×10^{3}	7500	Burkholder et al. (2019)	L	462
OHCCHO	4.1×10^{3}	7500	Burkholder et al. (2015)	L	462
(glyoxal)	4.1×10^{3}	7500	Sander et al. (2011)	L	462
[107-22-2]	4.9×10^{5}		Kampf et al. (2013)	M	462, 465
LEQAOMBKQFMDFZ-UHFFFAOYSA-N	4.1×10^{3}	7500	Ip et al. (2009)	M	462
			Volkamer et al. (2009)	M	466
	2.6×10^{5}		Kroll et al. (2005)	M	462, 467
	3.6×10^{3}		Zhou and Mopper (1990)	M	462, 71
	$>3.0\times10^{3}$		Betterton and Hoffmann (1988)	M	462
	1.4×10^{4}		Lee and Zhou (1993)	C	88, 462
	2.0×10^{2}		Keshavarz et al. (2022)	Q	
	1.6×10^{1}		Duchowicz et al. (2020)	Q	300
	8.9×10^{1}		Wang et al. (2017)	Q	81, 239
	9.6		Wang et al. (2017)	Q	81, 240
	1.2×10^{-2}		Wang et al. (2017)	Q	81, 241
	3.1×10^{4}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{3}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	246
	3.0×10^{3}		Duchowicz et al. (2020)	?	186, 21
	2.7×10^{5}		Woo and McNeill (2015)	?	468
propanal	9.9×10^{-2}	4300	Burkholder et al. (2019)	L	
C_2H_5CHO	9.9×10^{-2}	4300	Burkholder et al. (2015)	L	
(propionaldehyde)	1.3×10^{-1}	5500	Brockbank (2013)	L	1
[123-38-6]	9.9×10^{-2}	4300	Sander et al. (2011)	L	
NBBJYMSMWIIQGU-UHFFFAOYSA-N	9.9×10^{-2}	4300	Sander et al. (2006)	L	
	1.3×10^{-1}		Liu et al. (2015)	M	73
	9.1×10^{-2}		Kim and Kim (2014)	M	
	1.3×10^{-1}	5800	Ji and Evans (2007)	M	
	1.3×10^{-1}	5700	Zhou and Mopper (1990)	M	458
	6.1×10^{-2}		Richon et al. (1985)	M	38
	1.2×10^{-1}		Mazza (1980)	M	
	1.3×10^{-1}		Buttery et al. (1969)	M	
	7.5×10^{-2}		Buttery et al. (1965)	M	
	1.3×10^{-1}		Mackay et al. (2006c)	V	
	1.3×10^{-2}		Mackay et al. (1995)	V	
	3.2×10^{-2}	3200	Djerki and Laub (1988)	V	
	1.6×10^{-1}		Amoore and Buttery (1978)	V	
	4.3×10^{-2}		Yaws (2003)	X	259

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.2×10^{-2}	5600	Schaffer and Daubert (1969)	X	299
	2.7×10^{-2}	2400	Janini and Quaddora (1986)	X	299
	9.8×10^{-2}		Dupeux et al. (2022)	Q	260
	1.2×10^{-1}		Keshavarz et al. (2022)	Q	
	9.9×10^{-2}		Duchowicz et al. (2020)	Q	185
	8.0×10^{-2}		Wang et al. (2017)	Q	81, 239
	2.4×10^{-1}		Wang et al. (2017)	Q	81, 240
	8.0×10^{-2}		Wang et al. (2017)	Q	81, 241
	1.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Modarresi et al. (2007)	Q	68
		5500	Kühne et al. (2005)	Q	
	1.4×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	1.1×10^{-1}		English and Carroll (2001)	Q	231, 232
	5.8×10^{-2}		Katritzky et al. (1998)	Q	
	1.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	7.3×10^{-2}		Russell et al. (1992)	Q	280
	1.0×10^{-1}		Suzuki et al. (1992)	Q	233
	1.3×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	1.3×10^{-1}		Mackay et al. (2006c)	?	21
		5000	Kühne et al. (2005)	?	
	2.3×10^{-1}		Yaws (1999)	?	21
	1.3×10^{-1}		Abraham et al. (1990)	?	
propanedial $C_3H_4O_2$ (malonaldehyde) [542-78-9] WSMYVTOQOOLQHP-UHFFFAOYSA-N	7.3×10^{1}		Wang et al. (2017)	Q	81, 239
	6.0×10^{1}		Wang et al. (2017)	Q	81, 240
	4.1		Wang et al. (2017)	Q	81, 241
MCM:C32OH13CO $C_3H_4O_3$ NVXLIZQNSVLKPO-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	81, 239
	5.5×10^{3}		Wang et al. (2017)	Q	81, 240
	8.7		Wang et al. (2017)	Q	81, 241
MCM:CH3CHOHCHO $C_3H_6O_2$ BSABBBMNWQWLLU-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	81, 239
	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
	3.1		Wang et al. (2017)	Q	81, 241
MCM:HOC2H4CHO $C_3H_6O_2$ AKXKFZDCRYJKTF-UHFFFAOYSA-N	3.6×10^{1}	9900	Wieser et al. (2023)	Q	439
	2.2×10^{2}		Wang et al. (2017)	Q	81, 239
	8.3×10^{2}		Wang et al. (2017)	Q	81, 240
	6.6×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
butanal	9.5×10^{-2}	6200	Burkholder et al. (2019)	L	
C_3H_7CHO	9.5×10^{-2}	6200	Burkholder et al. (2015)	L	
(butyraldehyde)	9.1×10^{-2}	6000	Brockbank (2013)	L	
[123-72-8]	9.5×10^{-2}	6200	Sander et al. (2011)	L	
ZTQSAGDEMFDKMZ-UHFFFAOYSA-N	9.5×10^{-2}	6200	Sander et al. (2006)	L	
	6.1×10^{-2}		Kim and Kim (2014)	M	
	8.9×10^{-2}	6200	Ji and Evans (2007)	M	
	9.5×10^{-2}	6200	Zhou and Mopper (1990)	M	458
	8.6×10^{-2}		Buttery et al. (1969)	M	
	6.4×10^{-2}		Buttery et al. (1965)	M	
	6.5×10^{-2}		Mackay et al. (2006c)	V	
	6.5×10^{-2}		Mackay et al. (1995)	V	
	1.0×10^{-1}		Hwang et al. (1992)	V	
	8.7×10^{-2}	3500	Djerki and Laub (1988)	V	
	6.7×10^{-2}		Amoore and Buttery (1978)	V	
	8.4×10^{-2}		Yaws (2003)	X	259
	8.3×10^{-2}		Yaws (2003)	X	238
	5.4×10^{-2}	4000	Janini and Quaddora (1986)	X	299
	6.8×10^{-2}		Dupeux et al. (2022)	Q	260
	1.6×10^{-1}		Keshavarz et al. (2022)	Q	
	9.9×10^{-2}		Duchowicz et al. (2020)	Q	
	6.3×10^{-2}		Wang et al. (2017)	Q	81, 239
	1.4×10^{-1}		Wang et al. (2017)	Q	81, 240
	6.3×10^{-2}		Wang et al. (2017)	Q	81, 241
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	5.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
	9.0×10^{-2}		Hilal et al. (2008)	Q	
	1.1×10^{-1}		Modarresi et al. (2007)	Q	68
		5900	Kühne et al. (2005)	Q	
	6.7×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	5.3×10^{-2}		Yao et al. (2002)	Q	230
	8.6×10^{-2}		English and Carroll (2001)	Q	231, 232
	5.4×10^{-2}		Katritzky et al. (1998)	Q	
	9.5×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	8.6×10^{-2}		Russell et al. (1992)	Q	280
	7.9×10^{-2}		Suzuki et al. (1992)	Q	233
	8.6×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	8.6×10^{-2}		Mackay et al. (2006c)	?	21
		6400	Kühne et al. (2005)	?	
	8.4×10^{-2}		Yaws (1999)	?	21
	8.6×10^{-2}		Abraham et al. (1990)	?	

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methylpropanal	5.1×10^{-2}		Burkholder et al. (2019)	L	
C_4H_8O	5.1×10^{-2}		Brockbank (2013)	L	
(isobutyraldehyde)	3.2×10^{-2}	7600	Bruneel et al. (2016)	M	
[78-84-2]	5.9×10^{-3}	4500	Strekowski and George (2005)	M	
AMIMRNSIRUDHCM-UHFFFAOYSA-N	3.3×10^{-2}		Karl et al. (2003)	M	
	3.4×10^{-2}		Pollien et al. (2003)	M	
	5.0×10^{-2}		Amoore and Buttery (1978)	M	
	5.5×10^{-2}		Duchowicz et al. (2020)	V	187
	5.5×10^{-2}		HSDB (2015)	V	
	6.7×10^{-2}		Amoore and Buttery (1978)	V	
	5.8×10^{-2}		Yaws (2003)	X	259
	4.5×10^{-2}		Dupeux et al. (2022)	Q	260
	3.8×10^{-2}		Duchowicz et al. (2020)	Q	
	7.4×10^{-2}		Wang et al. (2017)	Q	81, 239
	1.1×10^{-1}		Wang et al. (2017)	Q	81, 240
	4.3×10^{-2}		Wang et al. (2017)	Q	81, 241
	7.0×10^{-2}		Hilal et al. (2008)	Q	
		5000	Kühne et al. (2005)	Q	
	5.2×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	3.7×10^{-2}		Yao et al. (2002)	Q	230, 268
	5.2×10^{-2}		English and Carroll (2001)	Q	231, 275
	5.4×10^{-2}		Katritzky et al. (1998)	Q	
	8.2×10^{-2}		Nirmalakhandan et al. (1997)	Q	
		5100	Kühne et al. (2005)	?	
	5.7×10^{-2}		Yaws (1999)	?	21
	5.1×10^{-2}		Abraham et al. (1990)	?	
2-methylpropanedial	6.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_2$	1.2×10^{1}		Wang et al. (2017)	Q	81, 240
[16002-19-0]	1.9		Wang et al. (2017)	Q	81, 241
VXYSFSCCSQAYJV-UHFFFAOYSA-N					
MCM:MALDIAL	2.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_2$	4.6×10^{2}		Wang et al. (2017)	Q	81, 240
JGEMYUOFGVHXKV-UHFFFAOYSA-N	6.5		Wang et al. (2017)	Q	81, 241
MCM:C3MDIALOH	1.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_3$	2.0×10^{3}		Wang et al. (2017)	Q	81, 240
SQHUBVCIVAIUAB-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	81, 241
MCM:C41OH	2.5×10^{7}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	3.7×10^{7}		Wang et al. (2017)	Q	81, 240
YTBSYETUWUMLBZ-UHFFFAOYSA-N	1.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C41OOH	3.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_5$	3.6×10^{8}		Wang et al. (2017)	Q	81, 240
ROHPNOOUQDXFHZ-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	81, 241

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C4OCCOHCOH	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	5.0×10^{4}		Wang et al. (2017)	Q	81, 240
DFFAMJFPVBTTBX-UHFFFAOYSA-N	3.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CHOC3DIOL	2.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	2.2×10^{5}		Wang et al. (2017)	Q	81, 240
CQSYGAZTCJHVFE-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HC3CCHO	3.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_2$	8.7×10^{1}		Wang et al. (2017)	Q	81, 240
PPNVQCFSKPIRKK-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	81, 241
MCM:HC3CHO	7.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_2$	3.7×10^{3}		Wang et al. (2017)	Q	81, 240
FXCMZPXXCRHRNK-UHFFFAOYSA-N	2.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HMACROH	1.5×10^{7}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	8.5×10^{7}		Wang et al. (2017)	Q	81, 240
OUEKYUKJSLEOIU-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HMACR	4.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_2$	2.0×10^{2}		Wang et al. (2017)	Q	81, 240
QVBICLGJAQXLSA-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO13C3CHO	2.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	2.3×10^{5}		Wang et al. (2017)	Q	81, 240
NKVLMFFGFYHDNE-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO2C3CHO	2.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_2$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
HSJKGGMUJITCBW-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO3C3CHO	1.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_2$	8.9×10^{1}		Wang et al. (2017)	Q	81, 240
UIKQNMXWCYQNCS-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	81, 241
MCM:HOC3H6CHO	1.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_2$	2.8×10^{3}		Wang et al. (2017)	Q	81, 240
PIAOXUVIBAKVSP-UHFFFAOYSA-N	6.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HOHOC4DIAL	6.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_4$	3.0×10^{6}		Wang et al. (2017)	Q	81, 240
UUWVJXZLAWXQBU-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HOIPRCHO	2.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_2$	6.8×10^{2}		Wang et al. (2017)	Q	81, 240
JTMCAHGCWBGWRV-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:IBUTALOH	6.6		Wang et al. (2017)	Q	81, 239
$C_4H_8O_2$	4.4×10^{1}		Wang et al. (2017)	Q	81, 240
HNVAGBIANFAIIL-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	81, 241

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MACROH	8.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	3.6×10^{4}		Wang et al. (2017)	Q	81, 240
JBCPUXACCOWZEB-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
pentanal	6.6×10^{-2}	6500	Brockbank (2013)	L	
C_4H_9CHO	6.8×10^{-2}		Liu et al. (2015)	M	73
(valeraldehyde)	3.9×10^{-2}		Kim and Kim (2014)	M	
[110-62-3]	7.1×10^{-2}	6100	Ji and Evans (2007)	M	
HGBOYTHUEUWSSQ-UHFFFAOYSA-N	6.3×10^{-2}	6300	Zhou and Mopper (1990)	M	458
	6.7×10^{-2}		Buttery et al. (1969)	M	
	5.8×10^{-2}		Buttery et al. (1965)	M	
	2.4×10^{-1}	3800	Djerki and Laub (1988)	V	
	6.4×10^{-2}		Amoore and Buttery (1978)	V	
	3.0×10^{-2}		Yaws (2003)	X	259
	3.0×10^{-2}		Yaws (2003)	X	238
	6.1×10^{-2}		Dupeux et al. (2022)	Q	260
	2.2×10^{-1}		Keshavarz et al. (2022)	Q	
	9.8×10^{-2}		Duchowicz et al. (2020)	Q	300
	5.8×10^{-2}		Wang et al. (2017)	Q	81, 239
	8.9×10^{-2}		Wang et al. (2017)	Q	81, 240
	3.2×10^{-2}		Wang et al. (2017)	Q	81, 241
	5.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	4.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
	7.2×10^{-2}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	68
		6200	Kühne et al. (2005)	Q	
	6.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.9×10^{-2}		Yao et al. (2002)	Q	230, 268
	6.7×10^{-2}		English and Carroll (2001)	Q	231, 232
	7.3×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	6.1×10^{-2}		Suzuki et al. (1992)	Q	233
	6.2×10^{-2}		Meylan and Howard (1991)	Q	
	6.7×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	6.7×10^{-2}		Mackay et al. (2006c)	?	21
		5500	Kühne et al. (2005)	?	
	3.0×10^{-2}		Yaws (1999)	?	21
	4.4×10^{-2}		Yaws and Yang (1992)	?	21, 38
	6.7×10^{-2}		Abraham et al. (1990)	?	

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methylbutanal	2.5×10^{-2}	5600	Brockbank (2013)	L	
$C_5H_{10}O$	2.3×10^{-2}		Pollien et al. (2003)	M	
[96-17-3]	5.9×10^{-2}		Wang et al. (2017)	Q	81, 239
BYGQBDHUGHBGMD-UHFFFAOYSA-N	8.7×10^{-2}		Wang et al. (2017)	Q	81, 240
	3.9×10^{-2}		Wang et al. (2017)	Q	81, 241
	9.5×10^{-3}		Hertel et al. (2007)	Q	469
3-methylbutanal	1.1×10^{-2}	10000	Bruneel et al. (2016)	M	33
$C_5H_{10}O$	2.4×10^{-2}	6100	Wieland et al. (2015)	M	470
(isovaleraldehyde)	2.1×10^{-2}		Kim and Kim (2014)	M	
[590-86-3]	2.6×10^{-2}		Pollien et al. (2003)	M	
YGHRJJRRZDOVPD-UHFFFAOYSA-N	2.0×10^{-2}		Nelson and Hoff (1968)	M	298
	2.4×10^{-2}		Duchowicz et al. (2020)	V	187
	2.5×10^{-2}		HSDB (2015)	V	
	5.2×10^{-2}		Yaws (2003)	X	238
	3.8×10^{-2}		Duchowicz et al. (2020)	Q	
	5.9×10^{-2}		Wang et al. (2017)	Q	81, 239
	1.1×10^{-1}		Wang et al. (2017)	Q	81, 240
	4.5×10^{-2}		Wang et al. (2017)	Q	81, 241
	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
	7.3×10^{-2}		Hilal et al. (2008)	Q	
	9.1×10^{-2}		Modarresi et al. (2007)	Q	68
	9.8×10^{-3}		Hertel et al. (2007)	Q	469
MCM:C4MDIAL	1.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_2$	6.5×10^{2}		Wang et al. (2017)	Q	81, 240
USBJWIKCHJDWPF-UHFFFAOYSA-N	2.8		Wang et al. (2017)	Q	81, 241
MCM:CO1M22CHO	3.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_2$	8.9		Wang et al. (2017)	Q	81, 240
WNBFTLCNQKKVHC-UHFFFAOYSA-N	3.4×10^{-1}		Wang et al. (2017)	Q	81, 241
2,2-dimethylpropanal	4.1×10^{-2}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O$	5.6×10^{-2}		Wang et al. (2017)	Q	81, 240
(pivaldehyde)	2.8×10^{-2}		Wang et al. (2017)	Q	81, 241
[630-19-3]					
FJJYHTVHBVXEEQ-UHFFFAOYSA-N					
MCM:C3EDIALOH	1.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	2.6×10^{3}		Wang et al. (2017)	Q	81, 240
QTDYRJFEJDMBDI-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
MCM:C3M3OH2CHO	1.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	6.5×10^{1}		Wang et al. (2017)	Q	81, 240
VKYKDJZVZBURQF-UHFFFAOYSA-N	6.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C42CHO	2.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	3.2×10^{5}		Wang et al. (2017)	Q	81, 240
NGVSSTUGOBBIBC-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C4M2AL2OH	3.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	5.0×10^{6}		Wang et al. (2017)	Q	81, 240
NUHRTSFMSDZSTE-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C4OHCHO	8.3		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	5.6×10^{1}		Wang et al. (2017)	Q	81, 240
SUTLBTHMXYSMSZ-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	81, 241
MCM:C514OH	1.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	8.7×10^{5}		Wang et al. (2017)	Q	81, 240
UIVALZXFWDRKKE-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C57OH	1.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	6.8×10^{7}		Wang et al. (2017)	Q	81, 240
ZKDSJDSEVDWBAC-UHFFFAOYSA-N	1.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C58OH	1.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	1.4×10^{8}		Wang et al. (2017)	Q	81, 240
HTPZSALIZDTBIL-UHFFFAOYSA-N	2.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C5DIALOH	3.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_3$	5.8×10^{4}		Wang et al. (2017)	Q	81, 240
KBKQEUDBRUGUIQ-UHFFFAOYSA-N	3.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:H13C43CHO	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	1.7×10^{5}		Wang et al. (2017)	Q	81, 240
KJLUILOCNALPNM-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:H2M2C3CHO	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	6.2×10^{2}		Wang et al. (2017)	Q	81, 240
FXFBPKDQLDOIRG-UHFFFAOYSA-N	2.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HC4ACHO	4.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_2$	4.6×10^{3}		Wang et al. (2017)	Q	81, 240
BSHDRMLUCYMQOP-UHFFFAOYSA-N	1.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HC4CCHO	1.2×10^{3}	11000	Wieser et al. (2023)	Q	439
$C_5H_8O_2$	4.8×10^{2}		Wang et al. (2017)	Q	81, 239
GCHJBJOOADXJFT-UHFFFAOYSA-N	4.1×10^{3}		Wang et al. (2017)	Q	81, 240
	5.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HM22CHO	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	3.7×10^{2}		Wang et al. (2017)	Q	81, 240
JJMOMMLADQPZNY-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO24C4CHO	2.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	3.6×10^{5}		Wang et al. (2017)	Q	81, 240
WDKLWOBHKQJYSU-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HO2C43CHO	2.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	6.9×10^{2}		Wang et al. (2017)	Q	81, 240
ZURZPPULRFXVLF-UHFFFAOYSA-N	3.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO2C4CHO	1.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	2.1×10^{3}		Wang et al. (2017)	Q	81, 240
HFZMJAMTNAAZQE-UHFFFAOYSA-N	4.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO3C4CHO	1.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	7.8×10^{2}		Wang et al. (2017)	Q	81, 240
WRWLNLBWBJEUPI-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HOBUT2CHO	1.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
PLBZJQQQFIOXRU-UHFFFAOYSA-N	2.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HOIBUTCHO	1.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	2.0×10^{3}		Wang et al. (2017)	Q	81, 240
RWXBAXNFTXQJAY-UHFFFAOYSA-N	4.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MBOBCO	7.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	4.4×10^{4}		Wang et al. (2017)	Q	81, 240
YDXYYBJRCIQQSF-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PROL1MCHO	5.8		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	4.2×10^{1}		Wang et al. (2017)	Q	81, 240
MEHIGMLPKIJWEA-UHFFFAOYSA-N	7.4×10^{-1}		Wang et al. (2017)	Q	81, 241
hexanal	4.5×10^{-2}	6400	Brockbank (2013)	L	
$C_5H_{11}CHO$	2.3×10^{-2}	5200	Kutsuna and Kaneyasu (2021)	M	
[66-25-1]	2.9×10^{-2}	8900	Bruneel et al. (2016)	M	
JARKCYVAAOWBJS-UHFFFAOYSA-N	4.7×10^{-2}		Souchon et al. (2004)	M	
	3.2×10^{-2}		Karl et al. (2003)	M	
	1.6×10^{-1}	4900	Meynier et al. (2003)	M	38
	2.7×10^{-2}		van Ruth et al. (2002)	M	14
	2.2×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 363
	1.6×10^{-2}		van Ruth et al. (2001)	M	14
	4.9×10^{-2}	6500	Zhou and Mopper (1990)	M	458
	4.6×10^{-2}		Buttery et al. (1969)	M	
	5.8×10^{-2}		Buttery et al. (1965)	M	
	3.5×10^{-2}		Amoore and Buttery (1978)	V	
	2.8×10^{-2}		Yaws (2003)	X	259
	2.8×10^{-2}		Yaws (2003)	X	238, 38
	4.8×10^{-2}		Sieg et al. (2008)	C	
	4.6×10^{-2}		Meynier et al. (2003)	C	
	3.1×10^{-2}		Nahon et al. (2000)	C	14
	4.2×10^{-2}		Dupeux et al. (2022)	Q	260
	3.0×10^{-1}		Keshavarz et al. (2022)	Q	
	9.8×10^{-2}		Duchowicz et al. (2020)	Q	300

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.6×10^{-2}		Wang et al. (2017)	Q	81, 239
	5.8×10^{-2}		Wang et al. (2017)	Q	81, 240
	5.5×10^{-2}		Wang et al. (2017)	Q	81, 241
	4.6×10^{-2}		Li et al. (2014)	Q	242
	4.3×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
	5.8×10^{-2}		Hilal et al. (2008)	Q	
	9.8×10^{-2}		Modarresi et al. (2007)	Q	68
	1.1×10^{-2}		Hertel et al. (2007)	Q	469
		6600	Kühne et al. (2005)	Q	
	4.6×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.6×10^{-2}		Yao et al. (2002)	Q	230
	5.2×10^{-2}		English and Carroll (2001)	Q	231, 261
	4.8×10^{-2}		Katritzky et al. (1998)	Q	
	5.8×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	4.6×10^{-2}		Suzuki et al. (1992)	Q	233
	4.6×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	4.6×10^{-2}		Mackay et al. (2006c)	?	21
		6900	Kühne et al. (2005)	?	
	3.8×10^{-2}		Yaws (1999)	?	21, 38
	1.9×10^{-2}		Yaws and Yang (1992)	?	21, 38
	4.6×10^{-2}		Abraham et al. (1990)	?	
pentanedial	3.0×10^{2}	9200	Olson (1998)	M	
$OHC(CH_2)_3CHO$	4.1×10^{2}		HSDB (2015)	Q	100
(glutaraldehyde)		8800	Kühne et al. (2005)	Q	
[111-30-8]		9100	Kühne et al. (2005)	?	
SXRSQZLOMIGNAQ-UHFFFAOYSA-N					
2-methylpentanal	5.3×10^{-2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O$	5.6×10^{-2}		Wang et al. (2017)	Q	81, 240
(2-methylvaleraldehyde)	3.5×10^{-2}		Wang et al. (2017)	Q	81, 241
[123-15-9]	2.7×10^{-2}		HSDB (2015)	Q	100
FTZILAQGHINQQR-UHFFFAOYSA-N		5700	Kühne et al. (2005)	Q	
		5300	Kühne et al. (2005)	?	
hexanedial	4.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	1.7×10^{2}		Wang et al. (2017)	Q	81, 240
(adipaldehyde)	3.2×10^{1}		Wang et al. (2017)	Q	81, 241
[1072-21-5]					
UMHJEEQLYBKSAN-UHFFFAOYSA-N					

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:M22C3CHO	3.2×10^{-2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O$	6.5×10^{-2}		Wang et al. (2017)	Q	81, 240
LTNUSYNQZJZUSY-UHFFFAOYSA-N	3.1×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:M2C43CHO	6.2×10^{-2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O$	6.0×10^{-2}		Wang et al. (2017)	Q	81, 240
AKUUEDVRXOZTBF-UHFFFAOYSA-N	3.7×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:M33C3CHO	3.2×10^{-2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O$	5.0×10^{-2}		Wang et al. (2017)	Q	81, 240
QYPLKDUOPJZROX-UHFFFAOYSA-N	2.6×10^{-2}		Wang et al. (2017)	Q	81, 241
3-methylpentanal	3.8×10^{-2}		Yaws (2003)	X	238
$C_6H_{12}O$	5.3×10^{-2}		Wang et al. (2017)	Q	81, 239
[15877-57-3]	7.8×10^{-2}		Wang et al. (2017)	Q	81, 240
YJWJGLQYQJGEEP-UHFFFAOYSA-N	4.5×10^{-2}		Wang et al. (2017)	Q	81, 241
	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
4-methylpentanal	3.8×10^{-2}		Yaws (2003)	X	238
$C_6H_{12}O$	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
[1119-16-0]					
JGEGJYXHCFUMJF-UHFFFAOYSA-N					
2-ethylbutanal	4.0×10^{-2}		Yaws (2003)	X	259
$C_6H_{12}O$	3.7×10^{-2}		Dupeux et al. (2022)	Q	260
[97-96-1]					
UNNGUFMVYQJGTD-UHFFFAOYSA-N					
MCM:C518CHO	3.2×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	5.3×10^{2}		Wang et al. (2017)	Q	81, 240
XEAYIEUKFACAKS-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C615OH	4.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	4.4×10^{4}		Wang et al. (2017)	Q	81, 240
LOUHJSYYTNSRBN-UHFFFAOYSA-N	3.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C623OH	3.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	6.2×10^{8}		Wang et al. (2017)	Q	81, 240
ASGSKBSLHTVURJ-UHFFFAOYSA-N	1.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C67OH	1.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	3.5×10^{5}		Wang et al. (2017)	Q	81, 240
SIBVVDHXFPINCX-UHFFFAOYSA-N	4.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C68OH	1.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	3.6×10^{5}		Wang et al. (2017)	Q	81, 240
RJKLRJTWLKKQSE-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C6DIALOH	1.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	4.7×10^{5}		Wang et al. (2017)	Q	81, 240
GATFIJYWERJMGU-UHFFFAOYSA-N	2.6×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CO1C6OH	1.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	1.9×10^{3}		Wang et al. (2017)	Q	81, 240
FPFTWHJPEMPAGE-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:CO1H63OH	4.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	2.5×10^{6}		Wang et al. (2017)	Q	81, 240
TWSXDPXQZVBPJU-UHFFFAOYSA-N	2.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:H2M2C4CHO	9.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
NEJZWIVQOAKZHY-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:H2M3C4CHO	1.5×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	1.8×10^{3}		Wang et al. (2017)	Q	81, 240
GUXDGBBNSMURMG-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:H3M3C4CHO	9.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	5.5×10^{2}		Wang et al. (2017)	Q	81, 240
HKXRCBUXVFAKDA-UHFFFAOYSA-N	1.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HM22C3CHO	9.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	1.1×10^{3}		Wang et al. (2017)	Q	81, 240
VOISQCUJWIZDHK-UHFFFAOYSA-N	5.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HM2C43CHO	1.5×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	1.7×10^{3}		Wang et al. (2017)	Q	81, 240
QQZFDCJFBSAIBQ-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HM33C3CHO	9.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	1.0×10^{3}		Wang et al. (2017)	Q	81, 240
YHMMFPKTSXQULG-UHFFFAOYSA-N	2.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO2C54CHO	1.5×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
ZHZOUKIXPREHLS-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO3C5CHO	1.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	1.5×10^{3}		Wang et al. (2017)	Q	81, 240
HAPLZPWSLJPZBM-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO5C5CHO	6.9		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	4.0×10^{1}		Wang et al. (2017)	Q	81, 240
BRZMRZVKWQWYPJ-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	81, 241
heptanal	3.4×10^{-2}	7500	Brockbank (2013)	L	
$C_6H_{13}CHO$	3.5×10^{-2}		Souchon et al. (2004)	M	
[111-71-7]	2.0×10^{-2}		van Ruth et al. (2002)	M	14
FXHGMKSSBGDXIY-UHFFFAOYSA-N	1.9×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 363
	1.1×10^{-2}		van Ruth et al. (2001)	M	14
	3.3×10^{-2}	7500	Zhou and Mopper (1990)	M	458
	3.7×10^{-2}		Buttery et al. (1969)	M	

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.0×10^{-2}		Buttery et al. (1965)	M	
	5.4×10^{-2}		Amoore and Buttery (1978)	V	
	2.1×10^{-2}		Yaws (2003)	X	259
	2.0×10^{-2}		Yaws (2003)	X	238, 38
	3.7×10^{-2}		Sieg et al. (2008)	C	
	3.0×10^{-2}		Dupeux et al. (2022)	Q	260
	5.3×10^{-2}		Keshavarz et al. (2022)	Q	
	9.8×10^{-2}		Duchowicz et al. (2020)	Q	185
	3.6×10^{-2}		Wang et al. (2017)	Q	81, 239
	4.3×10^{-2}		Wang et al. (2017)	Q	81, 240
	2.5×10^{-2}		Wang et al. (2017)	Q	81, 241
	3.7×10^{-2}		Li et al. (2014)	Q	242
	3.3×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
	3.7×10^{-2}		Hilal et al. (2008)	Q	
	8.1×10^{-2}		Modarresi et al. (2007)	Q	68
		6900	Kühne et al. (2005)	Q	
	3.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.2×10^{-2}		Yao et al. (2002)	Q	230
	3.9×10^{-2}		English and Carroll (2001)	Q	231, 275
	4.7×10^{-2}		Katritzky et al. (1998)	Q	
	4.5×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	3.6×10^{-2}		Suzuki et al. (1992)	Q	233
	3.7×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		7100	Kühne et al. (2005)	?	
	2.8×10^{-2}		Yaws (1999)	?	21, 38
	2.3×10^{-2}		Yaws and Yang (1992)	?	21, 38
	3.7×10^{-2}		Abraham et al. (1990)	?	
MCM:C622CHO	5.8×10^{3}	11000	Wieser et al. (2023)	Q	439
$C_7H_{12}O_2$	2.5×10^{2}		Wang et al. (2017)	Q	81, 239
JWVBPJJNIHELFZ-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
	7.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C624CHO	5.8×10^{3}	11000	Wieser et al. (2023)	Q	439
$C_7H_{12}O_2$	2.5×10^{2}		Wang et al. (2017)	Q	81, 239
AIMYSSDKEKDSEU-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 240
	2.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C728OH	2.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_4$	1.2×10^{9}		Wang et al. (2017)	Q	81, 240
RQDWEXZQVQBWBC-UHFFFAOYSA-N	2.2×10^{6}		Wang et al. (2017)	Q	81, 241

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C730OH	2.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_4$	3.4×10^{9}		Wang et al. (2017)	Q	81, 240
ROYLBPWMPALPRM-UHFFFAOYSA-N	1.3×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:H3M3C5CHO	7.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_2$	1.1×10^{3}		Wang et al. (2017)	Q	81, 240
PUMVOOYIPAYIQQ-UHFFFAOYSA-N	5.6×10^{1}		Wang et al. (2017)	Q	81, 241
octanal	2.0×10^{-2}	7300	Brockbank (2013)	L	
$C_7H_{15}CHO$	2.1×10^{-2}		van Ruth et al. (2002)	M	14
[124-13-0]	1.9×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 363
NUJGJRNETVAIRJ-UHFFFAOYSA-N	8.8×10^{-3}		van Ruth et al. (2001)	M	14
	2.1×10^{-2}		Li and Carr (1993)	M	
	2.1×10^{-2}	7400	Zhou and Mopper (1990)	M	458
	1.9×10^{-2}		Buttery et al. (1969)	M	
	7.5×10^{-2}		Buttery et al. (1965)	M	
	2.9×10^{-2}		Amoore and Buttery (1978)	V	
	1.3×10^{-2}		Yaws (2003)	X	259
	1.3×10^{-2}		Yaws (2003)	X	238, 38
	1.9×10^{-2}		Sieg et al. (2008)	C	
	1.9×10^{-2}		Nahon et al. (2000)	C	14
	2.8×10^{-2}		Dupeux et al. (2022)	Q	260
	7.1×10^{-2}		Keshavarz et al. (2022)	Q	
	9.7×10^{-2}		Duchowicz et al. (2020)	Q	
	2.4×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	7.0×10^{-2}		Modarresi et al. (2007)	Q	68
		7300	Kühne et al. (2005)	Q	
	5.2×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	2.0×10^{-2}		Yao et al. (2002)	Q	230
	3.1×10^{-2}		English and Carroll (2001)	Q	231, 232
	4.5×10^{-2}		Katritzky et al. (1998)	Q	
	3.6×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	2.8×10^{-2}		Suzuki et al. (1992)	Q	233
	1.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		6200	Kühne et al. (2005)	?	
	1.8×10^{-2}		Yaws (1999)	?	21, 38
	2.0		Yaws and Yang (1992)	?	21, 38
	1.9×10^{-2}		Abraham et al. (1990)	?	

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-ethylhexanal	1.2×10^{-2}	5400	Brockbank (2013)	L	
$C_8H_{16}O$	1.3×10^{-2}		Duchowicz et al. (2020)	V	187
[123-05-7]	1.2×10^{-2}		HSDB (2015)	V	
LGYNIFWIKSEESD-UHFFFAOYSA-N	2.4×10^{-2}		Yaws (2003)	X	259
	2.4×10^{-2}		Yaws (2003)	X	238
	2.1×10^{-2}		Dupeux et al. (2022)	Q	260
	3.8×10^{-2}		Duchowicz et al. (2020)	Q	
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.7×10^{-2}		Hilal et al. (2008)	Q	
	2.4×10^{-2}		Modarresi et al. (2007)	Q	68
MCM:C729CHO	8.0×10^{2}	10000	Wieser et al. (2023)	Q	439
$C_8H_{12}O_2$	7.1×10^{1}		Wang et al. (2017)	Q	81, 239
MEGRLTONSLAOOM-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	81, 240
	6.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C810OH	6.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_3$	1.7×10^{5}		Wang et al. (2017)	Q	81, 240
WBGXLUPQADVOIR-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C822OH	2.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_2$	1.8×10^{3}		Wang et al. (2017)	Q	81, 240
CCTLWIOCAVSPLW-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C824OH	3.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_3$	1.9×10^{5}		Wang et al. (2017)	Q	81, 240
RBBQERVBTKJTLF-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C826OH	7.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_4$	3.0×10^{8}		Wang et al. (2017)	Q	81, 240
LLAUXDLXTPQIPI-UHFFFAOYSA-N	2.6×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C830OH	2.5×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_2$	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
KODLEZWYEGWLGP-UHFFFAOYSA-N	6.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C831OH	6.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_3$	2.1×10^{5}		Wang et al. (2017)	Q	81, 240
YTEDFRLZFCPFBH-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C89OH	2.5×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_2$	2.3×10^{3}		Wang et al. (2017)	Q	81, 240
KMZPPEYMMZMCIQ-UHFFFAOYSA-N	2.2×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
nonanal	1.1×10^{-2}	6800	Brockbank (2013)	L	
$C_8H_{17}CHO$	1.0×10^{-2}	6700	Zhou and Mopper (1990)	M	458
[124-19-6]	1.3×10^{-2}		Buttery et al. (1969)	M	
GYHFUZHODSMOHU-UHFFFAOYSA-N	7.1×10^{-2}		Buttery et al. (1965)	M	
	1.3×10^{-2}		Amoore and Buttery (1978)	V	
	1.0×10^{-2}		Yaws (2003)	X	259
	1.0×10^{-2}		Yaws (2003)	X	238, 38
	1.4×10^{-2}		Sieg et al. (2008)	C	
	1.8×10^{-2}		Dupeux et al. (2022)	Q	260
	9.6×10^{-2}		Keshavarz et al. (2022)	Q	
	9.7×10^{-2}		Duchowicz et al. (2020)	Q	185
	1.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.4×10^{-2}		Hilal et al. (2008)	Q	
	5.9×10^{-2}		Modarresi et al. (2007)	Q	68
	1.3×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.8×10^{-2}		Yao et al. (2002)	Q	230
	2.3×10^{-2}		English and Carroll (2001)	Q	231, 232
	2.8×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	2.1×10^{-2}		Suzuki et al. (1992)	Q	233
	2.0×10^{-2}		Meylan and Howard (1991)	Q	
	1.3×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	1.5×10^{-2}		Yaws (1999)	?	21, 38
	6.9×10^{-3}		Yaws and Yang (1992)	?	21, 38
	1.3×10^{-2}		Abraham et al. (1990)	?	
3,5,5-trimethylhexanal $C_9H_{18}O$ [5435-64-3] WTPYRCJDOZVZON-UHFFFAOYSA-N	2.0×10^{-2}		HSDB (2015)	Q	100
decanal	6.3×10^{-3}	8900	Brockbank (2013)	L	
$C_9H_{19}CHO$	4.3×10^{-3}		Helburn et al. (2008)	M	
[112-31-2]	6.0×10^{-3}	8700	Zhou and Mopper (1990)	M	458
KSMVZQYAVGTKIV-UHFFFAOYSA-N	1.7×10^{-1}		Buttery et al. (1965)	M	
	1.3×10^{-2}		Yaws (2003)	X	259
	1.3×10^{-2}		Yaws (2003)	X	238
	5.5×10^{-3}		Sieg et al. (2008)	C	
	1.9×10^{-2}		Dupeux et al. (2022)	Q	260
	1.8×10^{-1}		Keshavarz et al. (2022)	Q	
	9.7×10^{-2}		Duchowicz et al. (2020)	Q	300
	2.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	8.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.6×10^{-2}		Hilal et al. (2008)	Q	
	5.1×10^{-2}		Modarresi et al. (2007)	Q	68
		7900	Kühne et al. (2005)	Q	
	5.6×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	3.8×10^{-2}		Katritzky et al. (1998)	Q	
	5.5×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		8500	Kühne et al. (2005)	?	
MCM:C918CHO $C_{10}H_{16}O_2$ GWMMOZICECYZLL-UHFFFAOYSA-N	1.8×10^{1}		Wang et al. (2017)	Q	81, 239
	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
	1.5×10^{1}		Wang et al. (2017)	Q	81, 241
hydroxycitronellal $C_{10}H_{20}O_2$ [107-75-5] WPFVBOQKRVRMJB-UHFFFAOYSA-N	9.4×10^{2}		Dupeux et al. (2022)	Q	260
undecanal $C_{11}H_{22}O$ [112-44-7] KMPQYAYAQWNLME-UHFFFAOYSA-N	7.0×10^{-3}		Yaws (2003)	X	259
	6.9×10^{-3}		Yaws (2003)	X	238
	1.5×10^{-2}		Dupeux et al. (2022)	Q	260
	2.2×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
		8300	Kühne et al. (2005)	Q	
		8300	Kühne et al. (2005)	?	
dodecanal $C_{12}H_{24}O$ [112-54-9] HFJRKMMYBMWEAD-UHFFFAOYSA-N	5.2×10^{-3}		Yaws (2003)	X	259
	5.2×10^{-3}		Yaws (2003)	X	238
	1.2×10^{-2}		Dupeux et al. (2022)	Q	260
	2.3×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
1-tridecanal $C_{13}H_{26}O$ [10486-19-8] BGEHHAVMRVXCGR-UHFFFAOYSA-N	5.8×10^{-3}		Yaws (2003)	X	259
	5.8×10^{-3}		Yaws (2003)	X	238
	9.6×10^{-3}		Dupeux et al. (2022)	Q	260
	2.4×10^{-3}		Gharagheizi et al. (2012)	Q	
	5.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
1-tetradecanal $C_{14}H_{28}O$ [124-25-4] UHUFTBALEZWWIH-UHFFFAOYSA-N	8.0×10^{-4}		Yaws (2003)	X	259
	6.2×10^{-3}		Dupeux et al. (2022)	Q	260
	2.6×10^{-3}		Gharagheizi et al. (2012)	Q	
aquaflora $C_{12}H_{18}O$ [1339119-15-1] BFTAXJRKNXWMMX-UHFFFAOYSA-N	5.2×10^{-1}		Dupeux et al. (2022)	Q	260

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
starfleur $C_{13}H_{24}O$ (3-(4-isobutylcyclohexyl)propanal) [1254940-85-6] XUTZHJNXAOHUTM-UHFFFAOYSA-N	1.4×10^{-1}		Dupeux et al. (2022)	Q	260
MCM:C126CO	8.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{18}O_2$	1.7×10^{2}		Wang et al. (2017)	Q	81, 240
IWMJDJFLMSAAES-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C126OH	2.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_2$	2.1×10^{3}		Wang et al. (2017)	Q	81, 240
PQYIIYBUHROKIY-UHFFFAOYSA-N	4.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C127OH	5.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_3$	7.1×10^{6}		Wang et al. (2017)	Q	81, 240
QHKXYVNBHFONML-UHFFFAOYSA-N	3.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C126CHO	6.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{20}O_2$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
ZDIXDRBTLRZYNM-UHFFFAOYSA-N	4.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C1311OH	4.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_3$	8.3×10^{6}		Wang et al. (2017)	Q	81, 240
CBUCUSJJCJUTML-UHFFFAOYSA-N	6.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C1313OH	7.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_4$	4.3×10^{8}		Wang et al. (2017)	Q	81, 240
XIWFBNXBOAYHAJ-UHFFFAOYSA-N	8.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C136OH	2.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_2$	2.0×10^{3}		Wang et al. (2017)	Q	81, 240
GEHGNVSPJQGFQG-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	81, 241
propenal	1.3×10^{-1}	5500	Burkholder et al. (2019)	L	471
CH_2CHCHO	7.2×10^{-2}	5100	Brockbank (2013)	L	
(acrolein)	7.2×10^{-2}	5100	Snider and Dawson (1985)	M	
[107-02-8]	1.0×10^{-1}		Mackay et al. (2006c)	V	
HGINCPLSRVDWNT-UHFFFAOYSA-N	2.3		Lide and Frederikse (1995)	V	
	1.0×10^{-2}		Mackay et al. (1995)	V	
	7.0×10^{-2}		Hwang et al. (1992)	V	
	1.3×10^{-1}		Suntio et al. (1988)	V	12
	1.0×10^{-1}	3800	Goldstein (1982)	X	299
	2.2		Howard (1989)	X	414
	8.1×10^{-2}		Gaffney and Senum (1984)	X	391
	1.8×10^{-1}		Suntio et al. (1988)	C	12
	1.4×10^{-1}		Ryan et al. (1988)	C	
	1.2×10^{-1}		Keshavarz et al. (2022)	Q	
	3.5×10^{-1}		Duchowicz et al. (2020)	Q	
	2.2×10^{-1}		Wang et al. (2017)	Q	81, 239

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.9×10^{-1}		Wang et al. (2017)	Q	81, 240
	2.1×10^{-1}		Wang et al. (2017)	Q	81, 241
	5.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	9.5×10^{-2}		Hilal et al. (2008)	Q	
	6.3×10^{-1}		Modarresi et al. (2007)	Q	68
		4600	Kühne et al. (2005)	Q	
	8.1×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	7.5×10^{-2}		Mackay et al. (2006c)	?	21
		3800	Kühne et al. (2005)	?	
	1.2×10^{-1}		Yaws (1999)	?	21, 12
2-methylpropenal	4.5×10^{-2}	4600	Burkholder et al. (2019)	L	
C_4H_6O	6.4×10^{-2}		Burkholder et al. (2015)	L	
(methacrolein)	4.5×10^{-2}	4600	Brockbank (2013)	L	
[78-85-3]	4.8×10^{-2}	4300	Ji and Evans (2007)	M	
STNJBCKSHOAVAJ-UHFFFAOYSA-N	6.4×10^{-2}		Iraci et al. (1999)	M	
	4.2×10^{-2}	5300	Allen et al. (1998)	M	
	5.2×10^{-2}		HSDB (2015)	V	
	4.7×10^{-2}		Yaws (2003)	X	259
	4.7×10^{-2}		Yaws (2003)	X	238
	7.3×10^{-2}		Dupeux et al. (2022)	Q	260
	1.6×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.5×10^{-1}		Wang et al. (2017)	Q	81, 239
	1.4×10^{-1}		Wang et al. (2017)	Q	81, 240
	8.3×10^{-2}		Wang et al. (2017)	Q	81, 241
	1.6×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	4.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
	9.5×10^{-2}		Hilal et al. (2008)	Q	
	1.1×10^{-1}		Modarresi et al. (2007)	Q	68
		4000	Kühne et al. (2005)	Q	
	4.3×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		4800	Kühne et al. (2005)	?	
	4.8×10^{-2}		Yaws (1999)	?	21

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-butenal	5.9×10^{-1}	3600	Goldstein (1982)	X	299
$CH_3CHCHCHO$	5.0×10^{-1}		Gaffney and Senum (1984)	X	391
(crotonaldehyde)	2.9×10^{-1}		Wang et al. (2017)	Q	81, 239
[4170-30-3]	1.6×10^{-1}		Wang et al. (2017)	Q	81, 240
MLUCVPSAIODCQM-UHFFFAOYSA-N	1.6		Wang et al. (2017)	Q	81, 241
	9.7×10^{-2}		Hilal et al. (2008)	Q	
	3.9×10^{-1}		Modarresi et al. (2007)	Q	68
			Burkholder et al. (2019)	W	472
(*E*)-2-butenal	5.4×10^{-1}	5300	Brockbank (2013)	L	1
$CH_3CHCHCHO$	5.0×10^{-1}		Buttery et al. (1971)	M	
(*trans*-crotonaldehyde)	4.4×10^{-2}		Mackay et al. (2006c)	V	
[123-73-9]	4.4×10^{-2}		Mackay et al. (1995)	V	
MLUCVPSAIODCQM-NSCUHMNNSA-N	7.6×10^{-1}		Yaws (2003)	X	259
	1.5		Dupeux et al. (2022)	Q	260
	1.6×10^{-1}		Keshavarz et al. (2022)	Q	
	1.2×10^{-1}		Duchowicz et al. (2020)	Q	300
	3.9×10^{-1}		Modarresi et al. (2007)	Q	68
		5000	Kühne et al. (2005)	Q	
	5.2×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.7×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	3.1×10^{-1}		Suzuki et al. (1992)	Q	233
	5.1×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		4300	Kühne et al. (2005)	?	
	5.9×10^{-1}		Yaws (1999)	?	21, 12
	5.1×10^{-1}		Abraham et al. (1990)	?	
2-hexenal	3.0×10^{-1}		Keshavarz et al. (2022)	Q	
$C_3H_7CHCHCHO$	1.2×10^{-1}		Duchowicz et al. (2020)	Q	
[505-57-7]	6.2×10^{-2}		Hilal et al. (2008)	Q	
MBDOYVRWFFCFHM-UHFFFAOYSA-N	2.5×10^{-1}		Modarresi et al. (2007)	Q	68
	8.6×10^{-2}		English and Carroll (2001)	Q	231, 261
	2.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
(*E*)-2-hexenal	1.4×10^{-1}		Karl et al. (2003)	M	
$C_3H_7CHCHCHO$	9.0×10^{-1}	5700	Meynier et al. (2003)	M	38
(*trans*-2-hexenal)	2.0×10^{-1}		Buttery et al. (1971)	M	
[6728-26-3]	2.0×10^{-1}		Meynier et al. (2003)	C	
MBDOYVRWFFCFHM-SNAWJCMRSA-N	2.1×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	1.7×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.8×10^{-1}		Suzuki et al. (1992)	Q	233

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(*E*,*E*)-2,4-hexadienal $CH_3CHCHCHCHCHO$ (*trans-trans*-2,4-hexadienal) [142-83-6] BATOPAZDIZEVQF-MQQKCMAXSA-N	1.0		Buttery et al. (1971)	M	
	3.0×10^{-1}		Keshavarz et al. (2022)	Q	
	1.4×10^{-1}		Duchowicz et al. (2020)	Q	185
	3.9×10^{-1}		Hilal et al. (2008)	Q	
	4.7×10^{-1}		Modarresi et al. (2007)	Q	68
	1.5		Suzuki et al. (1992)	Q	233
	1.0		Duchowicz et al. (2020)	?	186, 21
2-heptenal $C_7H_{12}O$ [2463-63-0] NDFKTBCGKNOHPJ-UHFFFAOYSA-N	5.0×10^{-2}		Hilal et al. (2008)	Q	
(*E*)-2-heptenal $C_7H_{12}O$ (*trans*-2-heptenal) [18829-55-5] NDFKTBCGKNOHPJ-AATRIKPKSA-N	1.3		Abney (2021)	Q	401
(*Z*)-4-heptenal $C_7H_{12}O$ (*cis*-4-heptenal) [6728-31-0] VVGOCOMZRGWHPI-ARJAWSKDSA-N	8.8×10^{-2}		Straver and de Loos (2005)	M	
2-octenal $C_8H_{14}O$ [2363-89-5] LVBXEMGDVWVTGY-UHFFFAOYSA-N	7.1×10^{-2}		Keshavarz et al. (2022)	Q	
	1.2×10^{-1}		Duchowicz et al. (2020)	Q	300
	4.1×10^{-2}		Hilal et al. (2008)	Q	
	1.9×10^{-1}		Modarresi et al. (2007)	Q	68
	5.2×10^{-2}		English and Carroll (2001)	Q	231, 232
	1.3×10^{-1}		Duchowicz et al. (2020)	?	186, 21
(*E*)-2-octenal $C_8H_{14}O$ (*trans*-2-octenal) [2548-87-0] LVBXEMGDVWVTGY-VOTSOKGWSA-N	1.3×10^{-1}		Buttery et al. (1971)	M	
	1.4×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	1.0×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.1×10^{-1}		Suzuki et al. (1992)	Q	233
			Betterton (1992)	W	473
2-ethyl-2-hexenal $C_8H_{14}O$ [645-62-5] PYLMCYQHBRSDND-UHFFFAOYSA-N	5.2×10^{-2}	5800	Brockbank (2013)	L	
(*E*)-2-nonenal $C_9H_{16}O$ (*trans*-2-nonenal) [18829-56-6] BSAIUMLZVGUGKX-BQYQJAHWSA-N	5.8×10^{-2}		Roberts and Pollien (1997)	M	

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
trans-2,*cis*-6-nonadienal $C_9H_{14}O$ [557-48-2] HZYHMHHBBBSGHB-ODYTWBPASA-N	8.2×10^{-2}	7100	Ömür-Özbek and Dietrich (2005)	M	
3,7-dimethyl-6-octenal $C_{10}H_{18}O$ (citronellal) [106-23-0] NEHNMFOYXAPHSD-UHFFFAOYSA-N	2.5×10^{-2} 3.8×10^{-2}	4500	van Roon et al. (2005) HSDB (2015)	V Q	 100
3,7-dimethyl-2,6-octadienal $C_{10}H_{16}O$ (citral) [5392-40-5] WTEVQBCEXWBHNA-UHFFFAOYSA-N	2.9×10^{-1} 5.2 2.3×10^{-1}	6700	Wu et al. (2022b) Dupeux et al. (2022) HSDB (2015)	M Q Q	 260 100
tillenal $C_{11}H_{18}O$ (3-(4,4-dimethyl-1-cyclohexen-1-yl)propanal) [850997-10-3] IHMKWBJKOWYASH-UHFFFAOYSA-N	3.4×10^{-1}		Dupeux et al. (2022)	Q	260
lilybelle $C_{12}H_{20}O$ [1378867-81-2] VZZSYXAVGYODQG-UHFFFAOYSA-N	4.5×10^{-1}		Dupeux et al. (2022)	Q	260
mugoxal $C_{13}H_{22}O$ (3-(4-*tert*-butylcyclohexen-1-yl)propanal) WGWWNPFQPHLSIM-UHFFFAOYSA-N	6.7×10^{-1}		Dupeux et al. (2022)	Q	260
orange oil $C_{15}H_{22}O$ [8028-48-6] NOPLRNXKHZRXHT-UHFFFAOYSA-N	6.3×10^{-4}		Maniere et al. (2011)	?	242, 166
benzaldehyde C_6H_5CHO [100-52-7] HUMNYLRZRPPJDN-UHFFFAOYSA-N	4.0×10^{-1} 3.8×10^{-1} 3.9×10^{-1} 3.2×10^{-1} 3.4×10^{-1} 3.5×10^{-1} 4.2×10^{-1} 3.7×10^{-1} 1.6×10^{-1} 1.6×10^{-1}	5200 5500 4800 6300 7000 4600 5100	Brockbank (2013) Staudinger and Roberts (2001) Staudinger and Roberts (1996) Allou et al. (2011) Souchon et al. (2004) Allen et al. (1998) Zhou and Mopper (1990) Betterton and Hoffmann (1988) Mackay et al. (2006c) Mackay et al. (1995)	L L L M M M M M V V	1, 474 458 462

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.6×10^{-1}		Hine and Mookerjee (1975)	V	
	3.5×10^{-1}	5400	Bagno et al. (1991)	T	475
	3.9×10^{-1}		Yaws (2003)	X	259
	3.6×10^{-1}		Gaffney and Senum (1984)	X	391
	3.7×10^{-1}		Schüürmann (2000)	C	21
	8.4×10^{-1}		Dupeux et al. (2022)	Q	260
	5.3×10^{-2}		Keshavarz et al. (2022)	Q	
	6.6×10^{-1}		Duchowicz et al. (2020)	Q	185
	3.0		Wang et al. (2017)	Q	81, 239
	1.3		Wang et al. (2017)	Q	81, 240
	1.6		Wang et al. (2017)	Q	81, 241
	3.6×10^{-1}		Li et al. (2014)	Q	242
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	7.7×10^{-1}		Hilal et al. (2008)	Q	
	1.2		Modarresi et al. (2007)	Q	68
	2.6×10^{-2}		Emel'yanenko et al. (2007)	Q	417
	2.6×10^{-2}		Hertel and Sommer (2006)	Q	417
		5800	Kühne et al. (2005)	Q	
	3.7×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	5.4×10^{-1}		English and Carroll (2001)	Q	231, 275
	2.4×10^{-1}		Katritzky et al. (1998)	Q	
	7.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	3.6×10^{-1}		Suzuki et al. (1992)	Q	233
	3.7×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	4.4×10^{-1}		Mackay et al. (2006c)	?	21
		5400	Kühne et al. (2005)	?	
	4.0×10^{-1}		Yaws (1999)	?	21
	3.6×10^{-1}		Abraham et al. (1990)	?	
phenylacetaldehyde	1.6		Dupeux et al. (2022)	Q	260
$C_6H_5CH_2CHO$	2.8		Wang et al. (2017)	Q	81, 239
[122-78-1]	3.6		Wang et al. (2017)	Q	81, 240
DTUQWGWMVIHBKE-UHFFFAOYSA-N	3.6		Wang et al. (2017)	Q	81, 241
	1.0×10^{-1}		Emel'yanenko et al. (2007)	Q	417
	1.0×10^{-1}		Hertel and Sommer (2005)	Q	417
2-methylbenzaldehyde	3.1×10^{-1}	6900	Ji et al. (2008)	M	
C_8H_8O	1.9		Wang et al. (2017)	Q	81, 239
(*o*-tolualdehyde)	1.7		Wang et al. (2017)	Q	81, 240
[529-20-4]	8.7×10^{-1}		Wang et al. (2017)	Q	81, 241
BTFQKIATRPGRBS-UHFFFAOYSA-N	3.3×10^{-1}		HSDB (2015)	Q	100

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methylbenzaldehyde	3.5×10^{-1}	7200	Brockbank (2013)	L	
C_8H_8O	3.0×10^{-1}	5800	Wu et al. (2022b)	M	
(*m*-tolualdehyde)	3.5×10^{-1}	7200	Ji et al. (2008)	M	
[620-23-5]	1.9		Wang et al. (2017)	Q	81, 239
OVWYEQOVUDKZNU-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 240
	1.7		Wang et al. (2017)	Q	81, 241
	3.3×10^{-1}		HSDB (2015)	Q	100
4-methylbenzaldehyde	5.3×10^{-1}	7200	Brockbank (2013)	L	
C_8H_8O	4.6×10^{-1}	6400	Wu et al. (2022b)	M	
(*p*-tolualdehyde)	5.3×10^{-1}	7200	Ji et al. (2008)	M	
[104-87-0]	5.7×10^{-1}		Duchowicz et al. (2020)	V	187
FXLOVSHXALFLKQ-UHFFFAOYSA-N	5.8×10^{-1}		HSDB (2015)	V	
	5.4×10^{-1}		Abraham et al. (1994a)	R	
	3.3×10^{-1}		Duchowicz et al. (2020)	Q	
	1.9		Wang et al. (2017)	Q	81, 239
	1.3		Wang et al. (2017)	Q	81, 240
	3.0		Wang et al. (2017)	Q	81, 241
	7.9×10^{-1}		Hilal et al. (2008)	Q	
	5.3×10^{-1}		Modarresi et al. (2007)	Q	68
	4.8×10^{-1}		English and Carroll (2001)	Q	231, 232
	6.5×10^{-1}		Katritzky et al. (1998)	Q	
	5.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	5.6×10^{-1}		Yaws (1999)	?	21
terephthaldialdehyde $C_8H_6O_2$ [623-27-8] KUCOHFSKRZZVRO-UHFFFAOYSA-N	1.6×10^{1}		Abraham et al. (2019)	Q	
2-hydroxybenzaldehyde	1.1	6200	Ji et al. (2008)	M	
$C_6H_4(OH)CHO$	1.8		Duchowicz et al. (2020)	V	187
(2-formylphenol; salicylaldehyde)	4.6		Duchowicz et al. (2020)	Q	
[90-02-8]	4.0×10^{3}		McFall et al. (2020)	Q	476
SMQUZDBALVYZAC-UHFFFAOYSA-N	6.2		Raventos-Duran et al. (2010)	Q	272, 244
	9.9		Raventos-Duran et al. (2010)	Q	245
	6.2		Raventos-Duran et al. (2010)	Q	246
	1.6×10^{1}		Hilal et al. (2008)	Q	
	1.8		Yaws (1999)	?	21, 477
3-hydroxybenzaldehyde	3.9×10^{3}		Gaffney and Senum (1984)	X	391
$C_6H_4(OH)CHO$	9.6×10^{3}		Keshavarz et al. (2022)	Q	
(3-formylphenol)	1.8×10^{4}		Duchowicz et al. (2020)	Q	300
[100-83-4]	1.2×10^{3}		Raventos-Duran et al. (2010)	Q	243, 244
IAVREABSGIHHMO-UHFFFAOYSA-N	1.6×10^{4}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{3}		Raventos-Duran et al. (2010)	Q	246
	5.3×10^{3}		Hilal et al. (2008)	Q	
	7.9×10^{2}		Modarresi et al. (2007)	Q	68

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{3}		Katritzky et al. (1998)	Q	
	3.0×10^{4}		Nirmalakhandan et al. (1997)	Q	
	3.9×10^{3}		Duchowicz et al. (2020)	?	186, 21
	3.8×10^{3}		Abraham et al. (1990)	?	
4-hydroxybenzaldehyde	1.9×10^{4}	8600	Parsons et al. (1971)	T	419
$C_6H_4(OH)CHO$	9.6×10^{3}		Keshavarz et al. (2022)	Q	
(4-formylphenol)	2.1×10^{4}		Duchowicz et al. (2020)	Q	
[123-08-0]	1.2×10^{3}		Gharagheizi et al. (2012)	Q	
RGHHSNMVTDWUBI-UHFFFAOYSA-N	1.2×10^{3}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{3}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{3}		Raventos-Duran et al. (2010)	Q	246
	8.8×10^{2}		Hilal et al. (2008)	Q	
	1.6×10^{3}		Modarresi et al. (2007)	Q	68
	3.0×10^{4}		Nirmalakhandan et al. (1997)	Q	
	1.9×10^{4}		Duchowicz et al. (2020)	?	186, 21
	1.9×10^{4}		Abraham et al. (1990)	?	
2-methoxybenzaldehyde	1.0×10^{1}	8900	Ji et al. (2008)	M	
$C_8H_8O_2$					
[135-02-4]					
PKZJLOCLABXVMC-UHFFFAOYSA-N					
3-methoxybenzaldehyde	5.1	8800	Ji et al. (2008)	M	
$C_8H_8O_2$					
[591-31-1]					
WMPDAIZRQDCGFH-UHFFFAOYSA-N					
4-methoxybenzaldehyde	2.4×10^{1}	8700	Ji et al. (2008)	M	
$C_8H_8O_2$					
[123-11-5]					
ZRSNZINYAWTAHE-UHFFFAOYSA-N					
3-phenyl-2-propenal	2.8		HSDB (2015)	V	
C_9H_8O	1.4	6300	van Roon et al. (2005)	V	
(cinnamaldehyde)					
[104-55-2]					
KJPRLNWUNMBNBZ-QPJJXVBHSA-N					
2,3-dimethylbenzaldehyde	1.2		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O$	2.1		Wang et al. (2017)	Q	81, 240
[5779-93-1]	7.6×10^{-1}		Wang et al. (2017)	Q	81, 241
UIFVCPMLQXKEEU-UHFFFAOYSA-N					
3,4-dimethylbenzaldehyde	1.2		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O$	1.5		Wang et al. (2017)	Q	81, 240
[5973-71-7]	3.8		Wang et al. (2017)	Q	81, 241
POQJHLBMLVTHAU-UHFFFAOYSA-N					

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,5-dimethylbenzaldehyde $C_9H_{10}O$ [5779-95-3] NBEFMISJJNGCIZ-UHFFFAOYSA-N	1.2 9.6×10^{-1} 2.0		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
2-naphthaldehyde $C_{11}H_8O$ [66-99-9] PJKVFARRVXDXAD-UHFFFAOYSA-N	6.0×10^{1}		Abraham et al. (2019)	Q	
cyclemax $C_{12}H_{16}O$ (4-(1-methylethyl)-benzenepropanal) [7775-00-0] RLEFOSDUWZYGOS-UHFFFAOYSA-N	7.8×10^{-1}		Dupeux et al. (2022)	Q	260
bourgeonal $C_{13}H_{18}O$ [18127-01-0] FZJUFJKVIYFBSY-UHFFFAOYSA-N	1.1		Dupeux et al. (2022)	Q	260
florhydral $C_{13}H_{18}O$ [125109-85-5] OHRBQTOZYGEWCJ-UHFFFAOYSA-N	4.9×10^{-1}		Dupeux et al. (2022)	Q	260
cyclamen aldehyde $C_{13}H_{18}O$ [103-95-7] ZFNVDHOSLNRHNN-UHFFFAOYSA-N	2.3×10^{-1}		Dupeux et al. (2022)	Q	260
mimosal $C_{13}H_{16}O$ (4-methyl-5-(4-methylphenyl)pent-4-enal) [1226911-69-8] LBKHGAIELUNYML-ZRDIBKRKSA-N	4.9		Dupeux et al. (2022)	Q	260
lilial $C_{14}H_{20}O$ [80-54-6] SDQFDHOLCGWZPU-UHFFFAOYSA-N	5.7×10^{-1}		Dupeux et al. (2022)	Q	260
hivernal $C_{14}H_{18}O$ [300371-33-9] GEPCDOWRWODJEY-UHFFFAOYSA-N	2.2		Dupeux et al. (2022)	Q	260

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
silvial $C_{14}H_{20}O$ [6658-48-6] YLIXVKUWWOQREC-UHFFFAOYSA-N	2.9×10^{-1}		Dupeux et al. (2022)	Q	260
mefloral $C_{14}H_{20}O$ [62518-65-4] GLZRHVTZLDNUQP-UHFFFAOYSA-N	3.2×10^{-1}		Dupeux et al. (2022)	Q	260
nympheal $C_{14}H_{20}O$ (3-(4-isobutyl-2-methylphenyl)propanal) [1637294-12-2] UKZXPOJABTXLMK-UHFFFAOYSA-N	8.2×10^{-1}		Dupeux et al. (2022)	Q	260
hexyl cinnamic aldehyde $C_{15}H_{20}O$ [101-86-0] GUUHFMWKWLOQMM-UHFFFAOYSA-N	1.0		Dupeux et al. (2022)	Q	260
α-amyl cinnamaldehyde $C_{14}H_{18}O$ [122-40-7] HMKKIXGYKWDQSV-KAMYIIQDSA-N	1.3		HSDB (2015)	Q	449
MCM:HCOCH2CO3H $C_3H_4O_4$ CFPRXLWZTODTLN-UHFFFAOYSA-N	8.0×10^{4} 3.6×10^{3} 3.2×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:PROPALOOH $C_3H_6O_3$ UTLVMFCPERHVKU-UHFFFAOYSA-N	6.9×10^{3} 8.7×10^{1} 3.6×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:BUTALAOOH $C_4H_8O_3$ UBMPIIYSSVMXGT-UHFFFAOYSA-N	5.5×10^{3} 4.6×10^{1} 1.2×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:BUTALO2H $C_4H_8O_3$ HFNSAVKBHMZYBR-UHFFFAOYSA-N	5.5×10^{3} 2.7×10^{3} 8.7×10^{2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:C3MDIALOOH $C_4H_6O_4$ WJWKLOFSCXWKQD-UHFFFAOYSA-N	3.0×10^{6} 4.7×10^{3} 7.3		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:CHOC2CO3H $C_4H_6O_4$ ZCKJJZIUFVHIST-UHFFFAOYSA-N	7.1×10^{4} 1.1×10^{4} 1.9×10^{2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:IBUTALBO2H	5.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	3.6×10^{3}		Wang et al. (2017)	Q	81, 240
OSYMKIVGDGNGKG-UHFFFAOYSA-N	5.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:IBUTALO2H	3.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	1.8×10^{1}		Wang et al. (2017)	Q	81, 240
UINKREZTGVLFAU-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MALDALCO3H	2.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_4$	3.5×10^{4}		Wang et al. (2017)	Q	81, 240
QFBRACYMKXGFRM-UHFFFAOYSA-N	3.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PRPAL2CO3H	7.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_4$	2.3×10^{3}		Wang et al. (2017)	Q	81, 240
IGHWWGZEWMXWCB-UHFFFAOYSA-N	8.0		Wang et al. (2017)	Q	81, 241
MCM:C3EDIALOOH	2.7×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	2.1×10^{3}		Wang et al. (2017)	Q	81, 240
IOKXWRCVGKGMQG-UHFFFAOYSA-N	4.9		Wang et al. (2017)	Q	81, 241
MCM:C3M3CHOOOH	3.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	8.7×10^{2}		Wang et al. (2017)	Q	81, 240
FJYKIGXUSFRBER-UHFFFAOYSA-N	3.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C4CHOAOOH	4.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	3.0×10^{1}		Wang et al. (2017)	Q	81, 240
ZCMMOPXACREGKB-UHFFFAOYSA-N	6.3		Wang et al. (2017)	Q	81, 241
MCM:C4CHOBOOH	4.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	1.5×10^{3}		Wang et al. (2017)	Q	81, 240
JELNOURJPXUYRE-UHFFFAOYSA-N	3.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C4CODBCO3H	2.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_4$	4.2×10^{4}		Wang et al. (2017)	Q	81, 240
JLZDPUBRQDSTHL-UHFFFAOYSA-N	6.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C514OOH	4.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	2.0×10^{6}		Wang et al. (2017)	Q	81, 240
PUFIIBDSTKVRQR-UHFFFAOYSA-N	6.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C5DIALOOH	1.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_4$	7.3×10^{4}		Wang et al. (2017)	Q	81, 240
MJFLAVCETRHPDB-UHFFFAOYSA-N	3.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:CHOC4OOH	4.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	5.3×10^{3}		Wang et al. (2017)	Q	81, 240
CTZAXNMAMSERLK-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CO1M22CO3H	4.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	8.0×10^{2}		Wang et al. (2017)	Q	81, 240
HHOOHNHNSGMLRV-UHFFFAOYSA-N	8.9		Wang et al. (2017)	Q	81, 241

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:IC4CHOAOOH	5.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	3.8×10^{1}		Wang et al. (2017)	Q	81, 240
MEJCTHPUJKQILI-UHFFFAOYSA-N	8.3		Wang et al. (2017)	Q	81, 241
MCM:MC3ODBCO3H	2.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_4$	3.9×10^{4}		Wang et al. (2017)	Q	81, 240
UTZOYJZISPOIDM-UHFFFAOYSA-N	3.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C522CO3H	1.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	8.0×10^{3}		Wang et al. (2017)	Q	81, 240
NCACXMVSAKPDND-UHFFFAOYSA-N	1.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C615OOH	2.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	2.2×10^{4}		Wang et al. (2017)	Q	81, 240
XHCYBISQWAKVQU-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C6DIALOOH	3.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	1.5×10^{6}		Wang et al. (2017)	Q	81, 240
UGGYJIUZOSPDSO-UHFFFAOYSA-N	5.4×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:CHOC4CO3H	4.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	3.7×10^{3}		Wang et al. (2017)	Q	81, 240
RHHSYYPMFOTTRH-UHFFFAOYSA-N	6.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO1C6OOH	3.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	3.4×10^{3}		Wang et al. (2017)	Q	81, 240
HEPNQRDDKATRCQ-UHFFFAOYSA-N	8.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C615CO3H	3.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	3.4×10^{5}		Wang et al. (2017)	Q	81, 240
DXQJLRIPGQOCBO-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C729OOH	7.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_3$	2.6×10^{3}		Wang et al. (2017)	Q	81, 240
PQESPNYRBXTFKD-UHFFFAOYSA-N	4.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C729CO3H	7.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
MJXLYBJUYDBXAC-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C810OOH	1.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_4$	5.5×10^{5}		Wang et al. (2017)	Q	81, 240
YJCLQCSGAKCWEJ-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C822OOH	8.8×10^{3}	11000	Wieser et al. (2023)	Q	439
$C_8H_{14}O_3$	6.0×10^{3}		Wang et al. (2017)	Q	81, 239
XWYULULFGKWPMD-UHFFFAOYSA-N	2.8×10^{3}		Wang et al. (2017)	Q	81, 240
	1.1×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C830OOH	6.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_3$	4.4×10^{3}		Wang et al. (2017)	Q	81, 240
QPQAMUJVCCDVQB-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C831OOH	1.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_4$	3.0×10^{5}		Wang et al. (2017)	Q	81, 240
IGXVNESWPQHYEP-UHFFFAOYSA-N	3.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C89OOH	6.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_3$	4.4×10^{3}		Wang et al. (2017)	Q	81, 240
TYPKFPBYWMWINI-UHFFFAOYSA-N	8.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C822CO3H	1.7×10^{4}	14000	Wieser et al. (2023)	Q	439
$C_9H_{14}O_4$	7.3×10^{4}		Wang et al. (2017)	Q	81, 239
DRDXOQWGQPPQFG-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 240
	3.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C830CO3H	7.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	2.8×10^{3}		Wang et al. (2017)	Q	81, 240
YIGLTTCQERBPNX-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C89CO3H	7.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	2.9×10^{3}		Wang et al. (2017)	Q	81, 240
QJRQWHYQDGSSTJ-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C126OOH	7.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_3$	4.9×10^{3}		Wang et al. (2017)	Q	81, 240
KEVCPNVRIXMZTI-UHFFFAOYSA-N	1.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C126CO3H	8.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{20}O_4$	1.9×10^{3}		Wang et al. (2017)	Q	81, 240
OZAZBNTYEOZXRC-UHFFFAOYSA-N	2.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C136OOH	5.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_3$	4.3×10^{3}		Wang et al. (2017)	Q	81, 240
MAMVWZJYPZZMSJ-UHFFFAOYSA-N	4.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C136CO3H	6.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_4$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
JKRMUSIUVDAEPW-UHFFFAOYSA-N	7.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HCOCOHCO3H	2.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_3H_4O_5$	1.3×10^{4}		Wang et al. (2017)	Q	81, 240
DIZMXPJJIVKAJT-UHFFFAOYSA-N	6.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HOCHOCOOH	2.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_4$	1.3×10^{5}		Wang et al. (2017)	Q	81, 240
GWWSSJVARZQKFN-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:OCCOHCOOH	1.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_4$	5.9×10^{4}		Wang et al. (2017)	Q	81, 240
UFAXCNDNIIDPQE-UHFFFAOYSA-N	2.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C4OCCOHOOH	1.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	1.2×10^{5}		Wang et al. (2017)	Q	81, 240
JJIHBDXOHFOUDV-UHFFFAOYSA-N	7.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:COCCOHCOOH	2.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	2.0×10^{5}		Wang et al. (2017)	Q	81, 240
XTEYRSCVGRLIOG-UHFFFAOYSA-N	8.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:COHM2CO3H	1.7×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_5$	4.6×10^{3}		Wang et al. (2017)	Q	81, 240
AEAZUHMXWJBPCW-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HMACROOH	3.9×10^{10}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_5$	2.4×10^{8}		Wang et al. (2017)	Q	81, 240
AWITZWJPGUOCMB-UHFFFAOYSA-N	4.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:MACROHOOH	6.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	7.1×10^{4}		Wang et al. (2017)	Q	81, 240
HWQXXVVDRNBYQB-UHFFFAOYSA-N	6.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:MACROOH	1.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	7.6×10^{4}		Wang et al. (2017)	Q	81, 240
MOSGWPXPTZVSII-UHFFFAOYSA-N	5.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MALDIALOOH	1.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_5$	6.2×10^{6}		Wang et al. (2017)	Q	81, 240
MNYHDFHIZDEDLP-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:ALC4DOLOOH	1.6×10^{10}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_5$	3.8×10^{8}		Wang et al. (2017)	Q	81, 240
BTJWWKUWEVGVGA-UHFFFAOYSA-N	5.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C4MALOHOOH	5.6×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	6.6×10^{6}		Wang et al. (2017)	Q	81, 240
NJMKFLHNNBFYIH-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C57OOH	1.3×10^{10}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_5$	8.5×10^{7}		Wang et al. (2017)	Q	81, 240
VJGRRPOTERGJKF-UHFFFAOYSA-N	1.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C58OOH	1.9×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_5$	3.7×10^{8}		Wang et al. (2017)	Q	81, 240
MTCQYLXAFMKVMT-UHFFFAOYSA-N	3.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:CHOC4OHOOH	1.5×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	1.4×10^{6}		Wang et al. (2017)	Q	81, 240
LTZYUHWRVSINRM-UHFFFAOYSA-N	1.6×10^{5}		Wang et al. (2017)	Q	81, 241

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HIEB1OOH	3.7×10^{13}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_6$	1.6×10^{11}		Wang et al. (2017)	Q	81, 240
COFCBVJXHDFSHS-UHFFFAOYSA-N	6.5×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:HIEB2OOH	2.4×10^{13}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_6$	1.0×10^{11}		Wang et al. (2017)	Q	81, 240
PKIUCWJPHHVKPZ-UHFFFAOYSA-N	1.2×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:HOC4CHOOOH	1.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	6.9×10^{5}		Wang et al. (2017)	Q	81, 240
LRYOXTYJCQGVIC-UHFFFAOYSA-N	1.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:IEB2OOH	1.3×10^{10}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_5$	3.7×10^{8}		Wang et al. (2017)	Q	81, 240
MCOKLECUTPXNOW-UHFFFAOYSA-N	2.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C1H4C5CO3H	1.6×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	5.9×10^{7}		Wang et al. (2017)	Q	81, 240
DOEHHISPDHWTCR-UHFFFAOYSA-N	2.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C623OOH	2.8×10^{10}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_5$	7.4×10^{8}		Wang et al. (2017)	Q	81, 240
OGBKQGQRAMSXTF-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C67OOH	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	4.2×10^{5}		Wang et al. (2017)	Q	81, 240
ONTGLCVTLGTTQS-UHFFFAOYSA-N	9.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C68OOH	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	4.6×10^{5}		Wang et al. (2017)	Q	81, 240
ITDKDNQPTMKBIM-UHFFFAOYSA-N	3.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CO1H63OOH	1.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	1.8×10^{7}		Wang et al. (2017)	Q	81, 240
KJWILEAANBSBHN-UHFFFAOYSA-N	3.8×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C728OOH	5.3×10^{10}	18000	Wieser et al. (2023)	Q	439
$C_7H_{14}O_5$	2.1×10^{10}		Wang et al. (2017)	Q	81, 239
WJYXJQPIZCIBJO-UHFFFAOYSA-N	1.7×10^{9}		Wang et al. (2017)	Q	81, 240
	1.4×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C730OOH	6.1×10^{10}	18000	Wieser et al. (2023)	Q	439
$C_7H_{14}O_5$	2.1×10^{10}		Wang et al. (2017)	Q	81, 239
YXKHJQXHKYJCPI-UHFFFAOYSA-N	1.1×10^{10}		Wang et al. (2017)	Q	81, 240
	2.6×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C824OOH	8.4×10^{6}	15000	Wieser et al. (2023)	Q	439
$C_8H_{14}O_4$	1.9×10^{7}		Wang et al. (2017)	Q	81, 239
FGEKWAMEWUMQIL-UHFFFAOYSA-N	6.3×10^{5}		Wang et al. (2017)	Q	81, 240
	6.3×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C826OOH	6.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_5$	5.1×10^{8}		Wang et al. (2017)	Q	81, 240
MATCTRFTDTXPPO-UHFFFAOYSA-N	1.7×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C127OOH	1.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_4$	1.9×10^{7}		Wang et al. (2017)	Q	81, 240
CZSOPCQUOGQYQQ-UHFFFAOYSA-N	2.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C1311OOH	1.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_4$	1.6×10^{7}		Wang et al. (2017)	Q	81, 240
GNGYVQPBVCXXTM-UHFFFAOYSA-N	1.2×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C1313OOH	6.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_5$	9.1×10^{8}		Wang et al. (2017)	Q	81, 240
ALNYAIDMJTUDIF-UHFFFAOYSA-N	1.9×10^{6}		Wang et al. (2017)	Q	81, 241

A3.6 Ketones (RCOR)

Table A3.6: Ketones (RCOR)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
propanone	2.7×10^{-1}	5500	Burkholder et al. (2019)	L	
CH_3COCH_3	2.7×10^{-1}	5500	Burkholder et al. (2015)	L	
(acetone)	2.9×10^{-1}	5300	Brockbank (2013)	L	1, 478
[67-64-1]	2.7×10^{-1}	5500	Sander et al. (2011)	L	
CSCPPACGZOOCGX-UHFFFAOYSA-N	3.3×10^{-1}	5300	Poulain et al. (2010)	L	
	2.8×10^{-1}	5100	Sander et al. (2006)	L	
	2.6×10^{-1}	5700	Fogg and Sangster (2003)	L	
	2.8×10^{-1}	4800	Staudinger and Roberts (2001)	L	
	2.7×10^{-1}	5000	Plyasunov and Shock (2001)	L	
	3.0×10^{-1}	4600	Staudinger and Roberts (1996)	L	
	2.9×10^{-1}	5100	Poulain et al. (2010)	M	
	3.3×10^{-1}	4500	O'Farrell and Waghorne (2010)	M	
	2.6×10^{-1}	5400	Ji and Evans (2007)	M	
	2.4×10^{-1}	4200	Falabella et al. (2006)	M	11, 340
	2.6×10^{-1}	6400	Strekowski and George (2005)	M	
	2.4×10^{-1}		Straver and de Loos (2005)	M	
	2.4×10^{-1}	4300	Chai et al. (2005)	M	11
	2.7×10^{-1}		Nozière and Riemer (2003)	M	80
	1.0×10^{-1}		Ayuttaya et al. (2001)	M	342
	9.4×10^{-4}		Ayuttaya et al. (2001)	M	343
	5.3×10^{-1}		Ayuttaya et al. (2001)	M	344
	9.6×10^{-2}		Welke et al. (1998)	M	
	2.7×10^{-1}	5300	Benkelberg et al. (1995)	M	
	2.7×10^{-1}		Hoff et al. (1993)	M	
	1.7×10^{-1}		Yu (1992)	M	12
	3.2×10^{-1}	5800	Betterton (1991)	M	
	3.5×10^{-1}	3800	Zhou and Mopper (1990)	M	458
	1.2×10^{-1}		Guitart et al. (1989)	M	14
	1.4×10^{-1}		Hellmann (1987)	M	88
	2.5×10^{-1}	4800	Snider and Dawson (1985)	M	
	3.2×10^{-1}	5400	Schoene and Steinhanses (1985)	M	
	1.9×10^{-1}		Richon et al. (1985)	M	38
	2.6×10^{-1}	5100	Lichtenbelt and Schram (1985)	M	479
	2.0×10^{-1}	7800	Ioffe et al. (1984)	M	
	1.5×10^{-1}		Sato and Nakajima (1979a)	M	14
	2.5×10^{-1}		Vitenberg et al. (1975)	M	
	2.5×10^{-1}		Vitenberg et al. (1974)	M	
	3.2×10^{-1}		Vitenberg et al. (1974)	M	
	2.5×10^{-1}		Buttery et al. (1969)	M	
	3.1×10^{-1}		Nelson and Hoff (1968)	M	298
	2.8×10^{-1}		Burnett (1963)	M	
	1.8×10^{-2}		Abraham and Acree (2007)	V	
	2.6×10^{-1}		Hwang et al. (1992)	V	

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.1×10^{-2}	3100	Djerki and Laub (1988)	V	
	2.4×10^{-1}		Rathbun and Tai (1982)	V	
	3.1×10^{-2}		Hine and Weimar (1965)	R	
	3.0×10^{-1}		Butler and Ramchandani (1935)	R	
	2.5×10^{-1}	4900	Bagno et al. (1991)	T	475
	2.1×10^{-1}		Yaws (2003)	X	259
	2.2×10^{-1}	5000	Schaffer and Daubert (1969)	X	299
	3.0×10^{-2}	3300	Janini and Quaddora (1986)	X	299
	3.0×10^{-1}		Gaffney and Senum (1984)	X	391
	2.7×10^{-1}		Cabani et al. (1981)	C	
	6.1×10^{-1}		Dupeux et al. (2022)	Q	260
	2.6×10^{-1}		Hayer et al. (2022)	Q	20
	1.2×10^{-1}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	6.6×10^{-2}		Wang et al. (2017)	Q	81, 239
	4.3×10^{-1}		Wang et al. (2017)	Q	81, 240
	7.1×10^{-1}		Wang et al. (2017)	Q	81, 241
	2.5×10^{-1}		Li et al. (2014)	Q	242
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	1.4×10^{-1}		Hilal et al. (2008)	Q	
	4.0×10^{-1}		Modarresi et al. (2007)	Q	68
		5500	Kühne et al. (2005)	Q	
	2.5×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.5×10^{-1}		English and Carroll (2001)	Q	231, 232
	2.4×10^{-2}		Katritzky et al. (1998)	Q	
	2.1×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.9×10^{-1}		Suzuki et al. (1992)	Q	233
	2.5×10^{-1}		Taft et al. (1985)	Q	
	2.8×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	2.5×10^{-1}		Mackay et al. (2006c)	?	21
		5100	Kühne et al. (2005)	?	
	1.5×10^{-1}		Yaws (1999)	?	21
	1.8×10^{-1}		Yaws et al. (1998)	?	
	1.6×10^{-1}		Abraham and Weathersby (1994)	?	21
	2.3×10^{-1}		Yaws and Yang (1992)	?	21
	2.5×10^{-1}		Abraham et al. (1990)	?	
propanone-2-13C CH_3COCH_3 (acetone-2-13C) [3881-06-9] CSCPPACGZOOCGX-LBPDFUHNSA-N	3.1×10^{-1}	5300	Hiatt (2013)	M	

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-hydroxypropanone	7.7×10^{1}		Lee and Zhou (1993)	C	88
CH_3COCH_2OH	8.3		Wang et al. (2017)	Q	81, 239
(hydroxyacetone)	1.4×10^{2}		Wang et al. (2017)	Q	81, 240
[116-09-6]	1.9×10^{1}		Wang et al. (2017)	Q	81, 241
XLSMFKSTNGKWQX-UHFFFAOYSA-N					
butanone	1.8×10^{-1}	5700	Burkholder et al. (2019)	L	
$C_2H_5COCH_3$	1.8×10^{-1}	5700	Burkholder et al. (2015)	L	
(methyl ethyl ketone; MEK)	1.8×10^{-1}	5600	Brockbank (2013)	L	1
[78-93-3]	1.8×10^{-1}	5700	Sander et al. (2011)	L	
ZWEHNKRNPOVVGH-UHFFFAOYSA-N	1.8×10^{-1}	5700	Sander et al. (2006)	L	
	1.9×10^{-1}	4600	Fogg and Sangster (2003)	L	
	1.8×10^{-1}	5400	Staudinger and Roberts (2001)	L	
	1.8×10^{-1}	5500	Plyasunov and Shock (2001)	L	
	2.0×10^{-1}	5000	Staudinger and Roberts (1996)	L	
	1.0×10^{-1}		Kim and Kim (2014)	M	
	9.5×10^{-2}		Helburn et al. (2008)	M	
	2.1×10^{-1}	5200	Ji and Evans (2007)	M	
	1.5×10^{-1}	4400	Falabella et al. (2006)	M	11, 340
	2.7×10^{-2}	12000	Strekowski and George (2005)	M	
	1.7×10^{-1}		Straver and de Loos (2005)	M	
	1.5×10^{-1}	4500	Chai et al. (2005)	M	11
			Cheng et al. (2004)	M	330
			Cheng et al. (2003)	M	330
	1.1×10^{-1}		Karl et al. (2003)	M	
	1.3×10^{-1}	4300	Hovorka et al. (2002)	M	11
	9.9×10^{-2}		van Ruth et al. (2002)	M	14
	1.0×10^{-1}		van Ruth and Villeneuve (2002)	M	14, 363
	9.0×10^{-2}		van Ruth et al. (2001)	M	14
	1.6×10^{-1}		Kim et al. (2000)	M	
	1.6×10^{-1}		Welke et al. (1998)	M	
	1.9×10^{-1}		Chaintreau et al. (1995)	M	
	1.4×10^{-1}	4700	Ettre et al. (1993)	M	11
	1.9×10^{-1}	5000	Zhou and Mopper (1990)	M	458
	6.8×10^{-2}	-5100	Ashworth et al. (1988)	M	33, 279
	1.3×10^{-1}		Hellmann (1987)	M	88
	1.8×10^{-1}		Park et al. (1987)	M	
	1.7×10^{-1}	5700	Snider and Dawson (1985)	M	
	1.4×10^{-1}		Hawthorne et al. (1985)	M	
	1.2×10^{-1}		Richon et al. (1985)	M	38
	3.2×10^{-1}		Ioffe et al. (1984)	M	81
	1.0×10^{-1}		Friant and Suffet (1979)	M	38
	9.8×10^{-2}		Sato and Nakajima (1979a)	M	14
	1.8×10^{-1}		Vitenberg et al. (1975)	M	
	1.1×10^{-1}		Vitenberg et al. (1974)	M	
	1.9×10^{-1}		Rohrschneider (1973)	M	

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.1×10^{-1}		Buttery et al. (1969)	M	
	1.1×10^{-2}		Abraham and Acree (2007)	V	
	2.8×10^{-1}		Mackay et al. (2006c)	V	
	2.8×10^{-1}		Mackay et al. (1995)	V	
	2.6×10^{-1}		Hwang et al. (1992)	V	
	8.6×10^{-2}	3700	Djerki and Laub (1988)	V	
	1.6×10^{-1}		Rathbun and Tai (1982)	V	
	7.1×10^{-2}		Hine and Weimar (1965)	R	
	2.1×10^{-1}	5500	Bagno et al. (1991)	T	475
		5500	Della Gatta et al. (1981)	T	
	7.6×10^{-2}		Yaws (2003)	X	259
	7.6×10^{-2}		Yaws (2003)	X	238
	7.1×10^{-2}	5800	Janini and Quaddora (1986)	X	299
	2.3×10^{-1}		Mackay et al. (1995)	C	
	4.1×10^{-1}		Harrison et al. (1993)	C	
	1.9×10^{-1}		Cabani et al. (1981)	C	
	2.3×10^{-1}		Dupeux et al. (2022)	Q	260
	1.8×10^{-1}		Hayer et al. (2022)	Q	20
	1.6×10^{-1}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	5.1×10^{-2}		Wang et al. (2017)	Q	81, 239
	2.5×10^{-1}		Wang et al. (2017)	Q	81, 240
	3.6×10^{-1}		Wang et al. (2017)	Q	81, 241
	2.1×10^{-1}		Li et al. (2014)	Q	242
	2.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	8.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
	1.3×10^{-1}		Hilal et al. (2008)	Q	
	3.0×10^{-1}		Modarresi et al. (2007)	Q	68
		5900	Kühne et al. (2005)	Q	
	1.7×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	1.4×10^{-1}		English and Carroll (2001)	Q	231, 232
	3.0×10^{-2}		Katritzky et al. (1998)	Q	
	1.6×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.5×10^{-1}		Suzuki et al. (1992)	Q	233
	1.7×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	1.0×10^{-1}		Mackay et al. (2006c)	?	21
		5300	Kühne et al. (2005)	?	
	3.3×10^{-1}		Yaws (1999)	?	21
	1.5×10^{-1}		Yaws et al. (1998)	?	
	1.0×10^{-1}		Abraham and Weathersby (1994)	?	21
	3.1×10^{-1}		Betterton (1991)	?	
	2.1×10^{-1}		Abraham et al. (1990)	?	

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
butanone-1,1,1,3,3-d5 $C_2H_5COCH_3$ (methyl ethyl ketone-d5; MEK-d5) [24313-50-6] ZWEHNKRNPOVVGH-PDWRLMEDSA-N	3.7×10^{-1}	8200	Hiatt (2013)	M	
2-pentanone	1.3×10^{-1}	6000	Brockbank (2013)	L	1
$C_3H_7COCH_3$	1.3×10^{-1}	5900	Plyasunov and Shock (2001)	L	
[107-87-9]	1.3×10^{-1}	5900	Hovorka et al. (2019)	M	
XNLICIUVMPYHGG-UHFFFAOYSA-N	1.6×10^{-1}	5700	Ji and Evans (2007)	M	
	1.0×10^{-1}	4600	Falabella et al. (2006)	M	11, 340
	8.6×10^{-2}		Straver and de Loos (2005)	M	
	1.0×10^{-1}	4800	Chai et al. (2005)	M	11
	1.1×10^{-1}		Kim et al. (2000)	M	
	1.2×10^{-1}		Shiu and Mackay (1997)	M	
	9.0×10^{-2}		Hawthorne et al. (1985)	M	
	6.4×10^{-2}		Sato and Nakajima (1979a)	M	14
	1.7×10^{-1}		Vitenberg et al. (1974)	M	
	1.1×10^{-1}		Vitenberg et al. (1974)	M	480
	1.6×10^{-1}		Buttery et al. (1969)	M	
	9.2×10^{-2}		Nelson and Hoff (1968)	M	298
	1.5×10^{-1}		Mackay et al. (2006c)	V	
	5.9×10^{-2}		Philippe et al. (2003)	V	14
	1.5×10^{-1}		Shiu and Mackay (1997)	V	
	1.5×10^{-1}		Mackay et al. (1995)	V	
	2.4×10^{-1}	4300	Djerki and Laub (1988)	V	
	2.6×10^{-1}		Rathbun and Tai (1982)	V	
	3.1×10^{-1}		Amoore and Buttery (1978)	V	
		5900	Della Gatta et al. (1981)	T	
	1.4×10^{-1}		Yaws (2003)	X	259
	9.1×10^{-2}	4600	Janini and Quaddora (1986)	X	299
	1.7×10^{-1}		Mackay et al. (1995)	C	
	2.5×10^{-1}		Dupeux et al. (2022)	Q	260
	8.7×10^{-2}		Hayer et al. (2022)	Q	20
	2.2×10^{-1}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	300
	4.3×10^{-2}		Wang et al. (2017)	Q	81, 239
	1.6×10^{-1}		Wang et al. (2017)	Q	81, 240
	1.8×10^{-1}		Wang et al. (2017)	Q	81, 241
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	1.0×10^{-1}		Hilal et al. (2008)	Q	
	1.7×10^{-1}		Modarresi et al. (2007)	Q	68
		6200	Kühne et al. (2005)	Q	
	1.4×10^{-1}		Yaffe et al. (2003)	Q	249, 273

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.9×10^{-2}		Katritzky et al. (1998)	Q	
	1.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.2×10^{-1}		Russell et al. (1992)	Q	280
	1.2×10^{-1}		Suzuki et al. (1992)	Q	233
	1.2×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	1.6×10^{-1}		Mackay et al. (2006c)	?	21
		6500	Kühne et al. (2005)	?	
	1.4×10^{-1}		Yaws (1999)	?	21
	1.3×10^{-1}		Yaws et al. (1998)	?	
	6.7×10^{-2}		Abraham and Weathersby (1994)	?	21
	1.5×10^{-1}		Abraham et al. (1990)	?	
	3.1×10^{-1}		Mackay and Yeun (1983)	?	
3-pentanone	8.9×10^{-2}	5800	Brockbank (2013)	L	1, 481
$C_2H_5COC_2H_5$	1.1×10^{-1}	6000	Plyasunov and Shock (2001)	L	
(diethyl ketone)	1.1×10^{-1}	5900	Hovorka et al. (2019)	M	
[96-22-0]	2.1×10^{-1}		O'Farrell and Waghorne (2010)	M	
FDPIMTJIUBPUKL-UHFFFAOYSA-N	1.6×10^{-1}	5600	Ji and Evans (2007)	M	
	7.0×10^{-2}		Sato and Nakajima (1979a)	M	14
	9.7×10^{-5}		Saylor et al. (1938)	M	38
	8.4×10^{-2}		Mackay et al. (2006c)	V	
	1.2×10^{-1}		Mackay et al. (1995)	V	
	8.4×10^{-2}		Mackay et al. (1995)	V	
	2.8×10^{-1}		Rathbun and Tai (1982)	V	
	1.3×10^{-1}	6000	Bagno et al. (1991)	T	475
		6000	Della Gatta et al. (1981)	T	
	8.2×10^{-2}		Yaws (2003)	X	259
	8.2×10^{-2}		Yaws (2003)	X	238
	2.0×10^{-1}	9200	Janini and Quaddora (1986)	X	299
	1.1×10^{-1}		Howard (1993)	X	414
	1.3×10^{-1}		Cabani et al. (1981)	C	
	8.6×10^{-2}		Dupeux et al. (2022)	Q	260
	2.2×10^{-1}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	4.3×10^{-2}		Wang et al. (2017)	Q	81, 239
	1.3×10^{-1}		Wang et al. (2017)	Q	81, 240
	6.6×10^{-2}		Wang et al. (2017)	Q	81, 241
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	7.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
	9.2×10^{-2}		Hilal et al. (2008)	Q	
	1.9×10^{-1}		Modarresi et al. (2007)	Q	68
		6200	Kühne et al. (2005)	Q	
	1.4×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	4.3×10^{-2}		Yao et al. (2002)	Q	230

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^{-1}		English and Carroll (2001)	Q	231, 275
	2.7×10^{-2}		Katritzky et al. (1998)	Q	
	1.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	2.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		6800	Kühne et al. (2005)	?	
	8.2×10^{-2}		Yaws (1999)	?	21
	1.2×10^{-1}		Yaws et al. (1998)	?	
	7.3×10^{-2}		Abraham and Weathersby (1994)	?	21
	1.3×10^{-1}		Abraham et al. (1990)	?	
1-cyclopropyl-ethanone	9.5×10^{-1}	5900	Bagno et al. (1991)	T	475
C_5H_8O		5900	Della Gatta et al. (1981)	T	
(cyclopropyl methyl ketone)	2.2×10^{-1}		Keshavarz et al. (2022)	Q	
[765-43-5]	9.9×10^{-2}		Duchowicz et al. (2020)	Q	300
HVCFCNAITDHQFX-UHFFFAOYSA-N	4.8×10^{-1}		Hilal et al. (2008)	Q	
	5.2×10^{-1}		Modarresi et al. (2007)	Q	68
	3.1×10^{-1}		English and Carroll (2001)	Q	231, 275
	6.4×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	9.7×10^{-1}		Duchowicz et al. (2020)	?	186, 21
3-methyl-2-butanone	1.1×10^{-1}	5800	Brockbank (2013)	L	1
$C_5H_{10}O$	9.1×10^{-2}	5700	Plyasunov and Shock (2001)	L	
(isopropyl methyl ketone)	9.3×10^{-2}	5600	Hovorka et al. (2019)	M	
[563-80-4]	1.0×10^{-1}		Duchowicz et al. (2020)	V	187
SYBYTAAJFKOIEJ-UHFFFAOYSA-N	8.7×10^{-2}		HSDB (2015)	V	
	9.6×10^{-2}		Cabani et al. (1981)	V	
	9.0×10^{-2}	5700	Bagno et al. (1991)	T	475
		5700	Della Gatta et al. (1981)	T	
	1.3×10^{-2}		Duchowicz et al. (2020)	Q	
	4.9×10^{-2}		Wang et al. (2017)	Q	81, 239
	1.3×10^{-1}		Wang et al. (2017)	Q	81, 240
	2.5×10^{-1}		Wang et al. (2017)	Q	81, 241
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	8.4×10^{-2}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	68
		5300	Kühne et al. (2005)	Q	
	9.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	6.4×10^{-2}		English and Carroll (2001)	Q	231, 232
	2.5×10^{-2}		Katritzky et al. (1998)	Q	
	1.0×10^{-1}		Nirmalakhandan et al. (1997)	Q	
		7200	Kühne et al. (2005)	?	
	1.1×10^{-1}		Yaws (1999)	?	21
	1.1×10^{-1}		Yaws et al. (1998)	?	
	9.7×10^{-2}		Abraham et al. (1990)	?	

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyclopentanone	1.2	5800	Brockbank (2013)	L	
C_5H_8O	2.8		O'Farrell and Waghorne (2010)	M	
[120-92-3]	8.2×10^{-1}	4900	Hovorka et al. (2002)	M	11
BGTOWKSIORTVQH-UHFFFAOYSA-N	8.2×10^{-1}		Hawthorne et al. (1985)	M	
	7.4×10^{-1}		Keshavarz et al. (2022)	Q	
	2.5×10^{-1}		Duchowicz et al. (2020)	Q	300
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	1.1		Hilal et al. (2008)	Q	
	4.7×10^{-1}		Modarresi et al. (2007)	Q	68
		5800	Kühne et al. (2005)	Q	
	1.0		Yaffe et al. (2003)	Q	249, 250
	7.5×10^{-1}		English and Carroll (2001)	Q	231, 261
	6.9×10^{-2}		Katritzky et al. (1998)	Q	
	7.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	9.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		5600	Kühne et al. (2005)	?	
	1.1		Abraham et al. (1990)	?	
2-hexanone	1.1×10^{-1}	6500	Brockbank (2013)	L	1
$C_6H_{12}O$	9.8×10^{-2}	6300	Plyasunov and Shock (2001)	L	
[591-78-6]	9.9×10^{-2}	6300	Hovorka et al. (2019)	M	
QQZOPKMRPOGIEB-UHFFFAOYSA-N	1.5×10^{-1}	8600	Hiatt (2013)	M	
	7.9×10^{-2}	4800	Falabella et al. (2006)	M	11, 340
	1.1×10^{-1}		Straver and de Loos (2005)	M	
	8.6×10^{-2}	5100	Chai et al. (2005)	M	11
	4.3×10^{-2}		Sato and Nakajima (1979a)	M	14
	1.1×10^{-1}		Duchowicz et al. (2020)	V	187
	1.1×10^{-1}		HSDB (2015)	V	
	1.1×10^{-1}		Mackay et al. (2006c)	V	
	1.1×10^{-1}		Mackay et al. (1995)	V	
	1.0×10^{-1}		Meylan and Howard (1991)	V	
	6.5×10^{-1}	4900	Djerki and Laub (1988)	V	
	1.0×10^{-1}		Cabani et al. (1981)	V	
		6200	Della Gatta et al. (1981)	T	
	1.2×10^{-1}		Yaws (2003)	X	259
	1.0×10^{-1}		Howard (1993)	X	414
	1.7×10^{-1}		Dupeux et al. (2022)	Q	260
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	3.8×10^{-2}		Wang et al. (2017)	Q	81, 239
	1.1×10^{-1}		Wang et al. (2017)	Q	81, 240
	1.7×10^{-1}		Wang et al. (2017)	Q	81, 241
	8.2×10^{-2}		Hilal et al. (2008)	Q	
	1.5×10^{-1}		Modarresi et al. (2007)	Q	68
		6600	Kühne et al. (2005)	Q	
	7.9×10^{-2}		Yaffe et al. (2003)	Q	249, 273

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.4×10^{-2}		English and Carroll (2001)	Q	231, 232
	2.4×10^{-2}		Katritzky et al. (1998)	Q	
	9.2×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	8.5×10^{-2}		Meylan and Howard (1991)	Q	
		6200	Kühne et al. (2005)	?	
	1.2×10^{-1}		Yaws (1999)	?	21
	1.2×10^{-1}		Yaws et al. (1998)	?	
	4.5×10^{-2}		Abraham and Weathersby (1994)	?	21
	1.0×10^{-1}		Abraham et al. (1990)	?	
2-hexanone-1,1,1,3,3-d5 $C_6H_{12}O$ [4840-82-8] QQZOPKMRPOGIEB-ZTIZGVCASA-N	1.7×10^{-1}	9000	Hiatt (2013)	M	
3-hexanone $C_6H_{12}O$ [589-38-8] PFCHFHIRKBAQGU-UHFFFAOYSA-N	7.9×10^{-2}	7100	Brockbank (2013)	L	
	7.5×10^{-2}		Plyasunov and Shock (2001)	L	
	7.6×10^{-2}	6400	Hovorka et al. (2019)	M	
			Dewulf et al. (1999)	M	364
	7.9×10^{-2}		Duchowicz et al. (2020)	V	187
	8.0×10^{-2}		Yaws (2003)	X	238
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	3.8×10^{-2}		Wang et al. (2017)	Q	81, 239
	8.9×10^{-2}		Wang et al. (2017)	Q	81, 240
	1.5×10^{-1}		Wang et al. (2017)	Q	81, 241
	6.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
	6.9×10^{-2}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Modarresi et al. (2007)	Q	68
		6600	Kühne et al. (2005)	Q	
	7.9×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.1×10^{-2}		Katritzky et al. (1998)	Q	
		5800	Kühne et al. (2005)	?	
	8.0×10^{-2}		Yaws (1999)	?	21
	8.0×10^{-2}		Yaws et al. (1998)	?	
3-methyl-2-pentanone $C_6H_{12}O$ [565-61-7] UIHCLUNTQKBZGK-UHFFFAOYSA-N	8.4×10^{-2}		Plyasunov and Shock (2001)	L	
	7.9×10^{-2}	6000	Hovorka et al. (2019)	M	
	1.3×10^{-1}		Duchowicz et al. (2020)	V	187
	1.3×10^{-2}		Duchowicz et al. (2020)	Q	
	4.0×10^{-2}		Wang et al. (2017)	Q	81, 239
	1.1×10^{-1}		Wang et al. (2017)	Q	81, 240
	1.8×10^{-1}		Wang et al. (2017)	Q	81, 241
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	7.3×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-1}		Modarresi et al. (2007)	Q	68

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.6×10^{-2}		Yaws et al. (1998)	?	
4-methyl-2-pentanone	6.9×10^{-2}	6200	Brockbank (2013)	L	1
$(CH_3)_2CHCH_2COCH_3$	6.9×10^{-2}	6000	Plyasunov and Shock (2001)	L	
(methyl isobutyl ketone; MIBK)	6.5×10^{-2}	6000	Hovorka et al. (2019)	M	
[108-10-1]	3.9×10^{-2}		Kim and Kim (2014)	M	
NTIZESTWPVYFNL-UHFFFAOYSA-N	1.0×10^{-1}	8700	Hiatt (2013)	M	
	3.9×10^{-2}		Kim et al. (2000)	M	
	4.7×10^{-2}		Welke et al. (1998)	M	
	4.3×10^{-2}	4600	Kolb et al. (1992)	M	278
	2.2×10^{-2}	110	Ashworth et al. (1988)	M	42, 279
	6.5×10^{-2}		Hellmann (1987)	M	88
	3.1×10^{-2}		Sato and Nakajima (1979a)	M	14
	7.2×10^{-2}		Duchowicz et al. (2020)	V	187
	7.0×10^{-2}		HSDB (2015)	V	
	6.5×10^{-2}		Mackay et al. (2006c)	V	
	6.5×10^{-2}		Mackay et al. (1995)	V	
	7.2×10^{-2}		Hwang et al. (1992)	V	
	1.4×10^{-1}		Rathbun and Tai (1982)	V	
	7.1×10^{-2}		Cabani et al. (1981)	V	
	7.3×10^{-2}		Yaws (2003)	X	259
	1.1×10^{-1}		Howard (1990)	X	414
	1.4×10^{-1}		Dupeux et al. (2022)	Q	260
	1.3×10^{-2}		Duchowicz et al. (2020)	Q	
	4.0×10^{-2}		Wang et al. (2017)	Q	81, 239
	1.3×10^{-1}		Wang et al. (2017)	Q	81, 240
	2.1×10^{-1}		Wang et al. (2017)	Q	81, 241
	8.8×10^{-2}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Modarresi et al. (2007)	Q	68
		6600	Kühne et al. (2005)	Q	
	7.3×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	5.1×10^{-2}		English and Carroll (2001)	Q	231, 261
	1.7×10^{-2}		Katritzky et al. (1998)	Q	
	7.9×10^{-2}		Nirmalakhandan et al. (1997)	Q	
		5700	Kühne et al. (2005)	?	
	7.3×10^{-2}		Yaws (1999)	?	21
	7.2×10^{-2}		Yaws et al. (1998)	?	
	3.2×10^{-2}		Abraham and Weathersby (1994)	?	21
	3.0×10^{-1}		Betterton (1991)	?	
	7.0×10^{-2}		Abraham et al. (1990)	?	

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-3-pentanone	5.3×10^{-2}		Plyasunov and Shock (2001)	L	
$C_6H_{12}O$	5.2×10^{-2}	6100	Hovorka et al. (2019)	M	
[565-69-5]	6.4×10^{-2}		Duchowicz et al. (2020)	V	187
HYTRYEXINDDXJK-UHFFFAOYSA-N	1.3×10^{-2}		Duchowicz et al. (2020)	Q	
	4.0×10^{-2}		Wang et al. (2017)	Q	81, 239
	9.3×10^{-2}		Wang et al. (2017)	Q	81, 240
	1.1×10^{-1}		Wang et al. (2017)	Q	81, 241
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	6.5×10^{-2}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Modarresi et al. (2007)	Q	68
	9.7×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	2.3×10^{-2}		Katritzky et al. (1998)	Q	
	6.4×10^{-2}		Yaws et al. (1998)	?	
3,3-dimethyl-2-butanone	4.3×10^{-2}	5800	Brockbank (2013)	L	1
$C_6H_{12}O$	4.5×10^{-2}	5700	Plyasunov and Shock (2001)	L	
(*tert*-butyl methyl ketone)	4.3×10^{-2}	5700	Hovorka et al. (2019)	M	
[75-97-8]	4.5×10^{-2}		Duchowicz et al. (2020)	V	187
PJGSXYOJTGTZAV-UHFFFAOYSA-N	4.5×10^{-2}		HSDB (2015)	V	
	7.6×10^{-2}	6000	Bagno et al. (1991)	T	475
		6000	Della Gatta et al. (1981)	T	
	5.5×10^{-3}		Duchowicz et al. (2020)	Q	
	2.8×10^{-2}		Wang et al. (2017)	Q	81, 239
	7.1×10^{-2}		Wang et al. (2017)	Q	81, 240
	1.8×10^{-1}		Wang et al. (2017)	Q	81, 241
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	4.7×10^{-2}		Hilal et al. (2008)	Q	
	2.8×10^{-1}		Modarresi et al. (2007)	Q	68
		5700	Kühne et al. (2005)	Q	
	7.9×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	4.5×10^{-2}		English and Carroll (2001)	Q	231, 232
	2.7×10^{-2}		Katritzky et al. (1998)	Q	
	7.9×10^{-2}		Nirmalakhandan et al. (1997)	Q	
		5400	Kühne et al. (2005)	?	
	6.4×10^{-2}		Yaws et al. (1998)	?	
cyclohexanone	1.5	6400	Brockbank (2013)	L	
$C_6H_{10}O$	8.6×10^{-1}	5100	Hovorka et al. (2002)	M	11
[108-94-1]	8.2×10^{-1}		Hawthorne et al. (1985)	M	
JHIVVAPYMSGYDF-UHFFFAOYSA-N	1.1		HSDB (2015)	V	
	3.8×10^{-1}		Mackay et al. (2006c)	V	
	3.8×10^{-1}		Mackay et al. (1995)	V	
	4.4×10^{-1}		Meylan and Howard (1991)	V	

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2		Yaws (2003)	X	259
	2.6		Dupeux et al. (2022)	Q	260
	1.0		Keshavarz et al. (2022)	Q	
	2.5×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.0×10^{-1}		Wang et al. (2017)	Q	81, 239
	2.0		Wang et al. (2017)	Q	81, 240
	5.9		Wang et al. (2017)	Q	81, 241
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	1.0		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	68
		6200	Kühne et al. (2005)	Q	
	1.2		Yaffe et al. (2003)	Q	249, 250
	9.0×10^{-1}		English and Carroll (2001)	Q	231, 232
	6.2×10^{-2}		Katritzky et al. (1998)	Q	
	5.6×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.9×10^{-1}		Meylan and Howard (1991)	Q	
	1.1		Duchowicz et al. (2020)	?	186, 21
		6300	Kühne et al. (2005)	?	
	1.8		Yaws (1999)	?	21
	1.6		Abraham et al. (1990)	?	
2-heptanone	6.8×10^{-2}	6800	Brockbank (2013)	L	1
$C_7H_{14}O$	7.2×10^{-2}	6800	Plyasunov and Shock (2001)	L	
[110-43-0]	5.9×10^{-2}	5300	Falabella et al. (2006)	M	11, 340
CATSNJVOTSVZJV-UHFFFAOYSA-N	6.8×10^{-2}	5700	Chai et al. (2005)	M	11
	3.9×10^{-2}		van Ruth et al. (2002)	M	14
	4.1×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 363
	2.5×10^{-2}		van Ruth et al. (2001)	M	14
	6.2×10^{-2}		Kim et al. (2000)	M	
	5.8×10^{-2}		Shiu and Mackay (1997)	M	
	3.7×10^{-2}		Sato and Nakajima (1979a)	M	14
	6.8×10^{-2}		Buttery et al. (1969)	M	
	7.5×10^{-2}		Mackay et al. (2006c)	V	
	7.5×10^{-2}		Shiu and Mackay (1997)	V	
	7.5×10^{-2}		Mackay et al. (1995)	V	
	1.8	5600	Djerki and Laub (1988)	V	
	1.7×10^{-1}		Rathbun and Tai (1982)	V	
	7.5×10^{-2}		Yaws (2003)	X	259
	7.4×10^{-2}		Yaws (2003)	X	238
	3.5×10^{-1}	4500	Janini and Quaddora (1986)	X	299
	1.5×10^{-1}		Dupeux et al. (2022)	Q	260
	5.3×10^{-2}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	185
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	5.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
	6.2×10^{-2}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	68
		6900	Kühne et al. (2005)	Q	
	1.2×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	6.5×10^{-2}		English and Carroll (2001)	Q	231, 275
	2.3×10^{-2}		Katritzky et al. (1998)	Q	
	7.2×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	6.2×10^{-2}		Russell et al. (1992)	Q	280
	6.9×10^{-2}		Suzuki et al. (1992)	Q	233
	5.8×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	6.8×10^{-2}		Mackay et al. (2006c)	?	21
		6900	Kühne et al. (2005)	?	
	7.5×10^{-2}		Yaws (1999)	?	21
	7.5×10^{-2}		Yaws et al. (1998)	?	
	3.9×10^{-2}		Abraham and Weathersby (1994)	?	21
	6.9×10^{-2}		Abraham et al. (1990)	?	
	1.1×10^{-1}		Mackay and Yeun (1983)	?	
3-heptanone	7.2×10^{-2}	7000	Brockbank (2013)	L	1
$C_7H_{14}O$	1.1×10^{-1}		HSDB (2015)	V	
[106-35-4]	4.9×10^{-2}		Yaws (2003)	X	259
NGAZZOYFWWSOGK-UHFFFAOYSA-N	5.0×10^{-2}		Yaws (2003)	X	238
	7.3×10^{-2}		Dupeux et al. (2022)	Q	260
	3.1×10^{-2}		Wang et al. (2017)	Q	81, 239
	6.0×10^{-2}		Wang et al. (2017)	Q	81, 240
	1.4×10^{-1}		Wang et al. (2017)	Q	81, 241
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	5.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
	1.3×10^{-1}		Modarresi et al. (2007)	Q	68
		6900	Kühne et al. (2005)	Q	
	1.2×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	1.4×10^{-2}		Katritzky et al. (1998)	Q	
		6000	Kühne et al. (2005)	?	
	2.4×10^{-2}		Yaws et al. (1998)	?	
4-heptanone	5.1×10^{-2}	6800	Brockbank (2013)	L	1, 482
$C_7H_{14}O$	6.1×10^{-2}	7000	Plyasunov and Shock (2001)	L	
[123-19-3]	1.8×10^{-1}		Duchowicz et al. (2020)	V	187
HCFAJYNVAYBARA-UHFFFAOYSA-N	4.1×10^{-2}		HSDB (2015)	V	
	5.6×10^{-2}		Cabani et al. (1981)	V	
	3.3×10^{-2}		Yaws (2003)	X	259
	3.3×10^{-2}		Yaws (2003)	X	238
	3.8×10^{-2}		Dupeux et al. (2022)	Q	260

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	5.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
	4.8×10^{-2}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	68
		6900	Kühne et al. (2005)	Q	
	5.8×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	6.5×10^{-2}		English and Carroll (2001)	Q	231, 232
	1.8×10^{-2}		Katritzky et al. (1998)	Q	
	7.7×10^{-2}		Nirmalakhandan et al. (1997)	Q	
		7800	Kühne et al. (2005)	?	
	2.3×10^{-2}		Yaws et al. (1998)	?	38
	5.6×10^{-2}		Abraham et al. (1990)	?	
3-methyl-2-hexanone	2.8×10^{-2}		Yaws (2003)	X	238
$C_7H_{14}O$	4.0×10^{-3}		Gharagheizi et al. (2012)	Q	
[2550-21-2]	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
GYWYASONLSQZBB-UHFFFAOYSA-N	3.2×10^{-2}		Yaws et al. (1998)	?	
4-methyl-2-hexanone	4.9×10^{-2}		Yaws (2003)	X	238
$C_7H_{14}O$	3.6×10^{-2}		Wang et al. (2017)	Q	81, 239
[105-42-0]	9.3×10^{-2}		Wang et al. (2017)	Q	81, 240
XUPXMIAWKPTZLZ-UHFFFAOYSA-N	2.1×10^{-1}		Wang et al. (2017)	Q	81, 241
	4.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
	3.3×10^{-2}		Yaws et al. (1998)	?	
5-methyl-2-hexanone	6.4×10^{-2}	6800	Brockbank (2013)	L	1
$C_7H_{14}O$	6.2×10^{-2}		Duchowicz et al. (2020)	V	187
[110-12-3]	6.2×10^{-2}		HSDB (2015)	V	
FFWSICBKRCICMR-UHFFFAOYSA-N	4.1×10^{-2}		Yaws (2003)	X	238
	1.3×10^{-2}		Duchowicz et al. (2020)	Q	
	3.6×10^{-2}		Wang et al. (2017)	Q	81, 239
	1.1×10^{-1}		Wang et al. (2017)	Q	81, 240
	3.8×10^{-1}		Wang et al. (2017)	Q	81, 241
	4.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
	7.7×10^{-2}		Hilal et al. (2008)	Q	
	1.1×10^{-1}		Modarresi et al. (2007)	Q	68
		6900	Kühne et al. (2005)	Q	
	7.3×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.2×10^{-2}		Katritzky et al. (1998)	Q	
		7600	Kühne et al. (2005)	?	
	2.7×10^{-2}		Yaws et al. (1998)	?	

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-3-hexanone	4.9×10^{-2}		Yaws (2003)	X	238
$C_7H_{14}O$	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
[7379-12-6]	4.1×10^{-2}		Yaws et al. (1998)	?	
HIGGFWFRAWSMBR-UHFFFAOYSA-N					
4-methyl-3-hexanone	3.1×10^{-2}		Yaws (2003)	X	238
$C_7H_{14}O$	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
[17042-16-9]	3.7×10^{-2}		Yaws et al. (1998)	?	
ULPMRIXXHGUZFA-UHFFFAOYSA-N					
5-methyl-3-hexanone	3.1×10^{-2}		Yaws (2003)	X	238
$C_7H_{14}O$	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
[623-56-3]	3.7×10^{-2}		Yaws et al. (1998)	?	
DXVYLFHTJZWTRF-UHFFFAOYSA-N					
3-ethyl-2-pentanone	2.9×10^{-2}		Yaws (2003)	X	238
$C_7H_{14}O$	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
[6137-03-7]	3.4×10^{-2}		Yaws et al. (1998)	?	
GSNKRSKIWFBWEG-UHFFFAOYSA-N					
3,3-dimethyl-2-pentanone	3.1×10^{-2}		Yaws (2003)	X	238
$C_7H_{14}O$	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
[20669-04-9]	4.5×10^{-2}		Yaws et al. (1998)	?	
QSHJLBQLQVSEFV-UHFFFAOYSA-N					
3,4-dimethyl-2-pentanone	3.2×10^{-2}		Yaws (2003)	X	238
$C_7H_{14}O$	3.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
[565-78-6]	4.3×10^{-2}		Yaws et al. (1998)	?	
QXHRQZNDMYRDPA-UHFFFAOYSA-N					
4,4-dimethyl-2-pentanone	3.6×10^{-2}		Yaws (2003)	X	238
$C_7H_{14}O$	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
[590-50-1]	5.5×10^{-2}		Yaws et al. (1998)	?	
AZASWMGVGQEVCS-UHFFFAOYSA-N					
2,2-dimethyl-3-pentanone	3.6×10^{-2}		Yaws (2003)	X	238
$C_7H_{14}O$	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
[564-04-5]	5.5×10^{-2}		Yaws et al. (1998)	?	
VLNUTKMHYLQCQB-UHFFFAOYSA-N					
2,4-dimethyl-3-pentanone	2.3×10^{-2}	6100	Brockbank (2013)	L	1
$C_7H_{14}O$	2.4×10^{-2}	6500	Plyasunov and Shock (2001)	L	
(diisopropyl ketone)	2.8×10^{-2}		Duchowicz et al. (2020)	V	187
[565-80-0]	4.1×10^{-2}		Cabani et al. (1981)	V	
HXVNBWAKAOHACI-UHFFFAOYSA-N	9.5×10^{-1}	6400	Bagno et al. (1991)	T	475
		6400	Della Gatta et al. (1981)	T	
	2.8×10^{-2}		Yaws (2003)	X	238
	4.9×10^{-3}		Duchowicz et al. (2020)	Q	
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
	3.5×10^{-2}		Hilal et al. (2008)	Q	
	1.5×10^{-1}		Modarresi et al. (2007)	Q	68
		6000	Kühne et al. (2005)	Q	
	2.8×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.4×10^{-2}		Yao et al. (2002)	Q	230
	1.4×10^{-2}		English and Carroll (2001)	Q	231, 232
	1.3×10^{-2}		Katritzky et al. (1998)	Q	
	6.0×10^{-2}		Nirmalakhandan et al. (1997)	Q	
		4900	Kühne et al. (2005)	?	
	2.8×10^{-2}		Yaws (1999)	?	21
	2.8×10^{-2}		Yaws et al. (1998)	?	
cycloheptanone $C_7H_{12}O$ [502-42-1] CGZZMOTZOONQIA-UHFFFAOYSA-N	7.0×10^{-1}		Hilal et al. (2008)	Q	
2-methylcyclohexanone $C_7H_{12}O$ [583-60-8] LFSAPCRASZRSKS-UHFFFAOYSA-N		5600	Kühne et al. (2005)	Q	
		4600	Kühne et al. (2005)	?	
3-methylcyclohexanone $C_7H_{12}O$ [591-24-2] UJBOOUHRTQVGRU-UHFFFAOYSA-N	6.7×10^{-2}		Duchowicz et al. (2020)	V	187
	9.9×10^{-2}		Duchowicz et al. (2020)	Q	
4-methylcyclohexanone $C_7H_{12}O$ [589-92-4] VGVHNLRUAMRIEW-UHFFFAOYSA-N		6500	Kühne et al. (2005)	Q	
		6100	Kühne et al. (2005)	?	
dicyclopropylmethanone $C_7H_{10}O$ (dicyclopropyl ketone) [1121-37-5] BIPUHAHGLJKIPK-UHFFFAOYSA-N	3.1	7300	Bagno et al. (1991)	T	475
		7300	Della Gatta et al. (1981)	T	
2-octanone $C_6H_{13}COCH_3$ [111-13-7] ZPVFWPFBNIEHGJ-UHFFFAOYSA-N	5.0×10^{-2}	7500	Brockbank (2013)	L	1, 483
	5.8×10^{-2}		Plyasunov and Shock (2001)	L	
	2.9×10^{-2}		van Ruth et al. (2002)	M	14
	3.1×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 363
	1.8×10^{-2}		van Ruth et al. (2001)	M	14
	5.2×10^{-2}		Buttery et al. (1969)	M	
	4.9×10^{-2}		Mackay et al. (2006c)	V	
	4.9×10^{-2}		Mackay et al. (1995)	V	
	5.5×10^{-2}		Rathbun and Tai (1982)	V	

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.1×10^{-2}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	185
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	5.1×10^{-2}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	68
		7300	Kühne et al. (2005)	Q	
	5.2×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	5.1×10^{-2}		English and Carroll (2001)	Q	231, 232
	2.0×10^{-2}		Katritzky et al. (1998)	Q	
	5.7×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	3.3×10^{-2}		Russell et al. (1992)	Q	280
	5.3×10^{-2}		Suzuki et al. (1992)	Q	233
	5.2×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	5.2×10^{-2}		Mackay et al. (2006c)	?	21
		7300	Kühne et al. (2005)	?	
	9.6×10^{-2}		Yaws (1999)	?	21, 12
	1.5×10^{-1}		Yaws et al. (1998)	?	12
	5.2×10^{-2}		Abraham et al. (1990)	?	
3-octanone $C_8H_{16}O$ [106-68-3] RHLVCLIPMVJYKS-UHFFFAOYSA-N	4.3×10^{-2}	6900	Brockbank (2013)	L	1
	2.9×10^{-2}	5800	Wu et al. (2022a)	M	484
	7.6×10^{-2}		HSDB (2015)	V	
	2.5×10^{-2}		Wang et al. (2017)	Q	81, 239
	4.2×10^{-2}		Wang et al. (2017)	Q	81, 240
	1.3×10^{-1}		Wang et al. (2017)	Q	81, 241
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.1×10^{-1}		Modarresi et al. (2007)	Q	68
4-octanone $C_8H_{16}O$ [589-63-9] YWXLSHOWXZUMSR-UHFFFAOYSA-N	3.6×10^{-2}		Hilal et al. (2008)	Q	
5-methyl-3-heptanone $C_8H_{16}O$ [541-85-5] PSBKJPTZCVYXSD-UHFFFAOYSA-N	5.0×10^{-2}		Ebert et al. (2023)	?	317
6-methyl-3-heptanone $C_8H_{16}O$ [624-42-0] CCCIYAQYQZQDIZ-UHFFFAOYSA-N	3.7×10^{-2}		HSDB (2015)	Q	100

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyclohexyl methyl ketone	2.9×10^{-1}	7200	Bagno et al. (1991)	T	475
$C_6H_{11}COCH_3$	7.1×10^{-2}		Keshavarz et al. (2022)	Q	
[823-76-7]	9.9×10^{-2}		Duchowicz et al. (2020)	Q	185
RIFKADJTWUGDOV-UHFFFAOYSA-N	4.1×10^{-1}		Hilal et al. (2008)	Q	
	4.2×10^{-1}		Modarresi et al. (2007)	Q	68
	2.3×10^{-1}		English and Carroll (2001)	Q	231, 232
	3.1×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	2.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2-nonanone	3.2×10^{-2}	7400	Brockbank (2013)	L	1, 485
$C_9H_{18}O$	3.7×10^{-2}	7500	Plyasunov and Shock (2001)	L	
[821-55-6]	4.1×10^{-2}		Li and Carr (1993)	M	
VKCYHJWLYTUGCC-UHFFFAOYSA-N	2.7×10^{-2}		Buttery et al. (1969)	M	
		7600	Abraham (1984)	V	
	2.1×10^{-2}		Yaws (2003)	X	259
	1.1×10^{-1}		Dupeux et al. (2022)	Q	260
	9.6×10^{-2}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	300
	4.1×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	4.1×10^{-2}		Hilal et al. (2008)	Q	
	1.0×10^{-1}		Modarresi et al. (2007)	Q	68
		7600	Kühne et al. (2005)	Q	
	2.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	3.9×10^{-2}		English and Carroll (2001)	Q	231, 232
	1.3×10^{-2}		Katritzky et al. (1998)	Q	
	4.4×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	4.0×10^{-2}		Suzuki et al. (1992)	Q	233
	2.7×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		8100	Kühne et al. (2005)	?	
	2.9×10^{-2}		Yaws et al. (1998)	?	
	2.7×10^{-2}		Abraham et al. (1990)	?	
3-nonanone	5.1×10^{-2}	6600	Brockbank (2013)	L	
$C_9H_{18}O$	2.2×10^{-2}		Wang et al. (2017)	Q	81, 239
[925-78-0]	3.2×10^{-2}		Wang et al. (2017)	Q	81, 240
IYTXKIXETAELAV-UHFFFAOYSA-N	1.2×10^{-1}		Wang et al. (2017)	Q	81, 241
5-nonanone	4.0×10^{-2}	8000	Brockbank (2013)	L	1
$C_9H_{18}O$	3.5×10^{-2}		Duchowicz et al. (2020)	V	187
(dibutyl ketone)	3.5×10^{-2}		HSDB (2015)	V	
[502-56-7]	3.4×10^{-2}		Meylan and Howard (1991)	V	
WSGCRAOTEDLMFQ-UHFFFAOYSA-N	3.7×10^{-2}		Cabani et al. (1981)	V	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	2.7×10^{-2}		Hilal et al. (2008)	Q	

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.0×10^{-2}		Modarresi et al. (2007)	Q	68
		7600	Kühne et al. (2005)	Q	
	2.7×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	3.9×10^{-2}		English and Carroll (2001)	Q	231, 232
	4.7×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	3.6×10^{-2}		Meylan and Howard (1991)	Q	
		7900	Kühne et al. (2005)	?	
	3.4×10^{-2}		Yaws et al. (1998)	?	38
	3.5×10^{-2}		Abraham et al. (1990)	?	
2,6-dimethyl-4-heptanone $C_9H_{18}O$ (diisobutyl ketone) [108-83-8] PTTPXKJBFFKCEK-UHFFFAOYSA-N	1.3×10^{-2}	7500	Brockbank (2013)	L	1
	1.3×10^{-2}		Plyasunov and Shock (2001)	L	
	8.4×10^{-2}		Duchowicz et al. (2020)	V	187
	8.2×10^{-2}		HSDB (2015)	V	
	4.9×10^{-3}		Duchowicz et al. (2020)	Q	
	3.1×10^{-2}		Hilal et al. (2008)	Q	
	1.1×10^{-1}		Modarresi et al. (2007)	Q	68
		7600	Kühne et al. (2005)	Q	
	8.6×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
		5500	Kühne et al. (2005)	?	
	8.3×10^{-2}		Yaws (1999)	?	21, 80
	9.2×10^{-2}		Yaws et al. (1998)	?	80
2,2,4,4-tetramethyl-3-pentanone $C_9H_{18}O$ (di-(*tert*-butyl) ketone) [815-24-7] UIQGEWJEWJMQSL-UHFFFAOYSA-N	2.3×10^{-2}		Bagno et al. (1991)	T	475
2-decanone $C_8H_{17}COCH_3$ [693-54-9] ZAJNGDIORYACQU-UHFFFAOYSA-N	1.8×10^{-2}		van Ruth et al. (2002)	M	14
	1.5×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 363
	1.5×10^{-2}		van Ruth et al. (2001)	M	14
	2.1×10^{-2}		Abraham (1984)	V	
	1.7×10^{-2}		Yaws (2003)	X	259
	9.2×10^{-2}		Dupeux et al. (2022)	Q	260
	4.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.4×10^{-2}		Hilal et al. (2008)	Q	
	8.0×10^{-2}		Modarresi et al. (2007)	Q	68
	2.7×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	3.1×10^{-2}		English and Carroll (2001)	Q	231, 261
	1.4×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.4×10^{-2}		Yaws et al. (1998)	?	
	2.1×10^{-2}		Abraham et al. (1990)	?	

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-undecanone $C_9H_{19}COCH_3$ [112-12-9] KYWIYKKSMDLRDC-UHFFFAOYSA-N	1.9×10^{-2}		Plyasunov and Shock (2001)	L	
	1.6×10^{-2}		Buttery et al. (1969)	M	
	1.8×10^{-2}		Yaws (2003)	X	259
	1.7×10^{-2}		Yaws (2003)	X	238
	7.6×10^{-2}		Dupeux et al. (2022)	Q	260
	1.8×10^{-1}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	300
	1.5×10^{-2}		Li et al. (2014)	Q	242
	4.1×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.7×10^{-2}		Hilal et al. (2008)	Q	
	6.3×10^{-2}		Modarresi et al. (2007)	Q	68
	1.6×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.3×10^{-2}		English and Carroll (2001)	Q	231, 232
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
	2.8×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	2.4×10^{-2}		Suzuki et al. (1992)	Q	233
	1.6×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	5.8×10^{-3}		Yaws et al. (1998)	?	
	1.5×10^{-2}		Abraham et al. (1990)	?	
6-undecanone $C_{11}H_{22}O$ [927-49-1] ZPQAKYPOZRXKFA-UHFFFAOYSA-N	1.5×10^{-2}		Hilal et al. (2008)	Q	
	6.9×10^{-2}		Modarresi et al. (2007)	Q	68
2-dodecanone $C_{12}H_{24}O$ [6175-49-1] LSKONYYRONEBKA-UHFFFAOYSA-N	4.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.1×10^{-3}		Yaws et al. (1998)	?	
2,6,8-trimethyl-4-nonanone $C_{12}H_{24}O$ [123-18-2] GFWVDQCGGDBTBS-UHFFFAOYSA-N			Brockbank (2013)	W	486
2-tridecanone $C_{13}H_{26}O$ [593-08-8] CYIFVRUOHKNECG-UHFFFAOYSA-N	4.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.7×10^{-4}		Yaws et al. (1998)	?	
2-tetradecanone $C_{14}H_{28}O$ [2345-27-9] POQLVOYRGNFGRM-UHFFFAOYSA-N	4.7×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.1×10^{-4}		Yaws et al. (1998)	?	

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-pentadecanone $C_{15}H_{30}O$ [2345-28-0] CJPNOLIZCWDHJK-UHFFFAOYSA-N	5.4×10^{-5}		Yaws et al. (1998)	?	
2-hexadecanone $C_{16}H_{32}O$ [18787-63-8] XCXKZBWAKKPFCJ-UHFFFAOYSA-N	1.7×10^{-5}		Yaws et al. (1998)	?	
2-heptadecanone $C_{17}H_{34}O$ [2922-51-2] TVTCXPXLRKTHAU-UHFFFAOYSA-N	3.9×10^{-6}		Yaws et al. (1998)	?	
menthone	5.7×10^{-2}		Marin et al. (1999)	M	
$C_{10}H_{18}O$	5.0×10^{-2}		Marin et al. (1999)	V	
[89-80-5]	6.2×10^{-2}		HSDB (2015)	Q	100
NFLGAXVYCFJBMK-UHFFFAOYSA-N	5.8×10^{-2}		Marin et al. (1999)	Q	
tricyclo[3.3.1.1(3,7)]decanone	1.4	5800	van Roon et al. (2005)	V	
$C_{10}H_{14}O$	7.5×10^{-1}		Cabani et al. (1981)	V	
(2-adamantanone)					
[700-58-3]					
IYKFYARMMIESOX-UHFFFAOYSA-N					
methyl cedryl ketone	6.1		Dupeux et al. (2022)	Q	260
$C_{17}H_{26}O$					
[32388-55-9]					
YBUIAJZFOGJGLJ-SWRJLBSHSA-N					
3-buten-2-one	4.0×10^{-1}		Burkholder et al. (2019)	L	
C_4H_6O	4.0×10^{-1}		Burkholder et al. (2015)	L	
(methyl vinyl ketone; MVK)	2.6×10^{-1}	4800	Ji and Evans (2007)	M	
[78-94-4]	4.0×10^{-1}		Iraci et al. (1999)	M	
FUSUHKVFWTUUBE-UHFFFAOYSA-N	2.1×10^{-1}	7800	Allen et al. (1998)	M	
	1.6×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.5×10^{-1}		Wang et al. (2017)	Q	81, 239
	3.1×10^{-1}		Wang et al. (2017)	Q	81, 240
	7.8×10^{-1}		Wang et al. (2017)	Q	81, 241
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	7.1×10^{-1}		Modarresi et al. (2007)	Q	68
		6000	Kühne et al. (2005)	Q	
	2.1×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		7800	Kühne et al. (2005)	?	

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.3×10^{-1}		Betterton (1991)	?	
methyl isopropenyl ketone	9.8×10^{-2}		Yaws (2003)	X	238
C_5H_8O	3.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[814-78-8]	9.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
ZGHFDIIVVIFNPS-UHFFFAOYSA-N	5.2×10^{-2}		Yao et al. (2002)	Q	230
	9.8×10^{-2}		Yaws (1999)	?	21
4-methyl-3-penten-2-one	2.7×10^{-1}		HSDB (2015)	V	
$C_6H_{10}O$	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
(mesityl oxide)	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	245
[141-79-7]	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	246
SHOJXDKTYKFBRD-UHFFFAOYSA-N	1.8×10^{-1}		Hilal et al. (2008)	Q	
	2.5×10^{-1}		Modarresi et al. (2007)	Q	68
	2.0×10^{-1}		Yaws (1999)	?	21, 12
1-phenylethanone	1.1	7900	Brockbank (2013)	L	1
$C_6H_5COCH_3$	1.1	7700	Staudinger and Roberts (2001)	L	
(acetophenone)	9.7×10^{-1}	6800	Hiatt (2013)	M	
[98-86-2]	1.2	7800	Ji et al. (2008)	M	
KWOLFJPFCHCOCG-UHFFFAOYSA-N	9.7×10^{-1}	12000	Allen et al. (1998)	M	
	9.3×10^{-1}		Shiu and Mackay (1997)	M	
	1.1	6000	Betterton (1991)	M	
	1.0		Mackay et al. (2006c)	V	
	1.0		Shiu and Mackay (1997)	V	
	1.0		Mackay et al. (1995)	V	
	9.2×10^{-1}		Hine and Mookerjee (1975)	V	
	9.5×10^{-1}	6400	Bagno et al. (1991)	T	475
	1.1		Yaws (2003)	X	259
	9.3×10^{-1}		Schüürmann (2000)	C	21
	1.8		Dupeux et al. (2022)	Q	260
	7.1×10^{-2}		Keshavarz et al. (2022)	Q	
	2.2×10^{-1}		Duchowicz et al. (2020)	Q	185
	2.0		Wang et al. (2017)	Q	81, 239
	2.0		Wang et al. (2017)	Q	81, 240
	4.6		Wang et al. (2017)	Q	81, 241
	9.2×10^{-1}		Li et al. (2014)	Q	242
	1.2		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	1.1		Hilal et al. (2008)	Q	
	2.9		Modarresi et al. (2007)	Q	68
		6100	Kühne et al. (2005)	Q	
	1.0		Yaffe et al. (2003)	Q	249, 250
	1.1		English and Carroll (2001)	Q	231, 232
	1.9×10^{-1}		Katritzky et al. (1998)	Q	
	5.3×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	9.2×10^{-1}		Suzuki et al. (1992)	Q	233

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.5×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		6700	Kühne et al. (2005)	?	
	1.1		Yaws (1999)	?	21
	9.2×10^{-1}		Abraham et al. (1990)	?	
1-phenylethanone-d5 $C_6D_5COCH_3$ (acetophenone-d5) [28077-64-7] KWOLFJPFCHCOCG-VIQYUKPQSA-N	2.3	10000	Hiatt (2013)	M	
4-methoxy-4-methyl-2-pentanone	5.1		Duchowicz et al. (2020)	V	187
$C_7H_{14}O_2$	5.1		HSDB (2015)	V	
[107-70-0]	2.2×10^{-1}		Duchowicz et al. (2020)	Q	
KOKPBCHLPVDQTK-UHFFFAOYSA-N	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	2.0		Raventos-Duran et al. (2010)	Q	245
	7.8		Raventos-Duran et al. (2010)	Q	246
	1.8		Hilal et al. (2008)	Q	
	2.4		Modarresi et al. (2007)	Q	68
2'-hydroxyacetophenone $C_8H_8O_2$ [118-93-4] JECYUBVRTQDVAT-UHFFFAOYSA-N	1.0	8400	Ji et al. (2008)	M	
6-methyl-5-hepten-2-one	1.2×10^{-1}	6200	Wu et al. (2022b)	M	
$C_8H_{14}O$	2.5×10^{-1}		Dupeux et al. (2022)	Q	260
[110-93-0]					
UHEPJGULSIKKTP-UHFFFAOYSA-N					
phenyl ethyl ketone	9.9×10^{-1}	7900	Ji et al. (2008)	M	
$C_9H_{10}O$	6.6×10^{-1}		Duchowicz et al. (2020)	V	187
(propiophenone)	7.6×10^{-2}		HSDB (2015)	V	
[93-55-0]	2.2×10^{-1}		Duchowicz et al. (2020)	Q	
KRIOVPPHQSLHCZ-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	81, 239
	1.4		Wang et al. (2017)	Q	81, 240
	9.1×10^{-1}		Wang et al. (2017)	Q	81, 241
	7.5×10^{-1}		Zhang et al. (2010)	Q	288, 289
	7.2×10^{-1}		Zhang et al. (2010)	Q	288, 290
	1.6		Zhang et al. (2010)	Q	288, 291
	9.7×10^{-1}		Zhang et al. (2010)	Q	288, 292
	8.6×10^{-1}		Hilal et al. (2008)	Q	
	8.0×10^{-1}		Modarresi et al. (2007)	Q	68
		6400	Kühne et al. (2005)	Q	
	7.9×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.9×10^{-1}		Katritzky et al. (1998)	Q	
		7700	Kühne et al. (2005)	?	

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2'-methylacetophenone	7.6×10^{-1}	7600	Ji et al. (2008)	M	
$C_9H_{10}O$	1.2		Wang et al. (2017)	Q	81, 239
[577-16-2]	2.4		Wang et al. (2017)	Q	81, 240
YXWWHNCQZBVZPV-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	81, 241
3'-methylacetophenone	1.5	7600	Ji et al. (2008)	M	
$C_9H_{10}O$					
[585-74-0]					
FSPSELPMWGWDRY-UHFFFAOYSA-N					
4'-methylacetophenone	1.8	8400	Ji et al. (2008)	M	
$C_9H_{10}O$	1.1		Abraham et al. (1994a)	R	
[122-00-9]	4.3		Abney (2021)	Q	401
GNKZMNRKLCTJAY-UHFFFAOYSA-N	1.2		Hilal et al. (2008)	Q	
	1.2		Yaffe et al. (2003)	Q	249, 250
	9.5×10^{-1}		English and Carroll (2001)	Q	231, 261
	3.8×10^{-1}		Nirmalakhandan et al. (1997)	Q	
2'-methoxyacetophenone	1.7×10^{1}	9500	Ji et al. (2008)	M	
$C_9H_{10}O_2$					
(2-methoxyphenyl methyl ketone)					
[579-74-8]					
DWPLEOPKBWNPQV-UHFFFAOYSA-N					
3'-methoxyacetophenone	1.9×10^{1}	9400	Ji et al. (2008)	M	
$C_9H_{10}O_2$					
(3-methoxyphenyl methyl ketone)					
[586-37-8]					
BAYUSCHCCGXLAY-UHFFFAOYSA-N					
4'-methoxyacetophenone	6.8×10^{-1}		Bagno et al. (1991)	T	475
$C_9H_{10}O_2$	6.9		Hilal et al. (2008)	Q	
(4-methoxyphenyl methyl ketone)	1.4		English and Carroll (2001)	Q	231, 232
[100-06-1]	1.3		Nirmalakhandan et al. (1997)	Q	
NTPLXRHDUXRPNE-UHFFFAOYSA-N					
2-methyl-5-(1-methylethenyl)-2-cyclohexen-1-one	4.9×10^{-1}		Amoore and Buttery (1978)	M	
$C_{10}H_{14}O$	5.5×10^{-1}		Amoore and Buttery (1978)	V	
(carvone)	8.0×10^{-1}		Hilal et al. (2008)	Q	
[6485-40-1]					
ULDHMXUKGWMISQ-SECBINFHSA-N					
benzophenone	1.7×10^{1}		Mackay et al. (2006c)	V	
$C_{13}H_{10}O$	6.1	9400	Bagno et al. (1991)	T	475
(diphenyl ketone)	1.7		Yaws (2003)	X	259
[119-61-9]	9.6		Dupeux et al. (2022)	Q	260
RWCCWEUUXYIKHB-UHFFFAOYSA-N	5.2		HSDB (2015)	Q	100
	5.1		Zhang et al. (2010)	Q	288, 289
	2.9		Zhang et al. (2010)	Q	288, 290

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.6×10^{1}		Zhang et al. (2010)	Q	288, 291
	3.4×10^{1}		Zhang et al. (2010)	Q	288, 292
	1.7		Yaws (1999)	?	21
2,4-dihydroxybenzophenone $C_{13}H_{10}O_3$ [131-56-6] ZXDDPOHVAMWLBH-UHFFFAOYSA-N	4.6×10^{5}		Abraham et al. (2019)	Q	
3,5,5-trimethyl-2-cyclohexen-1-one	1.5		Duchowicz et al. (2020)	V	187
$C_9H_{14}O$	1.5		HSDB (2015)	V	
(isophorone)	1.7		Mackay et al. (2006d)	V	
[78-59-1]	1.7		Hwang et al. (1992)	V	
HJOVHMDZYOCNQW-UHFFFAOYSA-N	1.7		Suntio et al. (1988)	V	12
	1.7	3900	Goldstein (1982)	X	299
	1.8		Suntio et al. (1988)	C	12
	1.7×10^{-2}		Duchowicz et al. (2020)	Q	
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	6.9×10^{-1}		Hilal et al. (2008)	Q	
	1.3		Modarresi et al. (2007)	Q	68
		7300	Kühne et al. (2005)	Q	
	1.5		Yaffe et al. (2003)	Q	249, 250
	1.2×10^{-1}		Katritzky et al. (1998)	Q	
		7400	Kühne et al. (2005)	?	
	1.5		Yaws (1999)	?	21
bicyclo[2.2.1]heptan-2-one $C_7H_{10}O$ (norcamphor; 2-norbornanone) [497-38-1] KPMKEVXVVHNIEY-UHFFFAOYSA-N	4.3×10^{-1}	5100	van Roon et al. (2005)	V	
4-methyl-1-(1-methylethyl)-bicyclo[3.1.0]hexan-3-one $C_{10}H_{16}O$ (thujone) [1125-12-8] USMNOWBWPHYOEA-UHFFFAOYSA-N	1.0×10^{-1}	4700	van Roon et al. (2005)	V	
isopropyl phenyl ketone	5.7×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{10}H_{12}O$	3.9×10^{-1}		Zhang et al. (2010)	Q	288, 290
[611-70-1]	1.7		Zhang et al. (2010)	Q	288, 291
BSMGLVDZZMBWQB-UHFFFAOYSA-N	8.2×10^{-1}		Zhang et al. (2010)	Q	288, 292

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
carvone $C_{10}H_{14}O$ [99-49-0] ULDHMXUKGWMISQ-UHFFFAOYSA-N	1.3×10^{-1}		HSDB (2015)	Q	100
thujone $C_{10}H_{16}O$ [76231-76-0] USMNOWBWPHYOEA-VWHDNNRLSA-N	6.2×10^{-1}		HSDB (2015)	Q	100
cis-jasmone $C_{11}H_{16}O$ [488-10-8] XMLSXPIVAXONDL-PLNGDYQASA-N	5.2		Dupeux et al. (2022)	Q	260
α-damascone $C_{13}H_{20}O$ [24720-09-0] CRIGTVCBMUKRSL-FNORWQNLSA-N	2.1×10^{1}		Abney (2021)	Q	401
(E)-β-damascenone $C_{13}H_{18}O$ [23726-93-4] POIARNZEYGURDG-FNORWQNLSA-N	3.2×10^{-1}	4600	Wieland et al. (2015)	M	487
9H-fluoren-9-one $C_{13}H_8O$ [486-25-9] YLQWCDOCJODRMT-UHFFFAOYSA-N	6.4 1.5×10^{1} 2.3×10^{1}		Abraham et al. (2019) HSDB (2015) Parnis et al. (2015)	Q Q Q	 100 371
anthrone $C_{14}H_{10}O$ [90-44-8] RJGDLRCDCYRQOQ-UHFFFAOYSA-N	1.2×10^{1}		HSDB (2015)	Q	100
1,2,3,5,6,7-hexahydro-1,1,2,3,3-pentamethyl-4H-inden-4-one $C_{14}H_{22}O$ [33704-61-9] MIZGSAALSYARKU-UHFFFAOYSA-N	7.0×10^{-2} 6.7×10^{-3} 2.0×10^{1} 4.8×10^{-2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
benzoin $C_{14}H_{12}O_2$ [119-53-9] ISAOCJYIOMOJEB-UHFFFAOYSA-N	2.2×10^{5}		Abraham et al. (2019)	Q	
methyl-alpha-ionone $C_{14}H_{22}O$ [93302-56-8] VPKMGDRERYMTJX-XEHSLEBBSA-N	1.2		Dupeux et al. (2022)	Q	260

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
iso-e super $C_{16}H_{26}O$ [54464-57-2] FVUGZKDGWGKCFE-UHFFFAOYSA-N	5.5×10^{-1}		Dupeux et al. (2022)	Q	260
2,4,6-trimethylbenzophenone	3.8		Zhang et al. (2010)	Q	288, 289
$C_{16}H_{16}O$	3.8		Zhang et al. (2010)	Q	288, 290
[954-16-5]	1.5×10^{1}		Zhang et al. (2010)	Q	288, 291
HPAFOABSQZMTHE-UHFFFAOYSA-N	6.0		Zhang et al. (2010)	Q	288, 292
1-(1,2,3,5,6,7,8,8a-octahydro-2,3,8,8-tetramethyl-2-naphthyl)ethan-1-one	2.5×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_{26}O$	3.0×10^{-1}		Zhang et al. (2010)	Q	288, 290
[68155-66-8]	1.1×10^{1}		Zhang et al. (2010)	Q	288, 291
NOMWSTMYQKABST-UHFFFAOYSA-N	4.0×10^{-2}		Zhang et al. (2010)	Q	288, 292
civetone $C_{17}H_{30}O$ [542-46-1] ZKVZSBSZTMPBQR-UPHRSURJSA-N	3.0		Dupeux et al. (2022)	Q	260
1-(2,3-dihydro-1,1,2,3,3,6-hexamethyl-1H-inden-5-yl)ethanone	3.1×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{17}H_{24}O$	2.0		Zhang et al. (2010)	Q	288, 290
[15323-35-0]	5.2		Zhang et al. (2010)	Q	288, 291
VDBHOHJWUDKDRW-UHFFFAOYSA-N	9.9×10^{-2}		Zhang et al. (2010)	Q	288, 292
celestolide	3.1×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{17}H_{24}O$	2.4		Zhang et al. (2010)	Q	288, 290
[13171-00-1]	3.1		Zhang et al. (2010)	Q	288, 291
IKTHMQYJOWTSJO-UHFFFAOYSA-N	8.8×10^{-2}		Zhang et al. (2010)	Q	288, 292
7H-benz[*de*]anthracen-7-one	1.5×10^{2}		HSDB (2015)	Q	100
$C_{17}H_{10}O$	8.0×10^{2}		Parnis et al. (2015)	Q	371
(benzanthrone) [82-05-3] HUKPVYBUJRAUAG-UHFFFAOYSA-N					
11H-benzo[*a*]fluoren-11-one $C_{17}H_{10}O$ [479-79-8] RNICURKFVSAHLQ-UHFFFAOYSA-N	7.2×10^{1}		Parnis et al. (2015)	Q	371
11H-benzo[*b*]fluoren-11-one $C_{17}H_{10}O$ [3074-03-1] MLMNDNOSVOKYMT-UHFFFAOYSA-N	5.4×10^{4}		Parnis et al. (2015)	Q	371

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benz[*a*]anthracene-7,12-dione $C_{18}H_{10}O_2$ [2498-66-0] LHMRXAIRPKSGDE-UHFFFAOYSA-N	4.2×10^{2}		Parnis et al. (2015)	Q	371
1-[2,3-dihydro-1,1,2,6-tetramethyl-3-(1-methylethyl)-1H-inden-5-yl]ethanone	2.3×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{18}H_{26}O$	3.2		Zhang et al. (2010)	Q	288, 290
[68140-48-7]	4.4		Zhang et al. (2010)	Q	288, 291
IMRYETFJNLKUHK-UHFFFAOYSA-N	1.3×10^{-1}		Zhang et al. (2010)	Q	288, 292
tonalide	7.0×10^{-2}		HSDB (2015)	V	
$C_{18}H_{26}O$	2.3×10^{-1}		Zhang et al. (2010)	Q	288, 289
[21145-77-7]	2.4		Zhang et al. (2010)	Q	288, 290
DNRJTBAOUJJKDY-UHFFFAOYSA-N	7.9		Zhang et al. (2010)	Q	288, 291
	7.9×10^{-2}		Zhang et al. (2010)	Q	288, 292
2,3-butanedione	7.3×10^{-1}	5700	Burkholder et al. (2019)	L	
$CH_3COCOCH_3$	7.3×10^{-1}	5700	Burkholder et al. (2015)	L	
(diacetyl; dimethylglyoxal)	7.3×10^{-1}	5700	Sander et al. (2011)	L	
[431-03-8]	1.4×10^{-1}	4900	Wu et al. (2022b)	M	
QSJXEFYPDANLFS-UHFFFAOYSA-N	4.2×10^{-1}	7200	Wieland et al. (2015)	M	488
	5.6×10^{-1}	6700	Strekowski and George (2005)	M	
	5.6×10^{-1}		Straver and de Loos (2005)	M	
	2.1×10^{-1}		van Ruth et al. (2002)	M	14
	2.0×10^{-1}		van Ruth and Villeneuve (2002)	M	14, 363
	2.0×10^{-1}		van Ruth et al. (2001)	M	14
	1.0		Marin et al. (1999)	M	
	3.7×10^{-1}		Roberts and Pollien (1997)	M	
	9.1×10^{-1}		Landy et al. (1995)	M	
	7.3×10^{-1}	5700	Betterton (1991)	M	
	5.7×10^{-1}		Snider and Dawson (1985)	M	
	6.1×10^{-1}		Marin et al. (1999)	V	
	1.9		Gaffney and Senum (1984)	X	448
	1.9		Gaffney and Senum (1984)	X	391
	1.6×10^{-1}		Keshavarz et al. (2022)	Q	
	2.2		Duchowicz et al. (2020)	Q	300
	3.6×10^{1}		Wang et al. (2017)	Q	81, 239
	9.1		Wang et al. (2017)	Q	81, 240
	1.9×10^{-1}		Wang et al. (2017)	Q	81, 241
	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	272, 244
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	246
	3.8		Hilal et al. (2008)	Q	
	1.4×10^{1}		Modarresi et al. (2007)	Q	68
		6500	Kühne et al. (2005)	Q	
	7.1×10^{-1}		Marin et al. (1999)	Q	

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.4×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		6000	Kühne et al. (2005)	?	
2,3-pentanedione	1.3×10^{-1}	6200	Wu et al. (2022b)	M	
$C_5H_8O_2$	3.2×10^{1}		Wang et al. (2017)	Q	81, 239
[600-14-6]	8.7		Wang et al. (2017)	Q	81, 240
TZMFJUDUGYTVRY-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	81, 241
2,4-pentanedione	8.5×10^{-1}	3800	Brockbank (2013)	L	
$C_5H_8O_2$	1.5		Nozière and Riemer (2003)	M	80
(acetylacetone)	9.9×10^{-1}	4400	Hovorka et al. (2002)	M	11
[123-54-6]	1.7		Hellmann (1987)	M	88
YRKCREAYFQTBPV-UHFFFAOYSA-N	4.3		HSDB (2015)	V	
	3.0		Yaws (2003)	X	238, 12
	3.2×10^{1}		Wang et al. (2017)	Q	81, 239
	4.5×10^{1}		Wang et al. (2017)	Q	81, 240
	2.5×10^{1}		Wang et al. (2017)	Q	81, 241
	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{2}		Raventos-Duran et al. (2010)	Q	246
	3.2		Gharagheizi et al. (2010)	Q	247
	1.7×10^{1}		Hilal et al. (2008)	Q	
	1.1×10^{1}		Modarresi et al. (2007)	Q	68
		7300	Kühne et al. (2005)	Q	
	1.1×10^{1}		Yao et al. (2002)	Q	230
		4400	Kühne et al. (2005)	?	
	2.2		Yaws (1999)	?	21, 12
1,2-naphthalenedione $C_{10}H_6O_2$ [524-42-5] KETQAJRQOHHATG-UHFFFAOYSA-N	2.3×10^{3}		HSDB (2015)	Q	100
1,4-naphthalenedione	5.0×10^{3}		HSDB (2015)	Q	100
$C_{10}H_6O_2$	1.6×10^{2}		Parnis et al. (2015)	Q	371
(1,4-naphthoquinone) [130-15-4] FRASJONUBLZVQX-UHFFFAOYSA-N					
menadione $C_{11}H_8O_2$ [58-27-5] MJVAVZPDRWSRRC-UHFFFAOYSA-N	3.2×10^{3}		HSDB (2015)	Q	100
2,6-di-*tert*-butyl-*p*-benzoquinone $C_{14}H_{20}O_2$ [719-22-2] RDQSIADLBQFVMY-UHFFFAOYSA-N	6.2×10^{2}		HSDB (2015)	Q	100

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
9,10-phenanthrenedione $C_{14}H_8O_2$ [84-11-7] YYVYAPXYZVYDHN-UHFFFAOYSA-N	3.7×10^{3}		HSDB (2015)	Q	449
9,10-anthracenedione	4.2×10^{2}		Duchowicz et al. (2020)	V	187
$C_{14}H_8O_2$	4.2×10^{2}		HSDB (2015)	V	
[84-65-1]	1.1×10^{-1}		Yaws (2003)	X	238
RZVHIXYEVGDQDX-UHFFFAOYSA-N	4.9×10^{2}		Duchowicz et al. (2020)	Q	
	1.6×10^{2}		Parnis et al. (2015)	Q	371
	3.1×10^{3}		Zhang et al. (2010)	Q	288, 289
	5.6×10^{2}		Zhang et al. (2010)	Q	288, 290
	1.7×10^{2}		Zhang et al. (2010)	Q	288, 291
	2.5×10^{4}		Zhang et al. (2010)	Q	288, 292
	1.1×10^{-1}		Gharagheizi et al. (2010)	Q	247
2-hydroxy-9,10-anthracenedione	5.4×10^{5}		Duchowicz et al. (2020)	V	187
$C_{14}H_8O_3$	2.8×10^{6}		Duchowicz et al. (2020)	Q	
[605-32-3]					
GCDBEYOJCZLKMC-UHFFFAOYSA-N					
1,4-dihydroxy-9,10-anthracenedione	1.2×10^{2}		Duchowicz et al. (2020)	V	187
$C_{14}H_8O_4$	1.4×10^{4}		Duchowicz et al. (2020)	Q	
[81-64-1]					
GUEIZVNYDFNHJU-UHFFFAOYSA-N					
benzil	3.0×10^{1}		Abraham et al. (2019)	Q	
$C_{14}H_{10}O_2$					
[134-81-6]					
WURBFLDFSFBTLW-UHFFFAOYSA-N					
dibenzoylmethane	7.5×10^{3}		Zhang et al. (2010)	Q	288, 289
$C_{15}H_{12}O_2$	8.0×10^{2}		Zhang et al. (2010)	Q	288, 290
[120-46-7]	6.9×10^{4}		Zhang et al. (2010)	Q	288, 291
NZZIMKJIVMHWJC-UHFFFAOYSA-N	1.3×10^{4}		Zhang et al. (2010)	Q	288, 292
2-methyl-9,10-anthracenedione	2.4×10^{2}		Parnis et al. (2015)	Q	371
$C_{15}H_{10}O_2$					
[84-54-8]					
NJWGQARXZDRHCD-UHFFFAOYSA-N					
2-ethyl-9,10-anthracenedione	2.6×10^{1}		Abraham et al. (2019)	Q	
$C_{16}H_{12}O_2$	2.1×10^{3}		Zhang et al. (2010)	Q	288, 289
[84-51-5]	4.2×10^{2}		Zhang et al. (2010)	Q	288, 290
SJEBAWHUJDUKQK-UHFFFAOYSA-N	1.6×10^{2}		Zhang et al. (2010)	Q	288, 291
	1.1×10^{4}		Zhang et al. (2010)	Q	288, 292

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
diphenadione $C_{23}H_{16}O_3$ [82-66-6] JYGLAHSAISAEAL-UHFFFAOYSA-N	6.4×10^{4} 2.9×10^{4}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
MCM:CH3COCO3H $C_3H_4O_4$ BXASKOSTAOGNPV-UHFFFAOYSA-N	6.6×10^{4} 4.7×10^{2} 4.5×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:HYPERACET $C_3H_6O_3$ LSIGHSKIPNHVEN-UHFFFAOYSA-N	5.0×10^{3} 2.1×10^{2} 1.4×10^{2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:BIACETOOH $C_4H_6O_4$ JYWVDPVJSGSFMT-UHFFFAOYSA-N	2.6×10^{6} 1.2×10^{4} 5.6×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:CO2C3CO3H $C_4H_6O_4$ SJOPHMGAZWPERQ-UHFFFAOYSA-N	5.1×10^{4} 6.2×10^{3} 2.8×10^{2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:MEKAOOH $C_4H_8O_3$ VEPDQRPXKSSVPR-UHFFFAOYSA-N	4.0×10^{3} 6.3×10^{3} 1.6×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:MEKBOOH $C_4H_8O_3$ ISENHDUDKGYVAU-UHFFFAOYSA-N	4.7×10^{3} 7.4×10^{1} 2.0×10^{2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:MEKCOOH $C_4H_8O_3$ PSPWSCBXMKHAFW-UHFFFAOYSA-N	4.0×10^{3} 1.0×10^{2} 1.4×10^{2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:MVKOOH $C_4H_6O_3$ PRFKYXWFQJOCGY-UHFFFAOYSA-N	1.1×10^{4} 2.6×10^{2} 9.3×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:C41CO3H $C_5H_8O_4$ FAYQBJFLFGEPOW-UHFFFAOYSA-N	4.8×10^{4} 2.0×10^{3} 3.3		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:C5CO14OOH $C_5H_6O_4$ FKGAAIITVQJZMS-UHFFFAOYSA-N	2.0×10^{5} 7.8×10^{4} 4.4		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:C5CO234 $C_5H_6O_3$ MVDYEFQVZNBPPH-UHFFFAOYSA-N	2.1×10^{4} 2.2×10^{3} 2.5×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C5CO234OOH	1.6×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_5$	3.0×10^{6}		Wang et al. (2017)	Q	81, 240
XNGUZQHZGCMOHY-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C5CO23OOH	2.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	5.3×10^{3}		Wang et al. (2017)	Q	81, 240
BRUGMCFWMGXRAP-UHFFFAOYSA-N	3.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO23C4CO3H	3.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_5$	4.5×10^{5}		Wang et al. (2017)	Q	81, 240
BRGQKBIYWSYIOL-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO23C54OOH	2.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	4.0×10^{3}		Wang et al. (2017)	Q	81, 240
QASRSSCEZIIDDC-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO24C53OOH	2.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	2.1×10^{4}		Wang et al. (2017)	Q	81, 240
AULGAHCEUUOLTF-UHFFFAOYSA-N	8.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO2C4CO3H	1.9×10^{4}	12000	Wieser et al. (2023)	Q	439
$C_5H_8O_4$	4.8×10^{4}		Wang et al. (2017)	Q	81, 239
COVHHGSUFOHLBW-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	81, 240
	7.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO3C4CO3H	4.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	2.5×10^{3}		Wang et al. (2017)	Q	81, 240
HMOQHHYQXPCOJD-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DIEKAOOH	3.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	3.6×10^{1}		Wang et al. (2017)	Q	81, 240
GVIFMISHBUBLQF-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DIEKBOOH	3.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	3.4×10^{3}		Wang et al. (2017)	Q	81, 240
PNIUWVGTVWVIRO-UHFFFAOYSA-N	3.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:MIPKAOOH	2.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	1.6×10^{1}		Wang et al. (2017)	Q	81, 240
UWVYZAHMDOAIIN-UHFFFAOYSA-N	9.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MIPKBOOH	3.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	3.2×10^{3}		Wang et al. (2017)	Q	81, 240
OWEKNVKRJSTQCB-UHFFFAOYSA-N	6.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MPRKAOOH	3.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	4.0×10^{1}		Wang et al. (2017)	Q	81, 240
RFXMBEJILJIJHO-UHFFFAOYSA-N	8.9×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MPRKBOOH	3.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	2.3×10^{3}		Wang et al. (2017)	Q	81, 240
BOKMIGXVNYNOOE-UHFFFAOYSA-N	8.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PE2ONE1OOH	3.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	5.8×10^{1}		Wang et al. (2017)	Q	81, 240
NFPIZNOAHNBIPJ-UHFFFAOYSA-N	3.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C23C54CO3H	3.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	1.7×10^{5}		Wang et al. (2017)	Q	81, 240
FOQTZZGGVXWRDJ-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C3COCCO3H	3.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
NQEGAXBMSWAEEJ-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C4DBDIKET	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_2$	1.8×10^{3}		Wang et al. (2017)	Q	81, 240
OTSKZNVDZOOHRX-UHFFFAOYSA-N	2.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C51CO3H	4.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	3.7×10^{3}		Wang et al. (2017)	Q	81, 240
JNOOBNCRVAKFDO-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C5CODBCO3H	1.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	5.6×10^{4}		Wang et al. (2017)	Q	81, 240
DSQMAYIDJPXZOY-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	81, 241
MCM:C5DBCOCO3H	1.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	5.4×10^{4}		Wang et al. (2017)	Q	81, 240
NVTHKHSWEWVMOZ-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	81, 241
MCM:C611OOH	1.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	3.1×10^{3}		Wang et al. (2017)	Q	81, 240
YTLUYDMGHZZGIK-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C619OOH	6.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	3.0×10^{6}		Wang et al. (2017)	Q	81, 240
CLPCTPYJHZPKKC-UHFFFAOYSA-N	1.9×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C627OOH	1.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	2.3×10^{5}		Wang et al. (2017)	Q	81, 240
BKNNHKNGGIDPKB-UHFFFAOYSA-N	5.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C62OOH	1.5×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	1.4×10^{6}		Wang et al. (2017)	Q	81, 240
NRJLAAIGKSDANL-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C6CO134OOH	2.5×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	2.3×10^{5}		Wang et al. (2017)	Q	81, 240
KXHHBNOARBHHNQ-UHFFFAOYSA-N	3.7×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C6CO34	2.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	5.4		Wang et al. (2017)	Q	81, 240
KVFQMAZOBTXCAZ-UHFFFAOYSA-N	1.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6CO34OOH	2.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	2.0×10^{3}		Wang et al. (2017)	Q	81, 240
GOPKJUXJYMJAQC-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C6CYTONOOH	4.8×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_5$	2.1×10^{9}		Wang et al. (2017)	Q	81, 240
JAWAIWJCDBIXQU-UHFFFAOYSA-N	2.6×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C6DCRBBOOH	1.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	2.9×10^{4}		Wang et al. (2017)	Q	81, 240
JRENYXREJDINFO-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	81, 241
MCM:CO234C6	1.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	1.1×10^{3}		Wang et al. (2017)	Q	81, 240
FYLKBSXPBXZFJV-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:CO234C6OOH	1.5×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
RXZSKHWIVPRCNE-UHFFFAOYSA-N	4.9		Wang et al. (2017)	Q	81, 241
MCM:CO235C6	1.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	3.1×10^{3}		Wang et al. (2017)	Q	81, 240
POASQEFMMPWSLD-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO235C6OOH	1.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	2.9×10^{6}		Wang et al. (2017)	Q	81, 240
OFEOQWJKJVUBKA-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CO23C65OOH	2.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	9.6×10^{4}		Wang et al. (2017)	Q	81, 240
QKJDOFMXAZMTSN-UHFFFAOYSA-N	3.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CO23C6	2.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	6.0		Wang et al. (2017)	Q	81, 240
MWVFCEVNXHTDNF-UHFFFAOYSA-N	7.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:CO24C63OOH	2.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	9.1×10^{3}		Wang et al. (2017)	Q	81, 240
BCTNDVKHSPOTQH-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO24C6	2.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	3.5×10^{1}		Wang et al. (2017)	Q	81, 240
NDOGLIPWGGRQCO-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO24C6OOH	2.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	1.3×10^{4}		Wang et al. (2017)	Q	81, 240
SLWLMHWJPVVUSV-UHFFFAOYSA-N	5.8×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CO24M3C5	3.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	2.1×10^{1}		Wang et al. (2017)	Q	81, 240
GSOHKPVFCOWKPU-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO25C6	2.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	4.9×10^{2}		Wang et al. (2017)	Q	81, 240
OJVAMHKKJGICOG-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CO25C6OOH	2.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	6.6×10^{4}		Wang et al. (2017)	Q	81, 240
JXALTZPWVLRWQW-UHFFFAOYSA-N	6.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:CO2C54CO3H	4.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	3.8×10^{3}		Wang et al. (2017)	Q	81, 240
CNZIZHTUCKWXKF-UHFFFAOYSA-N	4.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO2M33CO3H	2.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	7.1×10^{2}		Wang et al. (2017)	Q	81, 240
NINAOMADVJMMOS-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	81, 241
MCM:CO3C54CO3H	4.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	8.7×10^{2}		Wang et al. (2017)	Q	81, 240
VXADHVSNPNTBLA-UHFFFAOYSA-N	1.8		Wang et al. (2017)	Q	81, 241
MCM:CO3C5CO3H	3.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	5.3×10^{3}		Wang et al. (2017)	Q	81, 240
NEAYDZAAQZUWAX-UHFFFAOYSA-N	3.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CY6COCOOOH	6.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	1.1×10^{8}		Wang et al. (2017)	Q	81, 240
PCNCBCRTMCKUHD-UHFFFAOYSA-N	4.5×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:CY6DIONOOH	6.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	2.2×10^{7}		Wang et al. (2017)	Q	81, 240
WZMMYHNHRXLTAA-UHFFFAOYSA-N	5.8×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:CYC613DION	8.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_2$	2.5×10^{3}		Wang et al. (2017)	Q	81, 240
HJSLFCCWAKVHIW-UHFFFAOYSA-N	2.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:CYC6DIONE	8.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_2$	6.5×10^{2}		Wang et al. (2017)	Q	81, 240
OILAIQUEIWYQPH-UHFFFAOYSA-N	8.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CYHXONAOOH	9.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	4.8×10^{4}		Wang et al. (2017)	Q	81, 240
YLRYKXGGQIKRPE-UHFFFAOYSA-N	5.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:ECO3CO3H	2.0×10^{10}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_6$	2.6×10^{7}		Wang et al. (2017)	Q	81, 240
LOIDTPBEOYVNRI-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:EIPKAOOH	2.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	8.9		Wang et al. (2017)	Q	81, 240
UUAGRKYHKVSONO-UHFFFAOYSA-N	4.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:EIPKBOOH	2.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.7×10^{3}		Wang et al. (2017)	Q	81, 240
GSVDUVPILFIVQC-UHFFFAOYSA-N	5.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HEX2ONAOOH	2.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
BPODHSIMBCVMGL-UHFFFAOYSA-N	2.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HEX2ONBOOH	2.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	3.5×10^{3}		Wang et al. (2017)	Q	81, 240
XXENGSKOCXRCDY-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HEX2ONCOOH	2.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	2.8×10^{1}		Wang et al. (2017)	Q	81, 240
UIIPZQPVNWMUDI-UHFFFAOYSA-N	4.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HEX3ONAOOH	2.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
ZKBVMKAKXKAOJC-UHFFFAOYSA-N	6.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HEX3ONBOOH	2.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	2.2×10^{1}		Wang et al. (2017)	Q	81, 240
CFZVDJFTDOASSJ-UHFFFAOYSA-N	9.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HEX3ONCOOH	2.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	2.3×10^{1}		Wang et al. (2017)	Q	81, 240
RCWXBCITQMXQRJ-UHFFFAOYSA-N	5.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HEX3ONDOOH	2.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	2.2×10^{3}		Wang et al. (2017)	Q	81, 240
GTTLVNDFVPDHBU-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:M2BKAOOH	3.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
UYZBTKCJJDJNOE-UHFFFAOYSA-N	8.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:M2BKBOOH	2.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.1×10^{1}		Wang et al. (2017)	Q	81, 240
HXTZBJMRLHBTDT-UHFFFAOYSA-N	3.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MIBK3CO	3.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	5.1		Wang et al. (2017)	Q	81, 240
JENYBWHRLYZSSZ-UHFFFAOYSA-N	5.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:MIBK3COOOH	1.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	8.9×10^{2}		Wang et al. (2017)	Q	81, 240
REESTLWXXTVHDK-UHFFFAOYSA-N	6.8		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MIBKAOOH	2.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	8.5×10^{2}		Wang et al. (2017)	Q	81, 240
TVLYPTZVJFAYSU-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MIBKBOOH	3.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	3.2×10^{1}		Wang et al. (2017)	Q	81, 240
NTAUGUQNNYBRPR-UHFFFAOYSA-N	3.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MTBKOOH	2.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
FSDVGLADHCPPED-UHFFFAOYSA-N	5.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C235C6CO3H	1.6×10^{10}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_6$	4.4×10^{7}		Wang et al. (2017)	Q	81, 240
MCULIRAVDBAPRO-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C710OOH	1.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_3$	5.1×10^{2}		Wang et al. (2017)	Q	81, 240
WMYMHSKADBIKCY-UHFFFAOYSA-N	6.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C713OOH	1.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	1.2×10^{4}		Wang et al. (2017)	Q	81, 240
BVAIBJLRLSWCNT-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C714OOH	2.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	3.0×10^{4}		Wang et al. (2017)	Q	81, 240
FQLJODGQMVISEK-UHFFFAOYSA-N	2.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C715OOH	8.3×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	2.5×10^{5}		Wang et al. (2017)	Q	81, 240
IFAJGMRYFBSYLP-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C7236CO	6.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_3$	6.8×10^{4}		Wang et al. (2017)	Q	81, 240
ZXGNNLLPQXKXPQ-UHFFFAOYSA-N	8.7		Wang et al. (2017)	Q	81, 241
MCM:C726CO5OOH	7.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	1.0×10^{5}		Wang et al. (2017)	Q	81, 240
DRGOPDAWFSWANX-UHFFFAOYSA-N	6.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C727CO	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	5.6×10^{3}		Wang et al. (2017)	Q	81, 240
XDJAUXXWCBLXGT-UHFFFAOYSA-N	6.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C727OOH	2.0×10^{5}	13000	Wieser et al. (2023)	Q	439
$C_7H_{12}O_4$	1.8×10^{6}		Wang et al. (2017)	Q	81, 239
IMCLYNFQESJQRO-UHFFFAOYSA-N	4.3×10^{4}		Wang et al. (2017)	Q	81, 240
	9.8×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C73OOH	1.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
QFXLTANEYKLVBH-UHFFFAOYSA-N	7.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C74OOH	1.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	1.4×10^{6}		Wang et al. (2017)	Q	81, 240
ZLQFKUKGFNRBMM-UHFFFAOYSA-N	4.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C75OOH	2.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_3$	8.9×10^{2}		Wang et al. (2017)	Q	81, 240
YNKFHYFADYHYPZ-UHFFFAOYSA-N	1.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C7ADCCO3H	8.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	6.5×10^{4}		Wang et al. (2017)	Q	81, 240
KFHCVBUEDOHUEG-UHFFFAOYSA-N	5.0		Wang et al. (2017)	Q	81, 241
MCM:C7BDICARB	6.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_2$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
SGWFXGZCQBUONH-UHFFFAOYSA-N	3.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C7DCCO3H	1.4×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	1.5×10^{4}		Wang et al. (2017)	Q	81, 240
VBFDFNFUMYAFQG-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	81, 241
MCM:C7DDCCO3H	1.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	2.2×10^{4}		Wang et al. (2017)	Q	81, 240
ITRURPAVBUVUCD-UHFFFAOYSA-N	5.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C7EDICARB	9.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_2$	1.1×10^{3}		Wang et al. (2017)	Q	81, 240
YTVSAHBJOWKZHT-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C821OOH	1.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	2.6×10^{6}		Wang et al. (2017)	Q	81, 240
VNKKTGYQOPWEKF-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CO235C7	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	9.6×10^{2}		Wang et al. (2017)	Q	81, 240
PLNIROICNOROEN-UHFFFAOYSA-N	9.6		Wang et al. (2017)	Q	81, 241
MCM:CO245C7	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	9.6×10^{2}		Wang et al. (2017)	Q	81, 240
SOSHREJUCDQQIR-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO25C6CO3H	2.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	4.6×10^{6}		Wang et al. (2017)	Q	81, 240
NZAOVWOYFADSGM-UHFFFAOYSA-N	7.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:CO25C73OOH	1.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	2.8×10^{4}		Wang et al. (2017)	Q	81, 240
NWTMJMDPQCUZCE-UHFFFAOYSA-N	9.1×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CO25C74OOH	1.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	2.8×10^{4}		Wang et al. (2017)	Q	81, 240
VDRXHYKLZSMLBZ-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:CO25C7	2.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_2$	2.6×10^{2}		Wang et al. (2017)	Q	81, 240
HGRGPAAXHOTBAM-UHFFFAOYSA-N	8.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO3C75OOH	2.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_3$	8.0×10^{2}		Wang et al. (2017)	Q	81, 240
TVVPPVSOZMPRIM-UHFFFAOYSA-N	4.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:IC7DCCO3H	1.4×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	1.6×10^{4}		Wang et al. (2017)	Q	81, 240
JFPQYVJBAXIOAT-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:M3CO245C6	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	6.3×10^{2}		Wang et al. (2017)	Q	81, 240
FMABCBYNHKBBEH-UHFFFAOYSA-N	8.5		Wang et al. (2017)	Q	81, 241
MCM:M3CO25C6	2.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_2$	1.8×10^{2}		Wang et al. (2017)	Q	81, 240
NLLILAUVOOREKR-UHFFFAOYSA-N	8.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C5DBECO3H	6.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_5$	1.5×10^{6}		Wang et al. (2017)	Q	81, 240
QHSWUEYXPZRIAH-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
MCM:C5EDBCO3H	6.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_5$	1.6×10^{6}		Wang et al. (2017)	Q	81, 240
YXJCVNQUVAHMKT-UHFFFAOYSA-N	6.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C727CO3H	2.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	9.6×10^{5}		Wang et al. (2017)	Q	81, 240
FJTLPXSURBYIDW-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C7CO2M5OOH	4.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
GOMWBXPFFZKXIF-UHFFFAOYSA-N	2.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C7M2CO5OOH	4.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	7.6×10^{4}		Wang et al. (2017)	Q	81, 240
BVDWDBGMQXZSJX-UHFFFAOYSA-N	4.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C7M3CO	4.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_3$	8.1×10^{4}		Wang et al. (2017)	Q	81, 240
WFGYJTNUNWJHJN-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C7ODLBCO3H	8.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	1.2×10^{4}		Wang et al. (2017)	Q	81, 240
NMESNSUDSMNPLZ-UHFFFAOYSA-N	3.2×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C816CO	3.1×10^{2}	10000	Wieser et al. (2023)	Q	439
$C_8H_{12}O_2$	3.8×10^{1}		Wang et al. (2017)	Q	81, 239
FXXXYZSMIIVJDG-UHFFFAOYSA-N	3.0×10^{2}		Wang et al. (2017)	Q	81, 240
	6.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C816OOH	4.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_3$	2.0×10^{3}		Wang et al. (2017)	Q	81, 240
GWYFGLCLLKWWIQ-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C817OOH	1.2×10^{6}	13000	Wieser et al. (2023)	Q	439
$C_8H_{14}O_4$	1.5×10^{6}		Wang et al. (2017)	Q	81, 239
WQMXPSRLZZCZTO-UHFFFAOYSA-N	1.5×10^{6}		Wang et al. (2017)	Q	81, 240
	1.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C8236CO	4.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_3$	6.0×10^{4}		Wang et al. (2017)	Q	81, 240
IOHUPZZTKNTURH-UHFFFAOYSA-N	4.8		Wang et al. (2017)	Q	81, 241
MCM:C826CO3OOH	6.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	4.4×10^{4}		Wang et al. (2017)	Q	81, 240
JGDMXPACXAYITG-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C827OOH	9.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_4$	1.5×10^{4}		Wang et al. (2017)	Q	81, 240
MYZHYUNBFYQPIX-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C828OOH	6.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	3.1×10^{5}		Wang et al. (2017)	Q	81, 240
IPIPKWBUGMDLTO-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C83OOH	1.1×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	3.6×10^{5}		Wang et al. (2017)	Q	81, 240
MTDHYROWVQXAOV-UHFFFAOYSA-N	5.6		Wang et al. (2017)	Q	81, 241
MCM:C84OOH	1.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_4$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
HQUQRVBRCVTTSE-UHFFFAOYSA-N	7.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C85OOH	5.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_3$	5.5×10^{3}		Wang et al. (2017)	Q	81, 240
MGHQHHXZPXRHRQ-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C88CO	2.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_3$	7.4×10^{4}		Wang et al. (2017)	Q	81, 240
KYJUTSWXKQCOOZ-UHFFFAOYSA-N	3.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C88OOH	3.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	6.9×10^{5}		Wang et al. (2017)	Q	81, 240
LSPOECQNSUKNPK-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C8BCCO	2.0×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O$	9.6×10^{-1}		Wang et al. (2017)	Q	81, 240
BYOKRVKHSHTAOM-UHFFFAOYSA-N	3.7		Wang et al. (2017)	Q	81, 241
MCM:CO346C8	1.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_3$	1.1×10^{3}		Wang et al. (2017)	Q	81, 240
YUHNMHTZZXLCQZ-UHFFFAOYSA-N	7.3		Wang et al. (2017)	Q	81, 241
MCM:CO36C8	1.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_2$	1.5×10^{2}		Wang et al. (2017)	Q	81, 240
CVZGUJMLZZTPKH-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO3C85OOH	2.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{16}O_3$	5.9×10^{2}		Wang et al. (2017)	Q	81, 240
RPACFUNWVVDXHA-UHFFFAOYSA-N	3.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MXYQONE	2.1		Wang et al. (2017)	Q	81, 239
$C_8H_8O_2$	5.3×10^{3}		Wang et al. (2017)	Q	81, 240
SENUUPBBLQWHMF-UHFFFAOYSA-N	1.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:OXYQONE	2.1		Wang et al. (2017)	Q	81, 239
$C_8H_8O_2$	5.3×10^{3}		Wang et al. (2017)	Q	81, 240
AIACLXROWHONEE-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PEBQONE	2.7		Wang et al. (2017)	Q	81, 239
$C_8H_8O_2$	4.7×10^{3}		Wang et al. (2017)	Q	81, 240
IGRSQEOIAAGSGS-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PXYQONE	2.1		Wang et al. (2017)	Q	81, 239
$C_8H_8O_2$	5.3×10^{3}		Wang et al. (2017)	Q	81, 240
MYKLQMNSFPAPLZ-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C816CO3H	5.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	1.5×10^{3}		Wang et al. (2017)	Q	81, 240
IXOBJDNIWKDFSA-UHFFFAOYSA-N	3.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C817CO3H	3.4×10^{7}	16000	Wieser et al. (2023)	Q	439
$C_9H_{14}O_5$	1.7×10^{7}		Wang et al. (2017)	Q	81, 239
NVOUBBWYYUIRJW-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	81, 240
	2.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C827CO3H	1.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	6.0×10^{5}		Wang et al. (2017)	Q	81, 240
DZJUGPICXPPSEN-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C828CO3H	7.8×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_6$	2.0×10^{7}		Wang et al. (2017)	Q	81, 240
XCCOWFUPSKLDCA-UHFFFAOYSA-N	8.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C85CO3H	5.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	3.8×10^{3}		Wang et al. (2017)	Q	81, 240
DAYKQISVSRMABH-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C88CO3H	3.7×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	2.0×10^{7}		Wang et al. (2017)	Q	81, 240
KOEDWBONHQRVNE-UHFFFAOYSA-N	4.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C8M2CO6OOH	3.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	3.3×10^{4}		Wang et al. (2017)	Q	81, 240
LMHVWEUXUKAUEE-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C8M3CO	3.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	6.0×10^{4}		Wang et al. (2017)	Q	81, 240
VNKKGGMTAOGJCS-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C917OOH	2.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	1.2×10^{7}		Wang et al. (2017)	Q	81, 240
USPARXGTYFQAAO-UHFFFAOYSA-N	1.2×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C91OOH	1.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{18}O_3$	4.9×10^{2}		Wang et al. (2017)	Q	81, 240
LTHHCRGMHVQJHW-UHFFFAOYSA-N	4.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C923OOH	1.1×10^{4}	12000	Wieser et al. (2023)	Q	439
$C_9H_{16}O_3$	4.1×10^{3}		Wang et al. (2017)	Q	81, 239
ZSCOJLRNNZZYOH-UHFFFAOYSA-N	2.2×10^{3}		Wang et al. (2017)	Q	81, 240
	2.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C928OOH	8.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_4$	1.4×10^{6}		Wang et al. (2017)	Q	81, 240
NVMDAOHKHIQTQS-UHFFFAOYSA-N	1.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C94OOH	1.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_4$	9.3×10^{3}		Wang et al. (2017)	Q	81, 240
ZEMHBLLRPWJDGD-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C95OOH	8.7×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	2.3×10^{5}		Wang et al. (2017)	Q	81, 240
OKPNQXXXVOPUSS-UHFFFAOYSA-N	5.4		Wang et al. (2017)	Q	81, 241
MCM:C96OOH	4.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_3$	6.9×10^{3}		Wang et al. (2017)	Q	81, 240
UOSOYGOFRNBVGT-UHFFFAOYSA-N	4.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C9DC	1.2×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	2.3×10^{3}		Wang et al. (2017)	Q	81, 240
MRLMBLCAGJIZHM-UHFFFAOYSA-N	4.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C9DCCO	9.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_3$	7.6×10^{5}		Wang et al. (2017)	Q	81, 240
CNGBBXSWKSNDLL-UHFFFAOYSA-N	2.4×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C9DCOOH	1.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	8.3×10^{7}		Wang et al. (2017)	Q	81, 240
LVYPIBNFNZWAIN-UHFFFAOYSA-N	2.8×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:CO356C9	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_3$	1.1×10^{3}		Wang et al. (2017)	Q	81, 240
UAWDJSGDSYOWDW-UHFFFAOYSA-N	5.3		Wang et al. (2017)	Q	81, 241
MCM:CO36C9	1.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_2$	1.0×10^{2}		Wang et al. (2017)	Q	81, 240
NTESOQURXNMSRF-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:IPRBQONE	2.5		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_2$	2.4×10^{3}		Wang et al. (2017)	Q	81, 240
XLTSBDOZTUSCMX-UHFFFAOYSA-N	8.7		Wang et al. (2017)	Q	81, 241
MCM:LIMKET	6.4×10^{-1}	8000	Wieser et al. (2023)	Q	439
$C_9H_{14}O$	2.4×10^{-1}		Wang et al. (2017)	Q	81, 239
HOBBEYSRFFJETF-UHFFFAOYSA-N	9.8×10^{-1}		Wang et al. (2017)	Q	81, 240
	3.2		Wang et al. (2017)	Q	81, 241
MCM:METLQONE	1.8		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_2$	3.7×10^{3}		Wang et al. (2017)	Q	81, 240
FBVFNJVAQSWLOP-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NOPINAOOH	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_3$	2.9×10^{4}		Wang et al. (2017)	Q	81, 240
AGOGLNHOAIUZEO-UHFFFAOYSA-N	8.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NOPINBCO	1.2×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	2.2×10^{3}		Wang et al. (2017)	Q	81, 240
AQDJLLQBBRXMBZ-UHFFFAOYSA-N	4.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NOPINBOOH	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_3$	4.0×10^{4}		Wang et al. (2017)	Q	81, 240
ICIAOEDGJQUKIV-UHFFFAOYSA-N	9.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NOPINCOOH	8.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_3$	1.3×10^{4}		Wang et al. (2017)	Q	81, 240
YDBPVAMAGOPNKC-UHFFFAOYSA-N	7.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NOPINDCO	1.2×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_2$	5.0×10^{2}		Wang et al. (2017)	Q	81, 240
QEZVNLZLSDOZRT-UHFFFAOYSA-N	8.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NOPINDOOH	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_3$	5.4×10^{2}		Wang et al. (2017)	Q	81, 240
MUTHAEIFCDWSQQ-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NOPINONE	1.8×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O$	1.0		Wang et al. (2017)	Q	81, 240
XZFDKWMYCUEKSS-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:OETLQONE	1.8		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_2$	3.7×10^{3}		Wang et al. (2017)	Q	81, 240
CMBANAGVBLPIPT-UHFFFAOYSA-N	8.1		Wang et al. (2017)	Q	81, 241
MCM:PETLQONE	1.8		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_2$	3.7×10^{3}		Wang et al. (2017)	Q	81, 240
JUIQOKRNPGGIPV-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PPRBQONE	2.2		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_2$	3.0×10^{3}		Wang et al. (2017)	Q	81, 240
NBHAZVWKRHTWRW-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:TM124QONE	1.4		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_2$	4.1×10^{3}		Wang et al. (2017)	Q	81, 240
QIXDHVDGPXBRRD-UHFFFAOYSA-N	7.3		Wang et al. (2017)	Q	81, 241
MCM:C1011CO	3.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_2$	3.3×10^{2}		Wang et al. (2017)	Q	81, 240
HCTKOTXYXFZDNL-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C1011OOH	3.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_3$	4.3×10^{3}		Wang et al. (2017)	Q	81, 240
SNMQVMGNQAVOQP-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C101OOH	1.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{20}O_3$	4.4×10^{2}		Wang et al. (2017)	Q	81, 240
SFSDJTUNVGVIHA-UHFFFAOYSA-N	3.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C104OOH	1.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_4$	6.9×10^{3}		Wang et al. (2017)	Q	81, 240
NAKDXHBWPFMZPE-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C105OOH	7.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_5$	1.7×10^{5}		Wang et al. (2017)	Q	81, 240
SMUSKFONQIUMCM-UHFFFAOYSA-N	2.9		Wang et al. (2017)	Q	81, 241
MCM:C923CO3H	2.2×10^{4}	15000	Wieser et al. (2023)	Q	439
$C_{10}H_{16}O_4$	4.7×10^{4}		Wang et al. (2017)	Q	81, 239
JSHGCXGTVADTAK-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	81, 240
	3.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C928CO3H	9.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_5$	1.5×10^{6}		Wang et al. (2017)	Q	81, 240
LCMHUZKVXFPENZ-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C9M2CO6OOH	3.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_4$	1.9×10^{4}		Wang et al. (2017)	Q	81, 240
ACPAJMUJFSDSAX-UHFFFAOYSA-N	9.6×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C9M3CO	3.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{14}O_3$	3.5×10^{4}		Wang et al. (2017)	Q	81, 240
DYAPBQRZCBYWEA-UHFFFAOYSA-N	9.3		Wang et al. (2017)	Q	81, 241
MCM:CO356C10	8.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_3$	9.1×10^{2}		Wang et al. (2017)	Q	81, 240
OKXFSYMNZFSQOL-UHFFFAOYSA-N	4.7		Wang et al. (2017)	Q	81, 241
MCM:CO36C10	1.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_2$	8.0×10^{1}		Wang et al. (2017)	Q	81, 240
WYDYPTCJLWEFAY-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DEC3ONE	1.8×10^{-2}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{20}O$	2.6×10^{-2}		Wang et al. (2017)	Q	81, 240
XJLDYKIEURAVBW-UHFFFAOYSA-N	1.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:PERPINONIC	5.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_4$	3.0×10^{3}		Wang et al. (2017)	Q	81, 240
VFMYUIAYOIIENK-UHFFFAOYSA-N	5.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C1011CO3H	4.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_4$	2.5×10^{3}		Wang et al. (2017)	Q	81, 240
MDKPIQZZHUIYJQ-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C111OOH	1.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{22}O_3$	3.6×10^{2}		Wang et al. (2017)	Q	81, 240
AMIJEMPORNLGBW-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C114OOH	8.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{20}O_4$	5.4×10^{3}		Wang et al. (2017)	Q	81, 240
YQNGKLISCMALPY-UHFFFAOYSA-N	4.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C115OOH	6.3×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_5$	1.3×10^{5}		Wang et al. (2017)	Q	81, 240
VPBZYPGTLQIJKG-UHFFFAOYSA-N	6.0		Wang et al. (2017)	Q	81, 241
MCM:CO356C11	7.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_3$	7.8×10^{2}		Wang et al. (2017)	Q	81, 240
YADKKYWEPSBFCL-UHFFFAOYSA-N	4.9		Wang et al. (2017)	Q	81, 241
MCM:CO36C11	1.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{20}O_2$	6.5×10^{1}		Wang et al. (2017)	Q	81, 240
KWHQQLQVDJMZTG-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:UDEC3ONE	1.4×10^{-2}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{22}O$	2.1×10^{-2}		Wang et al. (2017)	Q	81, 240
YNMZZHPSYMOGCI-UHFFFAOYSA-N	1.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C121OOH	9.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{24}O_3$	2.8×10^{2}		Wang et al. (2017)	Q	81, 240
NWJGDRGQGOZUDJ-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C124OOH	6.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{22}O_4$	4.8×10^{3}		Wang et al. (2017)	Q	81, 240
DCPRRPHGFZBUMW-UHFFFAOYSA-N	9.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C125OOH	4.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_5$	1.1×10^{5}		Wang et al. (2017)	Q	81, 240
FTFXETPWXOMYNK-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO356C12	5.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_3$	7.3×10^{2}		Wang et al. (2017)	Q	81, 240
FQYVJQVZHPFSKC-UHFFFAOYSA-N	3.9		Wang et al. (2017)	Q	81, 241
MCM:CO36C12	8.5		Wang et al. (2017)	Q	81, 239
$C_{12}H_{22}O_2$	5.8×10^{1}		Wang et al. (2017)	Q	81, 240
RUTQSYKISNASLK-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DDEC3ONE	1.1×10^{-2}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{24}O$	1.7×10^{-2}		Wang et al. (2017)	Q	81, 240
PERIHWAPLOBAJM-UHFFFAOYSA-N	9.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C131OOH	1.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_4$	2.0×10^{6}		Wang et al. (2017)	Q	81, 240
HPZPYFVEAXAGHY-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:BCKET	2.3×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O$	2.6		Wang et al. (2017)	Q	81, 240
MBZBBVTYLUNZPJ-UHFFFAOYSA-N	2.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C131CO3H	1.7×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_5$	2.1×10^{6}		Wang et al. (2017)	Q	81, 240
LLSRBTGTUZNRQT-UHFFFAOYSA-N	8.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C141OOH	3.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{24}O_3$	4.9×10^{3}		Wang et al. (2017)	Q	81, 240
HKWHMEKBBPOBSQ-UHFFFAOYSA-N	7.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C141CO3H	4.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{24}O_4$	1.8×10^{3}		Wang et al. (2017)	Q	81, 240
ADRMPTUALHKSOU-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C619CO	5.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_3$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
NGHVTTBOPYXCFB-UHFFFAOYSA-N	1.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:CY6TRION	5.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_3$	4.6×10^{6}		Wang et al. (2017)	Q	81, 240
GKSCYYCYSPXQFY-UHFFFAOYSA-N	1.9×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PHCOMEOOH	1.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_8O_3$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
BXVCLOREWFXMNM-UHFFFAOYSA-N	3.7×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MPHCOMEOOH	9.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_3$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
NJDRUBYBGCJLGU-UHFFFAOYSA-N	3.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PHCOCOCOOH	9.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_8O_4$	4.7×10^{4}		Wang et al. (2017)	Q	81, 240
XMJMKOZGMVOAIC-UHFFFAOYSA-N	5.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PHCOCOME	1.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_8O_2$	9.1×10^{1}		Wang et al. (2017)	Q	81, 240
BVQVLAIMHVDZEL-UHFFFAOYSA-N	6.9		Wang et al. (2017)	Q	81, 241
MCM:PHCOETOOH	1.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_3$	6.0×10^{2}		Wang et al. (2017)	Q	81, 240
RYQHVKZCKUBIFL-UHFFFAOYSA-N	3.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DMPHCOME	7.4×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{12}O$	1.5		Wang et al. (2017)	Q	81, 240
BKIHFZLJJUNKMZ-UHFFFAOYSA-N	5.4		Wang et al. (2017)	Q	81, 241
MCM:DMPHCOMOOH	5.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{12}O_3$	8.5×10^{2}		Wang et al. (2017)	Q	81, 240
SEDWELDPOZYWLL-UHFFFAOYSA-N	3.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:EMPHCOME	6.5×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{14}O$	1.2		Wang et al. (2017)	Q	81, 240
CZNQKVDFQIGBEW-UHFFFAOYSA-N	5.0		Wang et al. (2017)	Q	81, 241
MCM:EMPHCOMOOH	5.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{14}O_3$	5.0×10^{2}		Wang et al. (2017)	Q	81, 240
OJNDCDHAKIGFTB-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:BIACETOH	5.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_3$	4.3×10^{3}		Wang et al. (2017)	Q	81, 240
NXIVQSJQXMAXJR-UHFFFAOYSA-N	3.7		Wang et al. (2017)	Q	81, 241
MCM:CO2H3CO3H	2.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_5$	1.7×10^{4}		Wang et al. (2017)	Q	81, 240
WNDCXKJVOGKFRM-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:H13CO2CO3H	1.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_6$	4.0×10^{5}		Wang et al. (2017)	Q	81, 240
RXVYYLAFXUAZCR-UHFFFAOYSA-N	1.7×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:H14CO23C4	2.1×10^{6}	17000	Wieser et al. (2023)	Q	439
$C_4H_6O_4$	6.5×10^{5}		Wang et al. (2017)	Q	81, 239
GJCZUCLKDGABDS-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	81, 240
	1.6×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:H1C23C4OOH	3.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_5$	6.0×10^{7}		Wang et al. (2017)	Q	81, 240
FQXHRCVOGVCTSR-UHFFFAOYSA-N	3.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HMVKAOOH	8.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	7.8×10^{4}		Wang et al. (2017)	Q	81, 240
XTELZFGIGJBUGR-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HMVKBOOH	1.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	2.0×10^{5}		Wang et al. (2017)	Q	81, 240
NGLQGLCPXKPDMS-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO12CO3C4	9.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	3.7×10^{4}		Wang et al. (2017)	Q	81, 240
SEYLPRWNVFCVRQ-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO14CO2C4	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	9.8×10^{5}		Wang et al. (2017)	Q	81, 240
XBJODPUPYBBDEM-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HOCO3C4OOH	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	1.9×10^{6}		Wang et al. (2017)	Q	81, 240
GQXQZBROPOTXJQ-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:MEKAOH	1.5×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_2$	1.2×10^{3}		Wang et al. (2017)	Q	81, 240
LVSQXDHWDCMMRJ-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MEKCOH	7.8		Wang et al. (2017)	Q	81, 239
$C_4H_8O_2$	7.8×10^{1}		Wang et al. (2017)	Q	81, 240
GFAZHVHNLUBROE-UHFFFAOYSA-N	8.3		Wang et al. (2017)	Q	81, 241
MCM:MVKOHAOH	6.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	3.7×10^{6}		Wang et al. (2017)	Q	81, 240
UQPHVQVXLPRNCX-UHFFFAOYSA-N	8.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:MVKOHAOOH	4.6×10^{8}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_5$	2.2×10^{7}		Wang et al. (2017)	Q	81, 240
MOVXURHCNUWOQO-UHFFFAOYSA-N	1.8×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:MVKOHBOOH	2.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_5$	2.7×10^{8}		Wang et al. (2017)	Q	81, 240
WSMWIMXDHMPHIN-UHFFFAOYSA-N	5.8×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:MVKOH	2.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_2$	2.3×10^{2}		Wang et al. (2017)	Q	81, 240
LHBQGXZUVXFJRH-UHFFFAOYSA-N	4.9		Wang et al. (2017)	Q	81, 241
MCM:C517OH	3.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	1.6×10^{6}		Wang et al. (2017)	Q	81, 240
NQMZUMSFJBKHAU-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C517OOH	1.1×10^{6}	13000	Wieser et al. (2023)	Q	439
$C_5H_{10}O_4$	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
OAFCGFSFCVGKSH-UHFFFAOYSA-N	4.9×10^{5}		Wang et al. (2017)	Q	81, 240
	1.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C519OOH	1.7×10^{5}	13000	Wieser et al. (2023)	Q	439
$C_5H_{10}O_4$	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
RDSFTYTWLRHJGZ-UHFFFAOYSA-N	4.0×10^{5}		Wang et al. (2017)	Q	81, 240
	8.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C51OH2CO	6.0		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	4.2×10^{1}		Wang et al. (2017)	Q	81, 240
WOVLKKLXYZJMSN-UHFFFAOYSA-N	9.6		Wang et al. (2017)	Q	81, 241
MCM:C51OH	1.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	2.1×10^{5}		Wang et al. (2017)	Q	81, 240
NJUQBPDKVORANW-UHFFFAOYSA-N	4.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C51OOH	1.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	2.1×10^{6}		Wang et al. (2017)	Q	81, 240
IZBMMNKBXWVQLB-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C521OH	1.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	4.8×10^{7}		Wang et al. (2017)	Q	81, 240
UOGQGBWLBZOULD-UHFFFAOYSA-N	9.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C521OOH	6.5×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	1.9×10^{7}		Wang et al. (2017)	Q	81, 240
INSNYERMNWOCIO-UHFFFAOYSA-N	2.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C524CO	3.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	1.9×10^{5}		Wang et al. (2017)	Q	81, 240
JVFYSLPFISVGRS-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C525OOH	3.8×10^{12}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_6$	2.0×10^{11}		Wang et al. (2017)	Q	81, 240
KYXSOONCNSTMJK-UHFFFAOYSA-N	3.1×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C53OH	1.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
PLVCXNLHUHTLCR-UHFFFAOYSA-N	6.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C53OOH	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	1.8×10^{6}		Wang et al. (2017)	Q	81, 240
VCGFNBZCPLQTJR-UHFFFAOYSA-N	6.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C55OOH	3.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	1.3×10^{6}		Wang et al. (2017)	Q	81, 240
IEXMEMALQGQSKE-UHFFFAOYSA-N	2.8×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C59OOH	1.1×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_5$	1.6×10^{8}		Wang et al. (2017)	Q	81, 240
JWNCLQLBUYGJMN-UHFFFAOYSA-N	3.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C5CO243OH	1.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
SLKPFOVYRYRNBA-UHFFFAOYSA-N	9.8		Wang et al. (2017)	Q	81, 241
MCM:C5OHCO4OOH	4.7×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	1.6×10^{6}		Wang et al. (2017)	Q	81, 240
DSLVXKSJLFFUGE-UHFFFAOYSA-N	4.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:CO2C5OH	3.6×10^{3}	9800	Wieser et al. (2023)	Q	439
$C_5H_{10}O_2$	1.2×10^{2}		Wang et al. (2017)	Q	81, 239
JSHPTIGHEWEXRW-UHFFFAOYSA-N	2.6×10^{3}		Wang et al. (2017)	Q	81, 240
	1.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:CO2H3MCO3H	1.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	3.2×10^{3}		Wang et al. (2017)	Q	81, 240
LZACDMRRAOGIBF-UHFFFAOYSA-N	3.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO3H4CO3H	1.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	1.0×10^{4}		Wang et al. (2017)	Q	81, 240
LAOPLCWFGWEKGR-UHFFFAOYSA-N	1.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DIEKAOH	7.3		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	6.8×10^{1}		Wang et al. (2017)	Q	81, 240
QMXCHEVUAIPIRM-UHFFFAOYSA-N	7.6		Wang et al. (2017)	Q	81, 241
MCM:H3C2C4CO3H	6.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	3.0×10^{6}		Wang et al. (2017)	Q	81, 240
NYZNEBYYPQANOB-UHFFFAOYSA-N	6.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HC23C4CO3H	4.5×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_6$	1.1×10^{8}		Wang et al. (2017)	Q	81, 240
UQNPRLJBDVQJQC-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HCOC5	1.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_2$	1.4×10^{2}		Wang et al. (2017)	Q	81, 240
LSMLKPXBSFFBNR-UHFFFAOYSA-N	3.4		Wang et al. (2017)	Q	81, 241
MCM:HMVKBCO3H	1.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	5.8×10^{6}		Wang et al. (2017)	Q	81, 240
VFNFGUWSZFHBRW-UHFFFAOYSA-N	2.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO13CO4C5	1.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	2.6×10^{5}		Wang et al. (2017)	Q	81, 240
CGPIPFJOMJUWGK-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HO14CO2C5	1.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	1.5×10^{6}		Wang et al. (2017)	Q	81, 240
XLDKDOKPMNKVMP-UHFFFAOYSA-N	4.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO14CO3C5	1.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	1.6×10^{6}		Wang et al. (2017)	Q	81, 240
YMIRTILUDYUWGY-UHFFFAOYSA-N	4.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO1CO24C5	4.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	3.2×10^{4}		Wang et al. (2017)	Q	81, 240
VBUBLWCIADYRMB-UHFFFAOYSA-N	4.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO1CO34C5	7.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	4.7×10^{4}		Wang et al. (2017)	Q	81, 240
LKLKMCUVBQDYFU-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO1CO3C5	1.2×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	4.6×10^{2}		Wang et al. (2017)	Q	81, 240
TYXULUBCBKMSSK-UHFFFAOYSA-N	6.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO2CO4C5	1.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
PCYZZYAEGNVNMH-UHFFFAOYSA-N	9.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HOCO3C5OOH	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	1.3×10^{6}		Wang et al. (2017)	Q	81, 240
ZLPJDXTYGYNOQK-UHFFFAOYSA-N	4.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HOCO4C5OOH	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	1.9×10^{6}		Wang et al. (2017)	Q	81, 240
MYGJVQXASPJPCS-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:MBOACO	2.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	9.8×10^{2}		Wang et al. (2017)	Q	81, 240
FEIUXLCYYBVUGD-UHFFFAOYSA-N	6.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:ME3CO2BUOL	7.3		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	4.6×10^{1}		Wang et al. (2017)	Q	81, 240
NBEGXSQMVJTIAR-UHFFFAOYSA-N	6.8		Wang et al. (2017)	Q	81, 241
MCM:MIPKAOH	4.5		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	4.4×10^{1}		Wang et al. (2017)	Q	81, 240
BNDRWEVUODOUDW-UHFFFAOYSA-N	7.6		Wang et al. (2017)	Q	81, 241
MCM:MIPKBOH	1.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	6.3×10^{2}		Wang et al. (2017)	Q	81, 240
VVSRECWZBBJOTG-UHFFFAOYSA-N	6.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MPRKAOH	7.3		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	8.5×10^{1}		Wang et al. (2017)	Q	81, 240
HDKKRASBPHFULQ-UHFFFAOYSA-N	4.9		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:BZOBIPEROH	6.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_4$	3.6×10^{3}		Wang et al. (2017)	Q	81, 240
OGRXSIBGKCRBOL-UHFFFAOYSA-N	1.7×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C4COMEOH	5.0		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	2.7×10^{1}		Wang et al. (2017)	Q	81, 240
FDJJNIXWMAWMBP-UHFFFAOYSA-N	8.0		Wang et al. (2017)	Q	81, 241
MCM:C4COMOH3OH	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	7.6×10^{5}		Wang et al. (2017)	Q	81, 240
NCEURKGQTPCVEC-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C4COMOHOOH	4.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	8.9×10^{5}		Wang et al. (2017)	Q	81, 240
JZGTXIGKACACHL-UHFFFAOYSA-N	3.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C4MOHOCO3H	1.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	5.4×10^{3}		Wang et al. (2017)	Q	81, 240
BJXKNHIKUQDPQL-UHFFFAOYSA-N	8.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C517CO3H	1.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	1.1×10^{7}		Wang et al. (2017)	Q	81, 240
HTNOTPIWPYZOLN-UHFFFAOYSA-N	7.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C519CO3H	1.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	1.6×10^{7}		Wang et al. (2017)	Q	81, 240
OBKQTPZEBCGGJT-UHFFFAOYSA-N	5.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C5COHOCO3H	5.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_6$	2.3×10^{5}		Wang et al. (2017)	Q	81, 240
BPYCYKKOURHNJX-UHFFFAOYSA-N	8.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C5O5OHCO3H	1.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	4.8×10^{3}		Wang et al. (2017)	Q	81, 240
GCQMJNYHSPBFDA-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C610OH	1.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	2.4×10^{5}		Wang et al. (2017)	Q	81, 240
YFEDHAOQJOZUIL-UHFFFAOYSA-N	2.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C610OOH	1.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	2.0×10^{6}		Wang et al. (2017)	Q	81, 240
VBEFRWQFSDXQDV-UHFFFAOYSA-N	6.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C611OH	5.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	3.0×10^{3}		Wang et al. (2017)	Q	81, 240
PYRMISJRKRVNPG-UHFFFAOYSA-N	3.5		Wang et al. (2017)	Q	81, 241
MCM:C612OH	9.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	6.0×10^{5}		Wang et al. (2017)	Q	81, 240
VCLSUNMNDIKRMY-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C612OOH	5.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	9.3×10^{5}		Wang et al. (2017)	Q	81, 240
OANIXDZJWBEQCD-UHFFFAOYSA-N	5.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C613OOH	1.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_5$	2.0×10^{8}		Wang et al. (2017)	Q	81, 240
MBLADDFAKVGAFO-UHFFFAOYSA-N	1.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C614CO	2.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	1.4×10^{6}		Wang et al. (2017)	Q	81, 240
DFWHGSVPVJPYJZ-UHFFFAOYSA-N	8.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C614OH	9.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	9.1×10^{6}		Wang et al. (2017)	Q	81, 240
WLPHOQAEOJPJID-UHFFFAOYSA-N	8.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C614OOH	7.8×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	8.3×10^{7}		Wang et al. (2017)	Q	81, 240
AZSLPKKGLPCKMI-UHFFFAOYSA-N	4.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C619OH	1.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	2.5×10^{6}		Wang et al. (2017)	Q	81, 240
WEYIBABPZCYASX-UHFFFAOYSA-N	4.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C61CO	3.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	2.2×10^{4}		Wang et al. (2017)	Q	81, 240
MGEAAKFVOQZVFH-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C61OH	1.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	3.6×10^{5}		Wang et al. (2017)	Q	81, 240
JOVKXRBMZIPRBZ-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C61OOH	1.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	1.7×10^{6}		Wang et al. (2017)	Q	81, 240
ZUQHNOSGBJLTRH-UHFFFAOYSA-N	3.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C621OOH	9.8×10^{11}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_6$	2.7×10^{10}		Wang et al. (2017)	Q	81, 240
OMSKVAAPFLCUBC-UHFFFAOYSA-N	3.5×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C624CO	2.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	6.3×10^{2}		Wang et al. (2017)	Q	81, 240
SAJQFIMRYKQCMA-UHFFFAOYSA-N	5.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C625OH	1.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	3.9×10^{8}		Wang et al. (2017)	Q	81, 240
UHZLCNNVPSWLBR-UHFFFAOYSA-N	2.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C625OOH	2.0×10^{10}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_5$	7.8×10^{8}		Wang et al. (2017)	Q	81, 240
RLEQEEKQTRHVBK-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C627OH	3.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	1.9×10^{5}		Wang et al. (2017)	Q	81, 240
YXADPHVQSSNJLB-UHFFFAOYSA-N	5.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C630OH	2.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	1.7×10^{6}		Wang et al. (2017)	Q	81, 240
LTOZVYXSZHIEKZ-UHFFFAOYSA-N	2.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C630OOH	1.8×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	2.2×10^{6}		Wang et al. (2017)	Q	81, 240
FPSNWVZQINIJKM-UHFFFAOYSA-N	1.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C63OH	1.4×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.2×10^{5}		Wang et al. (2017)	Q	81, 240
YEHSOHVSOJHCML-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C63OOH	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
RYUSCYCDUHZJRL-UHFFFAOYSA-N	1.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C64OH	8.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	2.2×10^{5}		Wang et al. (2017)	Q	81, 240
DWHFPVYPGLVOER-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C64OOH	7.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
WKWKMZOJIHCBFC-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C66CO	7.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	2.9×10^{4}		Wang et al. (2017)	Q	81, 240
PQXOVUFKUOIXAY-UHFFFAOYSA-N	4.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C66OH	1.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	9.3×10^{5}		Wang et al. (2017)	Q	81, 240
YKCRSYHGTATDJD-UHFFFAOYSA-N	6.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C66OOH	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	7.4×10^{5}		Wang et al. (2017)	Q	81, 240
ZIMKSIUZUDHWGV-UHFFFAOYSA-N	9.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C67CO3H	3.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	6.6×10^{5}		Wang et al. (2017)	Q	81, 240
BGZGHPIMJSIBNB-UHFFFAOYSA-N	3.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C69OH	1.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	8.9×10^{5}		Wang et al. (2017)	Q	81, 240
UAFCVHAXODPLTF-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C69OOH	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	1.3×10^{6}		Wang et al. (2017)	Q	81, 240
IBTXITPBBCYNLS-UHFFFAOYSA-N	6.8×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C6CO23HO5	7.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	2.6×10^{4}		Wang et al. (2017)	Q	81, 240
ZFXUWHPHUNDYBV-UHFFFAOYSA-N	5.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C6CO243OH	8.5×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	6.6×10^{3}		Wang et al. (2017)	Q	81, 240
YZRCADLLOAXRLD-UHFFFAOYSA-N	5.0		Wang et al. (2017)	Q	81, 241
MCM:C6CO34HO1	7.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	2.0×10^{4}		Wang et al. (2017)	Q	81, 240
LBGWMVXVPMPEID-UHFFFAOYSA-N	9.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C6CO3HO14	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	9.1×10^{5}		Wang et al. (2017)	Q	81, 240
AEYYIRCLAOJEMX-UHFFFAOYSA-N	9.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C6CO3HO25	1.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
AQJAHIKLRWQRAX-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C6CO3HO4	5.6		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	4.6×10^{1}		Wang et al. (2017)	Q	81, 240
SKCYVGUCBRYGTE-UHFFFAOYSA-N	6.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C6CO3OHOOH	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	6.3×10^{5}		Wang et al. (2017)	Q	81, 240
VJHRZIUXRMRGDC-UHFFFAOYSA-N	6.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C6HOCOOOH	9.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	7.4×10^{5}		Wang et al. (2017)	Q	81, 240
DEHZHOWOLMWYLS-UHFFFAOYSA-N	8.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:CO24M3C5OH	3.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
JUTFYFRULBWUNH-UHFFFAOYSA-N	2.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CO25C6OH	3.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	1.6×10^{5}		Wang et al. (2017)	Q	81, 240
MXGSILCFPNVDMX-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:CO2HO3C6	5.6		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	5.8×10^{1}		Wang et al. (2017)	Q	81, 240
UHSBCAJZDUQTHH-UHFFFAOYSA-N	4.1		Wang et al. (2017)	Q	81, 241
MCM:CO2HO4C6	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	7.8×10^{2}		Wang et al. (2017)	Q	81, 240
ODWYTDVNWFBCLV-UHFFFAOYSA-N	3.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO2HOC6OOH	9.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	1.0×10^{6}		Wang et al. (2017)	Q	81, 240
DONIGPAOCGSEHJ-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CO2M3C5OH	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	1.7×10^{3}		Wang et al. (2017)	Q	81, 240
YJCMJVMCCJIPRV-UHFFFAOYSA-N	4.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CO2MC5OH	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	1.9×10^{3}		Wang et al. (2017)	Q	81, 240
NZBRXFKHZBOFBW-UHFFFAOYSA-N	5.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CY6DIONOH	2.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	6.5×10^{7}		Wang et al. (2017)	Q	81, 240
ACRUCDPQQCIOID-UHFFFAOYSA-N	2.9×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:CYHXOLACO	1.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
ODZTXUXIYGJLMC-UHFFFAOYSA-N	6.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CYHXONAOH	3.5×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	3.5×10^{4}		Wang et al. (2017)	Q	81, 240
TWEVQGUWCLBRMJ-UHFFFAOYSA-N	8.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:DMK2OH	2.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	4.2×10^{6}		Wang et al. (2017)	Q	81, 240
RQDWELNLPMBYMA-UHFFFAOYSA-N	2.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DMKCOOH	6.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	3.2×10^{5}		Wang et al. (2017)	Q	81, 240
OKDWWGVTKQPUTM-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DMKOHOOH	4.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	7.3×10^{6}		Wang et al. (2017)	Q	81, 240
WAHPQVAXIMVNLL-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:EIPKAOH	3.9		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	3.3×10^{1}		Wang et al. (2017)	Q	81, 240
SYAVYWAMVZKGTF-UHFFFAOYSA-N	4.5		Wang et al. (2017)	Q	81, 241
MCM:EIPKBOH	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	3.1×10^{2}		Wang et al. (2017)	Q	81, 240
JYEMLYGXHDIVRA-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:H13M3CO4C5	9.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.7×10^{5}		Wang et al. (2017)	Q	81, 240
NBNMOYHUQSLZCQ-UHFFFAOYSA-N	3.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:H3C25C6OH	5.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	4.8×10^{7}		Wang et al. (2017)	Q	81, 240
XLUGOLRJPRATMY-UHFFFAOYSA-N	3.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:H3C25C6OOH	2.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	5.0×10^{7}		Wang et al. (2017)	Q	81, 240
XIJKANBCMKWKRM-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HEX3ONAOH	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	6.5×10^{2}		Wang et al. (2017)	Q	81, 240
XHYXKWWFNRBCGE-UHFFFAOYSA-N	4.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HEX3ONCOH	5.6		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	4.2×10^{1}		Wang et al. (2017)	Q	81, 240
ZWBUSAWJHMPOEJ-UHFFFAOYSA-N	3.5		Wang et al. (2017)	Q	81, 241
MCM:HEX3ONDOH	9.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	2.6×10^{2}		Wang et al. (2017)	Q	81, 240
ITHSWIXXHGKFJW-UHFFFAOYSA-N	5.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO1CO24C6	3.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
NUDMYLMVZRZHHU-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO1CO4C6	9.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
APQMHEQLBDXGMP-UHFFFAOYSA-N	4.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO2CO5C6	2.8×10^{3}	10000	Wieser et al. (2023)	Q	439
$C_6H_{12}O_2$	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
ZSDLLTJVENEIDW-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	81, 240
	6.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:M2BKAOH	1.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	6.9×10^{2}		Wang et al. (2017)	Q	81, 240
ZXZUCILLTLHIBZ-UHFFFAOYSA-N	4.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:M2BKBOH	3.9		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	4.4×10^{1}		Wang et al. (2017)	Q	81, 240
KHCUSEDRQWYNDS-UHFFFAOYSA-N	3.6		Wang et al. (2017)	Q	81, 241
MCM:MBKCOOHOOH	2.5×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	2.1×10^{6}		Wang et al. (2017)	Q	81, 240
VGLNQNYMXFMHPV-UHFFFAOYSA-N	4.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MIBKAOH3CO	2.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	4.6×10^{2}		Wang et al. (2017)	Q	81, 240
NARMPYMUEZMSEV-UHFFFAOYSA-N	2.4		Wang et al. (2017)	Q	81, 241
MCM:MIBKBOH	6.5		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	6.3×10^{1}		Wang et al. (2017)	Q	81, 240
IGPIDYBTABPKQT-UHFFFAOYSA-N	2.6		Wang et al. (2017)	Q	81, 241
MCM:MIBKHO14	9.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	8.1×10^{5}		Wang et al. (2017)	Q	81, 240
UZSRJTNVDUYOLE-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MIBKHO4OOH	5.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
FGHCAVJLMYVGOV-UHFFFAOYSA-N	1.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:MIBKOH34	5.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	4.1×10^{4}		Wang et al. (2017)	Q	81, 240
OSPIOFUQWMUWOI-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MIBKOHAOOH	8.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	1.8×10^{5}		Wang et al. (2017)	Q	81, 240
WIXFQYMFSUQGGT-UHFFFAOYSA-N	4.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MIBKOHBOOH	7.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	2.9×10^{5}		Wang et al. (2017)	Q	81, 240
NCKNZQNPSVRYAP-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:MTBKOH	7.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	3.8×10^{2}		Wang et al. (2017)	Q	81, 240
DYAWMXSWDGPGOI-UHFFFAOYSA-N	3.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PBZQCO	8.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_4O_4$	3.6×10^{9}		Wang et al. (2017)	Q	81, 240
LTWQMQDFZHUKCN-UHFFFAOYSA-N	3.4×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PBZQOH	3.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_4$	5.0×10^{8}		Wang et al. (2017)	Q	81, 240
KGAUAKJVBKFEJK-UHFFFAOYSA-N	1.5×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PBZQOOH	5.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_5$	1.9×10^{9}		Wang et al. (2017)	Q	81, 240
GWWKDNIKIVTFLV-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C61CO3H	7.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_6$	4.6×10^{5}		Wang et al. (2017)	Q	81, 240
LNQZNTUCDYUQNY-UHFFFAOYSA-N	4.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C62CO3H	8.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_6$	5.1×10^{5}		Wang et al. (2017)	Q	81, 240
OTMFEIRKQNFPTO-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C711OOH	5.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_4$	7.4×10^{5}		Wang et al. (2017)	Q	81, 240
CHMPWQJFRSDBMP-UHFFFAOYSA-N	5.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C712OH	8.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_3$	3.6×10^{5}		Wang et al. (2017)	Q	81, 240
XKQDJNZCXUTPAB-UHFFFAOYSA-N	5.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C712OOH	6.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_4$	7.6×10^{5}		Wang et al. (2017)	Q	81, 240
ISDXEEIPAJYQKS-UHFFFAOYSA-N	8.0×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C713OH	2.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_3$	4.0×10^{4}		Wang et al. (2017)	Q	81, 240
KKMPMNHIJNYFMY-UHFFFAOYSA-N	2.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C714OH	3.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_3$	6.8×10^{4}		Wang et al. (2017)	Q	81, 240
BDJIDAHXOAZMLT-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C719OH	5.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	7.1×10^{10}		Wang et al. (2017)	Q	81, 240
SNLGDBZBHBGDGF-UHFFFAOYSA-N	2.3×10^{8}		Wang et al. (2017)	Q	81, 241
MCM:C719OOH	7.1×10^{10}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	5.8×10^{11}		Wang et al. (2017)	Q	81, 240
RIQZESWBZQGTOF-UHFFFAOYSA-N	2.0×10^{9}		Wang et al. (2017)	Q	81, 241
MCM:C71OOH	8.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_4$	4.1×10^{5}		Wang et al. (2017)	Q	81, 240
NBQALOYIKVIATH-UHFFFAOYSA-N	3.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C726CO3OH	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	9.1×10^{4}		Wang et al. (2017)	Q	81, 240
KXKCGTAVIRFZLI-UHFFFAOYSA-N	6.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C72OH	1.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_3$	1.9×10^{5}		Wang et al. (2017)	Q	81, 240
NSVUCXUEJIZYCX-UHFFFAOYSA-N	8.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C72OOH	9.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_4$	9.3×10^{5}		Wang et al. (2017)	Q	81, 240
HOCRXLJRXJDOAI-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C76OOH	8.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_4$	8.0×10^{5}		Wang et al. (2017)	Q	81, 240
RNKPJWWQPAQZAU-UHFFFAOYSA-N	1.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C77CO	2.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_3$	8.1×10^{3}		Wang et al. (2017)	Q	81, 240
LRWMVVHMPWURQP-UHFFFAOYSA-N	7.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C77OH	8.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_3$	3.2×10^{5}		Wang et al. (2017)	Q	81, 240
BWFQHNYIFKCYIN-UHFFFAOYSA-N	8.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C77OOH	6.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_4$	6.5×10^{5}		Wang et al. (2017)	Q	81, 240
VLZZBCPZVYCEGU-UHFFFAOYSA-N	4.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C78CO	4.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_3$	1.8×10^{4}		Wang et al. (2017)	Q	81, 240
XZDSUXRHWGXGLP-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C78OH	9.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_3$	3.0×10^{5}		Wang et al. (2017)	Q	81, 240
RHPFPSWJNNLJIH-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C78OOH	5.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_4$	3.7×10^{5}		Wang et al. (2017)	Q	81, 240
CHSMMMZNDOATLZ-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C79OOH	2.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	1.0×10^{7}		Wang et al. (2017)	Q	81, 240
PAASZTKJDWJXEO-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C7BDCOH	1.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	3.6×10^{6}		Wang et al. (2017)	Q	81, 240
IQLAANIUQOXZGT-UHFFFAOYSA-N	7.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C7BDCOOH	2.3×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	2.5×10^{6}		Wang et al. (2017)	Q	81, 240
YSGKLAZJXASOJQ-UHFFFAOYSA-N	2.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C7EDCCO	5.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	2.2×10^{5}		Wang et al. (2017)	Q	81, 240
ZZJOBVIMQADRSG-UHFFFAOYSA-N	8.7		Wang et al. (2017)	Q	81, 241
MCM:C7EDCOH	2.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	2.7×10^{6}		Wang et al. (2017)	Q	81, 240
ILHMXLYATWSMQV-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C7EDCOOH	3.7×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	4.6×10^{6}		Wang et al. (2017)	Q	81, 240
GFYCWCYSZRNKIC-UHFFFAOYSA-N	4.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:CO25C73OH	3.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_3$	8.3×10^{4}		Wang et al. (2017)	Q	81, 240
SUAOXERUOLNODJ-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:CO25C74OH	3.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_3$	8.5×10^{4}		Wang et al. (2017)	Q	81, 240
WVDVIEDFZYMNAI-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:H2M2CO5C6	6.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_2$	1.5×10^{3}		Wang et al. (2017)	Q	81, 240
GNNBSAPGFGNCCT-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:H2M3CO5C6	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_2$	1.7×10^{3}		Wang et al. (2017)	Q	81, 240
JXXNGUYHZPNXHL-UHFFFAOYSA-N	2.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:H2M4CO5C6	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_2$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
ZIVAMUMQDXZFCR-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:H3C25CCO3H	3.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_6$	9.8×10^{8}		Wang et al. (2017)	Q	81, 240
ARDZNQBCJILRHG-UHFFFAOYSA-N	6.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HCC7CO	9.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_2$	4.6×10^{4}		Wang et al. (2017)	Q	81, 240
WVMVYBISUAVCBD-UHFFFAOYSA-N	1.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HO2CO35C7	3.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_3$	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
LULWLYVLBHVZLB-UHFFFAOYSA-N	5.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO2CO5C7	8.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_2$	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
DWMNUVZLRBCGOL-UHFFFAOYSA-N	2.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO3CO6C7	2.1×10^{3}	11000	Wieser et al. (2023)	Q	439
$C_7H_{14}O_2$	8.7×10^{1}		Wang et al. (2017)	Q	81, 239
MQRALIJAASQPNT-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PTLQCO	5.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_6O_4$	6.2×10^{9}		Wang et al. (2017)	Q	81, 240
QCLUMLMJJNMFFX-UHFFFAOYSA-N	6.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PTLQOH	2.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_4$	5.1×10^{8}		Wang et al. (2017)	Q	81, 240
FWCZASAULMADEU-UHFFFAOYSA-N	1.2×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PTLQOOH	3.6×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_5$	1.8×10^{9}		Wang et al. (2017)	Q	81, 240
ULCYCDVSDDOIBS-UHFFFAOYSA-N	3.8×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:TLCOBIPEOH	3.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_4$	7.3×10^{2}		Wang et al. (2017)	Q	81, 240
BTRXIMYXFXXDNL-UHFFFAOYSA-N	2.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:TLOBIPEROH	3.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_4$	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
OGIZZGFCOPEREO-UHFFFAOYSA-N	1.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C6MOCOCO3H	2.1×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_6$	1.7×10^{9}		Wang et al. (2017)	Q	81, 240
UAMJQIWVNIVSAA-UHFFFAOYSA-N	4.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C7CO2M5OH	7.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_3$	2.0×10^{4}		Wang et al. (2017)	Q	81, 240
VIGCXZSBZQABDL-UHFFFAOYSA-N	2.8×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C7CO2OCO3H	2.1×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_6$	2.0×10^{9}		Wang et al. (2017)	Q	81, 240
PYNUJNZYCLWJPS-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C7M2CO5OH	9.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_3$	8.5×10^{4}		Wang et al. (2017)	Q	81, 240
IWFVDGADKJRMAI-UHFFFAOYSA-N	2.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C817OH	5.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_3$	4.9×10^{5}		Wang et al. (2017)	Q	81, 240
HXKXVESDDNIBIQ-UHFFFAOYSA-N	2.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C818CO	6.5×10^{6}	16000	Wieser et al. (2023)	Q	439
$C_8H_{12}O_4$	3.6×10^{7}		Wang et al. (2017)	Q	81, 239
CRQAGKNTHDNGEW-UHFFFAOYSA-N	1.7×10^{7}		Wang et al. (2017)	Q	81, 240
	1.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C818OH	8.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_4$	2.9×10^{8}		Wang et al. (2017)	Q	81, 240
GYBDPSWJEGVQPC-UHFFFAOYSA-N	7.4×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C818OOH	5.7×10^{8}	17000	Wieser et al. (2023)	Q	439
$C_8H_{14}O_5$	5.0×10^{9}		Wang et al. (2017)	Q	81, 239
DLMBPALZQHFDOH-UHFFFAOYSA-N	1.0×10^{8}		Wang et al. (2017)	Q	81, 240
	9.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C819OOH	2.1×10^{7}	17000	Wieser et al. (2023)	Q	439
$C_8H_{14}O_5$	3.5×10^{9}		Wang et al. (2017)	Q	81, 239
JRXMSSDNDAZISI-UHFFFAOYSA-N	6.3×10^{7}		Wang et al. (2017)	Q	81, 240
	6.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C81OOH	6.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{16}O_4$	3.3×10^{5}		Wang et al. (2017)	Q	81, 240
SFFBCYBCCUXGLX-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C820OOH	2.3×10^{12}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_6$	1.4×10^{9}		Wang et al. (2017)	Q	81, 240
MPCACGHSMGOFNV-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C826CO3OH	1.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_3$	5.6×10^{4}		Wang et al. (2017)	Q	81, 240
GGSZUEZFMJTLBX-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C827OH	1.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_3$	5.4×10^{4}		Wang et al. (2017)	Q	81, 240
VYHQZXLAUHJBAB-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C829OH	1.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_4$	1.0×10^{8}		Wang et al. (2017)	Q	81, 240
ZFRREEXTYBESJX-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C829OOH	2.8×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_5$	8.0×10^{7}		Wang et al. (2017)	Q	81, 240
PFFZQAOPEABNHW-UHFFFAOYSA-N	9.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C82OOH	8.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{16}O_4$	6.8×10^{5}		Wang et al. (2017)	Q	81, 240
AQECYOJQUIJAFS-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C84OH	2.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_3$	4.1×10^{4}		Wang et al. (2017)	Q	81, 240
HXKSWDLNZPICFQ-UHFFFAOYSA-N	5.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C88OH	6.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_3$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
DCTATDQRTQNXHW-UHFFFAOYSA-N	3.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:EBZOBPEROH	2.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_4$	8.3×10^{2}		Wang et al. (2017)	Q	81, 240
YDVGTQTYIBCIQC-UHFFFAOYSA-N	6.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:HO34CO6C8	1.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_{16}O_3$	1.7×10^{5}		Wang et al. (2017)	Q	81, 240
GQDVWZAGWHUXKX-UHFFFAOYSA-N	3.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO3CO46C8	2.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_3$	8.3×10^{3}		Wang et al. (2017)	Q	81, 240
LLYUJOAMIUBKSA-UHFFFAOYSA-N	3.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO3CO6C8	8.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_8H_{16}O_2$	9.6×10^{2}		Wang et al. (2017)	Q	81, 240
VJDZJBNTVLGPEM-UHFFFAOYSA-N	8.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MXYOBPEROH	1.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_4$	3.0×10^{2}		Wang et al. (2017)	Q	81, 240
BQJOHFWATKFGAQ-UHFFFAOYSA-N	4.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:MXYQOH	1.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_4$	3.0×10^{8}		Wang et al. (2017)	Q	81, 240
DNSXSYZLXRHYTM-UHFFFAOYSA-N	3.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:MXYQOOH	1.9×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_5$	3.0×10^{8}		Wang et al. (2017)	Q	81, 240
UAWVAAITGKOKNW-UHFFFAOYSA-N	5.9×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:OXYQCO	3.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_8O_4$	6.2×10^{9}		Wang et al. (2017)	Q	81, 240
QSCBEAAIZXLBQA-UHFFFAOYSA-N	1.8×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:OXYQOH	1.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_4$	3.5×10^{8}		Wang et al. (2017)	Q	81, 240
LJMMKZLQFVIDLQ-UHFFFAOYSA-N	7.6×10^{4}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:OXYQOOH	2.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_5$	1.2×10^{9}		Wang et al. (2017)	Q	81, 240
NOWQTCYBLCRAEJ-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PXYQOH	1.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_4$	3.0×10^{8}		Wang et al. (2017)	Q	81, 240
RORXCXPFLRGHQV-UHFFFAOYSA-N	5.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:PXYQOOH	1.9×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_5$	4.2×10^{8}		Wang et al. (2017)	Q	81, 240
FYDHRLZPZZTRLJ-UHFFFAOYSA-N	2.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C6EO2HCO3H	1.7×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_6$	1.6×10^{9}		Wang et al. (2017)	Q	81, 240
KMUWHHLOUXRZEC-UHFFFAOYSA-N	3.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C7MJPCO3H	1.7×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_6$	1.2×10^{9}		Wang et al. (2017)	Q	81, 240
HVGFJXMJLWNDQT-UHFFFAOYSA-N	6.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C7MOCOCO3H	1.4×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_6$	2.3×10^{9}		Wang et al. (2017)	Q	81, 240
UXMGGYROBLVMKA-UHFFFAOYSA-N	9.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C8M2CO6OH	7.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_3$	4.8×10^{4}		Wang et al. (2017)	Q	81, 240
AUYUFIFJEJTOMG-UHFFFAOYSA-N	8.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C917OH	9.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_3$	4.3×10^{6}		Wang et al. (2017)	Q	81, 240
DVAQWOBQFULNSX-UHFFFAOYSA-N	3.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C920OOH	6.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_4$	1.6×10^{6}		Wang et al. (2017)	Q	81, 240
CXKZGZZGALDRTB-UHFFFAOYSA-N	6.9×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C921OOH	1.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_5$	3.2×10^{9}		Wang et al. (2017)	Q	81, 240
MIFQELLQXZRDIQ-UHFFFAOYSA-N	7.1×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C922OOH	3.6×10^{11}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_6$	7.8×10^{9}		Wang et al. (2017)	Q	81, 240
IOTRHTNOHNKLJT-UHFFFAOYSA-N	6.6×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C923OH	5.3×10^{3}	12000	Wieser et al. (2023)	Q	439
$C_9H_{16}O_2$	1.5×10^{2}		Wang et al. (2017)	Q	81, 239
VZYSLJNPEGILSI-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 240
	7.4×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C924CO	1.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_3$	5.6×10^{4}		Wang et al. (2017)	Q	81, 240
IEIWFPIZSBHOOD-UHFFFAOYSA-N	4.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C924OH	3.8×10^{5}	16000	Wieser et al. (2023)	Q	439
$C_9H_{16}O_3$	2.2×10^{4}		Wang et al. (2017)	Q	81, 239
OXSRPARPRXNCEH-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	81, 240
	2.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C924OOH	3.0×10^{6}	16000	Wieser et al. (2023)	Q	439
$C_9H_{16}O_4$	1.2×10^{7}		Wang et al. (2017)	Q	81, 239
BVODBOGLMHSHGK-UHFFFAOYSA-N	3.1×10^{5}		Wang et al. (2017)	Q	81, 240
	5.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C925OOH	9.1×10^{12}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_6$	5.0×10^{10}		Wang et al. (2017)	Q	81, 240
BGVLBDREANINMN-UHFFFAOYSA-N	1.6×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C927OH	2.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_3$	1.2×10^{7}		Wang et al. (2017)	Q	81, 240
JILOVKBSEAXPMT-UHFFFAOYSA-N	9.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C927OOH	7.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_4$	8.9×10^{6}		Wang et al. (2017)	Q	81, 240
UVVCFFCMOUIWEJ-UHFFFAOYSA-N	6.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C928OH	2.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_3$	3.8×10^{5}		Wang et al. (2017)	Q	81, 240
QGCNXROUFNWXOO-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C929CO	2.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	5.4×10^{6}		Wang et al. (2017)	Q	81, 240
BWILLNTUIBCKIM-UHFFFAOYSA-N	3.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C929OH	4.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_4$	5.9×10^{8}		Wang et al. (2017)	Q	81, 240
PMWQIXWFMSCXRH-UHFFFAOYSA-N	6.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C929OOH	2.9×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_5$	3.3×10^{8}		Wang et al. (2017)	Q	81, 240
IKUORCWWMOEDGL-UHFFFAOYSA-N	1.2×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C92OOH	5.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{18}O_4$	2.9×10^{5}		Wang et al. (2017)	Q	81, 240
MOTPUWPPGZYDTM-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C93CO	2.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_3$	6.6×10^{3}		Wang et al. (2017)	Q	81, 240
NCWLHDSPZIENNF-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C93OH	8.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{18}O_3$	1.5×10^{5}		Wang et al. (2017)	Q	81, 240
XOZZRVPGLURXSY-UHFFFAOYSA-N	2.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C93OOH	6.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{18}O_4$	3.3×10^{5}		Wang et al. (2017)	Q	81, 240
DSWUVSMVGXSNEV-UHFFFAOYSA-N	8.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C94OH	2.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_3$	2.6×10^{4}		Wang et al. (2017)	Q	81, 240
RCWXDPYULCSTKX-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C96OH	1.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_2$	3.3×10^{3}		Wang et al. (2017)	Q	81, 240
RRFQMYCDTHUGSU-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C97OH	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_3$	1.2×10^{6}		Wang et al. (2017)	Q	81, 240
QWYKJUJQBVIHQW-UHFFFAOYSA-N	8.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C97OOH	8.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_4$	3.9×10^{5}		Wang et al. (2017)	Q	81, 240
AXRJNDGSGFVBSX-UHFFFAOYSA-N	1.9×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C98OH	9.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_4$	1.0×10^{8}		Wang et al. (2017)	Q	81, 240
BWKWRXKCGJAJAO-UHFFFAOYSA-N	4.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C98OOH	2.9×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_5$	3.3×10^{7}		Wang et al. (2017)	Q	81, 240
MEUGYCLQCHCPCY-UHFFFAOYSA-N	1.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C9DCOH	4.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	1.9×10^{7}		Wang et al. (2017)	Q	81, 240
DIFRJFLUSYQBJM-UHFFFAOYSA-N	4.9×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:HO4CO7C9	6.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{18}O_2$	8.3×10^{2}		Wang et al. (2017)	Q	81, 240
BPRAKHMXALGYKO-UHFFFAOYSA-N	7.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:IPBZOBPROH	2.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	7.1×10^{2}		Wang et al. (2017)	Q	81, 240
WRQNGVASMLSOGA-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:IPRBQCO	4.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_4$	2.6×10^{9}		Wang et al. (2017)	Q	81, 240
UYSSVGYDANWBFJ-UHFFFAOYSA-N	1.2×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:IPRBQOH	1.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	1.7×10^{8}		Wang et al. (2017)	Q	81, 240
BQKYQBQGKYWJSQ-UHFFFAOYSA-N	7.6×10^{4}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:IPRBQOOH	2.9×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	6.9×10^{8}		Wang et al. (2017)	Q	81, 240
CCPBRYDTGCPJNX-UHFFFAOYSA-N	1.2×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:LMKAOH	2.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_3$	6.2×10^{6}		Wang et al. (2017)	Q	81, 240
RDFFVUMNEKCADL-UHFFFAOYSA-N	1.2×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:LMKAOOH	1.5×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_4$	2.7×10^{7}		Wang et al. (2017)	Q	81, 240
ZYSXBTHWQDNLBX-UHFFFAOYSA-N	3.6×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:LMKBCO	5.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_3$	3.7×10^{5}		Wang et al. (2017)	Q	81, 240
QJYRJOZGIVJKQK-UHFFFAOYSA-N	2.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:LMKBOOH	1.5×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_4$	2.6×10^{7}		Wang et al. (2017)	Q	81, 240
PMLHMEIQMSUJKR-UHFFFAOYSA-N	8.9×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:METLOBPROH	1.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	1.8×10^{2}		Wang et al. (2017)	Q	81, 240
ZSTYNOBMCJBFRA-UHFFFAOYSA-N	2.5×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:METLQOH	1.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	2.0×10^{8}		Wang et al. (2017)	Q	81, 240
YIUSRNITCRMQJW-UHFFFAOYSA-N	2.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:METLQOOH	1.7×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	1.3×10^{8}		Wang et al. (2017)	Q	81, 240
JBNOKZJMGKNXDA-UHFFFAOYSA-N	5.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NOPINAOH	5.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_2$	2.5×10^{4}		Wang et al. (2017)	Q	81, 240
CVWGOJDPALGYKB-UHFFFAOYSA-N	4.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NOPINBOH	5.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_2$	3.2×10^{4}		Wang et al. (2017)	Q	81, 240
FPBMXOVOMRHDTB-UHFFFAOYSA-N	2.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NOPINCOH	3.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_2$	9.3×10^{3}		Wang et al. (2017)	Q	81, 240
OXRZVROAQQDWAA-UHFFFAOYSA-N	3.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NOPINDOH	2.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_2$	7.3×10^{2}		Wang et al. (2017)	Q	81, 240
MLOBETUCFXAOOL-UHFFFAOYSA-N	8.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:OETLQCO	3.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_4$	4.7×10^{9}		Wang et al. (2017)	Q	81, 240
WOEKXHYIEUECKR-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:OETLQOH	1.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	2.0×10^{8}		Wang et al. (2017)	Q	81, 240
DZHQWTGZQAKVBN-UHFFFAOYSA-N	5.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:OETLQOOH	1.9×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	8.0×10^{8}		Wang et al. (2017)	Q	81, 240
KKWSBZSFLIKUTL-UHFFFAOYSA-N	2.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PBZOBPEROH	2.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	5.5×10^{2}		Wang et al. (2017)	Q	81, 240
JGNLEXNHGWFGHL-UHFFFAOYSA-N	5.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:PETLQOH	1.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	2.2×10^{8}		Wang et al. (2017)	Q	81, 240
KZOAJFYPECZGSC-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:PETLQOOH	1.7×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	2.0×10^{8}		Wang et al. (2017)	Q	81, 240
BJRXYYOXPIRVAX-UHFFFAOYSA-N	2.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:TM123OBPOH	1.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	1.7×10^{2}		Wang et al. (2017)	Q	81, 240
WQSRSICCLTUNRX-UHFFFAOYSA-N	4.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:TM124QOH	8.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	1.7×10^{8}		Wang et al. (2017)	Q	81, 240
GVKLCWOTVYVOTB-UHFFFAOYSA-N	2.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:TM124QOOH	1.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	2.6×10^{8}		Wang et al. (2017)	Q	81, 240
SLEWHRYFRSXVOQ-UHFFFAOYSA-N	3.2×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:TM135OBPOH	1.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	1.9×10^{2}		Wang et al. (2017)	Q	81, 240
MWFXWFJYOSXFGA-UHFFFAOYSA-N	4.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:APINBCO	1.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_2$	4.4×10^{2}		Wang et al. (2017)	Q	81, 240
VZRRCQOUNSHSGB-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C1011OH	1.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_2$	2.1×10^{3}		Wang et al. (2017)	Q	81, 240
FSFKNSSBELMLGT-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C102OOH	4.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{20}O_4$	2.6×10^{5}		Wang et al. (2017)	Q	81, 240
QHLMVJFPSLBXKZ-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C103CO	2.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_3$	5.4×10^{3}		Wang et al. (2017)	Q	81, 240
QIIAZEBRWZSMOM-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C103OH	7.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{20}O_3$	1.3×10^{5}		Wang et al. (2017)	Q	81, 240
SXEGIXJYQPFAQK-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C103OOH	5.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{20}O_4$	3.0×10^{5}		Wang et al. (2017)	Q	81, 240
DOFXWCNTKGZWNU-UHFFFAOYSA-N	1.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C104OH	2.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_3$	1.9×10^{4}		Wang et al. (2017)	Q	81, 240
FHITZQAABUJLCH-UHFFFAOYSA-N	4.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C920CO3H	6.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_5$	9.1×10^{5}		Wang et al. (2017)	Q	81, 240
OFVMBWQGLFFRLM-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C9M2CO6OH	5.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_3$	2.4×10^{4}		Wang et al. (2017)	Q	81, 240
SLPXKTFAPIGCFF-UHFFFAOYSA-N	4.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DMEOBPROH	1.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{14}O_4$	1.3×10^{2}		Wang et al. (2017)	Q	81, 240
ZCTKJUASOMJGQC-UHFFFAOYSA-N	9.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO5CO8C10	5.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{20}O_2$	7.4×10^{2}		Wang et al. (2017)	Q	81, 240
GDOWVFFRHQHNBZ-UHFFFAOYSA-N	8.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:LIMBCO	1.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_2$	3.5×10^{2}		Wang et al. (2017)	Q	81, 240
JEQLRDRDFLXSHY-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C112OOH	3.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{22}O_4$	2.4×10^{5}		Wang et al. (2017)	Q	81, 240
IFXOTQISYXBGBQ-UHFFFAOYSA-N	5.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C113CO	1.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{20}O_3$	4.5×10^{3}		Wang et al. (2017)	Q	81, 240
VJVDGYIYRBYKOQ-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C113OH	5.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{22}O_3$	1.1×10^{5}		Wang et al. (2017)	Q	81, 240
IBMABDXBRFZEGO-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C113OOH	4.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{22}O_4$	3.0×10^{5}		Wang et al. (2017)	Q	81, 240
PBWNXGFXFCLKSE-UHFFFAOYSA-N	8.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C114OH	1.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{20}O_3$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
UGVQLPIEIICAJP-UHFFFAOYSA-N	3.7×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DETLOBPROH	8.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{16}O_4$	9.1×10^{1}		Wang et al. (2017)	Q	81, 240
QNKVJNYVFVQVHN-UHFFFAOYSA-N	1.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HO6CO9C11	4.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{22}O_2$	6.5×10^{2}		Wang et al. (2017)	Q	81, 240
HEIFQPPUFKWMSE-UHFFFAOYSA-N	5.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C122OOH	3.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{24}O_4$	2.3×10^{5}		Wang et al. (2017)	Q	81, 240
PWTYXUGOJRDLPW-UHFFFAOYSA-N	9.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C123CO	1.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{22}O_3$	4.1×10^{3}		Wang et al. (2017)	Q	81, 240
IVLDSNPYDYHHKW-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C123OH	4.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{24}O_3$	9.6×10^{4}		Wang et al. (2017)	Q	81, 240
FTSJAGYKUWYWCN-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C123OOH	4.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{24}O_4$	2.8×10^{5}		Wang et al. (2017)	Q	81, 240
YANZHJXFRFYAEY-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C124OH	1.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{22}O_3$	1.3×10^{4}		Wang et al. (2017)	Q	81, 240
ABVYFIKKAQHKSN-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO7CO10C12	3.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{24}O_2$	5.1×10^{2}		Wang et al. (2017)	Q	81, 240
AJDNADCNQXGLCC-UHFFFAOYSA-N	4.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C131OH	5.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_3$	2.3×10^{5}		Wang et al. (2017)	Q	81, 240
AONUZHGLRYBQFR-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C132OH	5.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_4$	4.1×10^{8}		Wang et al. (2017)	Q	81, 240
FIXMRMMYQTVSPU-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C132OOH	2.9×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_5$	1.7×10^{8}		Wang et al. (2017)	Q	81, 240
VUANIPKMYHABIK-UHFFFAOYSA-N	1.1×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C133CO	7.1×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{20}O_5$	4.6×10^{9}		Wang et al. (2017)	Q	81, 240
NSPNCPQPMIIWRH-UHFFFAOYSA-N	4.7×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C133OH	3.2×10^{10}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_5$	6.0×10^{10}		Wang et al. (2017)	Q	81, 240
PJPMMZIOBGUFRQ-UHFFFAOYSA-N	8.9×10^{4}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C133OOH	8.5×10^{11}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_6$	3.7×10^{10}		Wang et al. (2017)	Q	81, 240
TWNMHUJEMNHLMV-UHFFFAOYSA-N	5.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C134CO	4.7×10^{12}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{18}O_6$	2.3×10^{11}		Wang et al. (2017)	Q	81, 240
XVPKZNMZKWIEGC-UHFFFAOYSA-N	2.1×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C134OH	1.0×10^{12}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{20}O_6$	1.1×10^{13}		Wang et al. (2017)	Q	81, 240
CKMYGJKMMJWXII-UHFFFAOYSA-N	8.7×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C134OOH	6.8×10^{14}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{20}O_7$	1.7×10^{12}		Wang et al. (2017)	Q	81, 240
RYVAPXIZXOQMSU-UHFFFAOYSA-N	2.3×10^{8}		Wang et al. (2017)	Q	81, 241
MCM:C135OOH	5.0×10^{17}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{18}O_8$	6.6×10^{13}		Wang et al. (2017)	Q	81, 240
VAECXYXKQRKKGE-UHFFFAOYSA-N	9.6×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:BCKAOH	2.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{24}O_3$	8.3×10^{6}		Wang et al. (2017)	Q	81, 240
ARSAOHGCYSGONM-UHFFFAOYSA-N	7.6×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:BCKAOOH	1.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{24}O_4$	4.0×10^{6}		Wang et al. (2017)	Q	81, 240
OXLVMLPVWDEZIL-UHFFFAOYSA-N	7.8×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:BCKBCO	5.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_3$	7.6×10^{5}		Wang et al. (2017)	Q	81, 240
IWYBCVOMQFEOMA-UHFFFAOYSA-N	2.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:BCKBOOH	1.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{24}O_4$	2.6×10^{6}		Wang et al. (2017)	Q	81, 240
SISQWITWYDFXLW-UHFFFAOYSA-N	3.7×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C141OH	1.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{24}O_2$	2.3×10^{3}		Wang et al. (2017)	Q	81, 240
OMNNANPOKVZFEY-UHFFFAOYSA-N	7.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C142OH	2.7×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{24}O_3$	8.5×10^{6}		Wang et al. (2017)	Q	81, 240
TZIWCZUVZZOIAP-UHFFFAOYSA-N	2.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C142OOH	7.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{24}O_4$	1.8×10^{7}		Wang et al. (2017)	Q	81, 240
OJVOLXXWTGQGEJ-UHFFFAOYSA-N	1.9×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C143CO	2.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_4$	5.1×10^{8}		Wang et al. (2017)	Q	81, 240
IPHIBGAHOYIGTO-UHFFFAOYSA-N	5.4×10^{6}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C143OH	9.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{24}O_4$	5.0×10^{9}		Wang et al. (2017)	Q	81, 240
PUMKKTACSBJGTI-UHFFFAOYSA-N	2.3×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C143OOH	2.5×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{24}O_5$	3.4×10^{9}		Wang et al. (2017)	Q	81, 240
FMXAUTXFPHKMFA-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C145OH	1.0×10^{12}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{24}O_6$	3.1×10^{13}		Wang et al. (2017)	Q	81, 240
CADDZNHIARUDOF-UHFFFAOYSA-N	1.5×10^{9}		Wang et al. (2017)	Q	81, 241
MCM:C145OOH	1.5×10^{15}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{24}O_7$	4.9×10^{13}		Wang et al. (2017)	Q	81, 240
CEBXMSFHIDLJKH-UHFFFAOYSA-N	1.8×10^{10}		Wang et al. (2017)	Q	81, 241
MCM:BCBCO	1.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{24}O_2$	6.5×10^{2}		Wang et al. (2017)	Q	81, 240
VLNGGDKMXDHPMK-UHFFFAOYSA-N	8.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PHCOMEOH	3.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_8O_2$	1.2×10^{3}		Wang et al. (2017)	Q	81, 240
ZWVHTXAYIKBMEE-UHFFFAOYSA-N	6.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MPHCOMEOH	1.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_2$	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
CEJINNSYZFLSCS-UHFFFAOYSA-N	4.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PHCOETOH	2.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_2$	7.4×10^{2}		Wang et al. (2017)	Q	81, 240
WLVPRARCUSRDNI-UHFFFAOYSA-N	6.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DMPHCOMOH	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{12}O_2$	7.8×10^{2}		Wang et al. (2017)	Q	81, 240
DBYMZNOFJHQFFD-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:EMPHCOMOH	8.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{14}O_2$	4.5×10^{2}		Wang et al. (2017)	Q	81, 240
MHJXTDDYZBYNEF-UHFFFAOYSA-N	8.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ALCOCH2OOH	4.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_3H_4O_4$	7.6×10^{3}		Wang et al. (2017)	Q	81, 240
RQBGWFCHIWSUOK-UHFFFAOYSA-N	3.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C33CO	4.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_3H_2O_3$	2.8×10^{3}		Wang et al. (2017)	Q	81, 240
ICQNCHSXWNQIHC-UHFFFAOYSA-N	4.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C312COCO3H	4.7×10^{7}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_5$	3.2×10^{5}		Wang et al. (2017)	Q	81, 240
GUGBJTDAGNLAJO-UHFFFAOYSA-N	8.0×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C413COOOH	3.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_4$	3.5×10^{4}		Wang et al. (2017)	Q	81, 240
XUKQQLOKOLCMAI-UHFFFAOYSA-N	4.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C4CO2OOH	3.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_4$	2.6×10^{4}		Wang et al. (2017)	Q	81, 240
NOBUEMWCPQFCCN-UHFFFAOYSA-N	2.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C4CODIAL	4.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_3$	5.0×10^{3}		Wang et al. (2017)	Q	81, 240
OWIMZZMOFXSCLT-UHFFFAOYSA-N	2.5		Wang et al. (2017)	Q	81, 241
MCM:CO23C3CHO	3.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_3$	3.3×10^{3}		Wang et al. (2017)	Q	81, 240
LVZOZHOAAHWEOQ-UHFFFAOYSA-N	1.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:CO2C3CHO	4.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_2$	6.0×10^{1}		Wang et al. (2017)	Q	81, 240
PKQIDSVLSKFZQC-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO2C4DIAL	2.8×10^{7}		Wang et al. (2017)	Q	81, 239
$C_4H_2O_4$	5.0×10^{5}		Wang et al. (2017)	Q	81, 240
OURVMEXCDVXLPR-UHFFFAOYSA-N	1.0×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:EGLYOX	4.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_2$	8.0		Wang et al. (2017)	Q	81, 240
RWHQMRRVZJSKGX-UHFFFAOYSA-N	2.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:VGLYOX	1.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_2$	2.6×10^{1}		Wang et al. (2017)	Q	81, 240
SDQVYUNYDAWYIK-UHFFFAOYSA-N	3.5×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C4CO2DCO3H	1.7×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_4O_5$	5.1×10^{6}		Wang et al. (2017)	Q	81, 240
AXIVSVGHKYPZBE-UHFFFAOYSA-N	8.1		Wang et al. (2017)	Q	81, 241
MCM:C4MCO2OOH	2.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	3.6×10^{3}		Wang et al. (2017)	Q	81, 240
RKGLOUQDKXPRQL-UHFFFAOYSA-N	6.3		Wang et al. (2017)	Q	81, 241
MCM:C511OOH	3.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	7.8×10^{4}		Wang et al. (2017)	Q	81, 240
NBNOBTZXOPWFTP-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C5124COOOH	2.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_5$	3.0×10^{6}		Wang et al. (2017)	Q	81, 240
BXDCDQOWFJMSCY-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C512OOH	2.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	9.3×10^{5}		Wang et al. (2017)	Q	81, 240
UGOJGQBYBBLKDX-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C515CO	2.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_4O_4$	1.0×10^{6}		Wang et al. (2017)	Q	81, 240
OONLUXUUWPUJOU-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C515OOH	2.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_5$	3.5×10^{6}		Wang et al. (2017)	Q	81, 240
KCJJHAINVUWKSI-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C54CO	2.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_4O_4$	5.8×10^{5}		Wang et al. (2017)	Q	81, 240
KDLDWLXQVYMIBX-UHFFFAOYSA-N	5.8×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C5CO23CHO	2.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_3$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
IPHREVVCPNNUEQ-UHFFFAOYSA-N	1.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C5COCHOOOH	2.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	2.3×10^{5}		Wang et al. (2017)	Q	81, 240
QJMOTDLHJFXUFN-UHFFFAOYSA-N	5.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C5DIALCO	1.4×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_4O_3$	4.9×10^{4}		Wang et al. (2017)	Q	81, 240
SFSCHQJUYKUKJM-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	81, 241
MCM:C5DICARB	1.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_2$	1.1×10^{3}		Wang et al. (2017)	Q	81, 240
GBLMMVFQENXAFZ-UHFFFAOYSA-N	2.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CHOC3COOOH	3.8×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_5$	7.4×10^{5}		Wang et al. (2017)	Q	81, 240
KFSMXRNQWYDJRM-UHFFFAOYSA-N	3.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CO12C4CHO	3.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_3$	9.3×10^{3}		Wang et al. (2017)	Q	81, 240
VUSMENNBCBGZQI-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO13C4CHO	3.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_3$	6.5×10^{3}		Wang et al. (2017)	Q	81, 240
SSMCSEDSANTCBB-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CO23C4CHO	2.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_3$	3.8×10^{3}		Wang et al. (2017)	Q	81, 240
QGGCMCHYJIPQCE-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	81, 241
MCM:CO24C4CHO	2.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_3$	4.3×10^{3}		Wang et al. (2017)	Q	81, 240
XHTYNUBGBUBFOA-UHFFFAOYSA-N	9.3		Wang et al. (2017)	Q	81, 241
MCM:CO2C43CHO	4.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_2$	1.7×10^{1}		Wang et al. (2017)	Q	81, 240
KNTLTMLEQPLVDA-UHFFFAOYSA-N	4.9		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CO2C4CHO	5.5×10^{2}	8400	Wieser et al. (2023)	Q	439
$C_5H_8O_2$	3.9×10^{1}		Wang et al. (2017)	Q	81, 239
KEHNRUNQZGRQHU-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	81, 240
	7.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO3C4CHO	3.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_2$	2.6×10^{1}		Wang et al. (2017)	Q	81, 240
ZNNXJRURXWWGLN-UHFFFAOYSA-N	6.5		Wang et al. (2017)	Q	81, 241
MCM:IPRGLYOX	4.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_2$	4.9		Wang et al. (2017)	Q	81, 240
FTDZDHIBENIBKZ-UHFFFAOYSA-N	1.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:PGLYOX	3.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_2$	5.8		Wang et al. (2017)	Q	81, 240
GDTHVMAIBQVUMV-UHFFFAOYSA-N	1.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C23C54CHO	2.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	7.4×10^{2}		Wang et al. (2017)	Q	81, 240
CBIOWOAHGWGTSI-UHFFFAOYSA-N	2.8		Wang et al. (2017)	Q	81, 241
MCM:C3COCCHO	3.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	2.2×10^{1}		Wang et al. (2017)	Q	81, 240
PVLKSJIUOKAUMV-UHFFFAOYSA-N	7.6		Wang et al. (2017)	Q	81, 241
MCM:C45IC5CHO	2.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	8.0×10^{2}		Wang et al. (2017)	Q	81, 240
WETHXHAOPNKQLZ-UHFFFAOYSA-N	4.5×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C4ECO2OOH	1.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	1.8×10^{3}		Wang et al. (2017)	Q	81, 240
CMRDMVGIWXQQFX-UHFFFAOYSA-N	3.6		Wang et al. (2017)	Q	81, 241
MCM:C511CHO	3.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
SLKPDJWOVVFRFW-UHFFFAOYSA-N	1.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C511CO3H	3.5×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	1.6×10^{6}		Wang et al. (2017)	Q	81, 240
PKVJBWZRBQBAMT-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C512CO3H	3.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	1.6×10^{6}		Wang et al. (2017)	Q	81, 240
OPLKNVAQLNTMAR-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C515CHO	2.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_4$	8.7×10^{5}		Wang et al. (2017)	Q	81, 240
JHVNJBQABGTRPH-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C515CO3H	2.2×10^{10}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_6$	1.1×10^{8}		Wang et al. (2017)	Q	81, 240
XPLLKUAMAYNXAT-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C5CO2DCO3H	1.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_5$	4.5×10^{6}		Wang et al. (2017)	Q	81, 240
DHHXAZIZMIZDQV-UHFFFAOYSA-N	3.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C5DCO2CO3H	1.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_5$	4.2×10^{6}		Wang et al. (2017)	Q	81, 240
GJOWGOOSLUXRQO-UHFFFAOYSA-N	6.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C5MDICARB	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_2$	1.0×10^{3}		Wang et al. (2017)	Q	81, 240
PFLPZDBOPDYOJU-UHFFFAOYSA-N	5.6		Wang et al. (2017)	Q	81, 241
MCM:C5TRONCO3H	2.2×10^{10}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_6$	4.6×10^{7}		Wang et al. (2017)	Q	81, 240
GGHLQXKHXYQGCE-UHFFFAOYSA-N	1.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C6125CO	9.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_3$	6.2×10^{4}		Wang et al. (2017)	Q	81, 240
RFTMILUWMDIPHH-UHFFFAOYSA-N	5.4		Wang et al. (2017)	Q	81, 241
MCM:C6135COOOH	1.7×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	4.8×10^{6}		Wang et al. (2017)	Q	81, 240
HGYTXVUJMUREIP-UHFFFAOYSA-N	2.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C6145COOOH	1.7×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	7.8×10^{6}		Wang et al. (2017)	Q	81, 240
DSJLQKNTJKMXRQ-UHFFFAOYSA-N	2.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C615CO2OOH	1.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	1.2×10^{5}		Wang et al. (2017)	Q	81, 240
MOFLPBJDWVVKPL-UHFFFAOYSA-N	2.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C615CO	2.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	2.8×10^{2}		Wang et al. (2017)	Q	81, 240
BRRWJVYIMRBLKB-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	81, 241
MCM:C616OOH	2.4×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	1.7×10^{7}		Wang et al. (2017)	Q	81, 240
RZNSBZRPHHAABM-UHFFFAOYSA-N	3.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C617OOH	1.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	6.2×10^{3}		Wang et al. (2017)	Q	81, 240
VPKXUGZDYIOAPR-UHFFFAOYSA-N	4.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C618OOH	1.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	2.8×10^{3}		Wang et al. (2017)	Q	81, 240
AMQFKFSLRYYJMS-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C620OOH	2.4×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	1.0×10^{7}		Wang et al. (2017)	Q	81, 240
UWWRYJPKFSIPFS-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C626OOH	2.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	2.3×10^{6}		Wang et al. (2017)	Q	81, 240
DHTMLHKAZOWLFT-UHFFFAOYSA-N	4.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C65OOH	1.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	1.6×10^{4}		Wang et al. (2017)	Q	81, 240
LHKMAYQHAYSMQO-UHFFFAOYSA-N	5.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C6CO134	2.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
VIOZHXSHLWOADQ-UHFFFAOYSA-N	6.2		Wang et al. (2017)	Q	81, 241
MCM:C6CO4DB	8.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_4O_4$	2.3×10^{6}		Wang et al. (2017)	Q	81, 240
OGFBTMOHTIWBJU-UHFFFAOYSA-N	1.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6COALCO3H	3.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	4.3×10^{6}		Wang et al. (2017)	Q	81, 240
WRLXIVUJPLXKIG-UHFFFAOYSA-N	6.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C6COCHOOOH	2.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	1.5×10^{6}		Wang et al. (2017)	Q	81, 240
DQAWORJSQGOPLV-UHFFFAOYSA-N	5.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C6CODIAL	2.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	3.2×10^{4}		Wang et al. (2017)	Q	81, 240
PAXFMQWEAJBIJB-UHFFFAOYSA-N	2.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C6DICARB	1.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_2$	6.5×10^{2}		Wang et al. (2017)	Q	81, 240
GVKYFODEMNCLGS-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	81, 241
MCM:CO123C5CHO	2.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_4$	1.7×10^{6}		Wang et al. (2017)	Q	81, 240
GLSSGXNNMIEKBR-UHFFFAOYSA-N	1.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CO235C5CHO	1.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_4$	2.1×10^{5}		Wang et al. (2017)	Q	81, 240
GPIFCHFPYCMSRY-UHFFFAOYSA-N	4.7		Wang et al. (2017)	Q	81, 241
MCM:CO24M3CHO	2.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	8.0×10^{2}		Wang et al. (2017)	Q	81, 240
OQYGUGGUHGKPLC-UHFFFAOYSA-N	2.7		Wang et al. (2017)	Q	81, 241
MCM:CO2C4GLYOX	2.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	7.4×10^{3}		Wang et al. (2017)	Q	81, 240
YEJDUVJLIVLCFZ-UHFFFAOYSA-N	8.1×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CO2C54CHO	3.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	1.8×10^{2}		Wang et al. (2017)	Q	81, 240
IDAHIBMEKOEBRG-UHFFFAOYSA-N	5.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO2M33CHO	2.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	1.1×10^{1}		Wang et al. (2017)	Q	81, 240
HOOWKSPRVCRTJK-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	81, 241
MCM:CO2M3C4CHO	3.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	1.8×10^{2}		Wang et al. (2017)	Q	81, 240
GQHWESFTVGVFIA-UHFFFAOYSA-N	4.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO35C5CHO	2.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
KXLMWINKDVAJKB-UHFFFAOYSA-N	2.6		Wang et al. (2017)	Q	81, 241
MCM:CO3C54CHO	3.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	1.6×10^{1}		Wang et al. (2017)	Q	81, 240
HFHZCESKBNQESK-UHFFFAOYSA-N	1.8		Wang et al. (2017)	Q	81, 241
MCM:CO3C5CHO	3.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_2$	2.3×10^{2}		Wang et al. (2017)	Q	81, 240
KKOFYQBBUSZDKJ-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO45C5CHO	2.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	9.1×10^{2}		Wang et al. (2017)	Q	81, 240
WXTRRXXKCNKUIA-UHFFFAOYSA-N	8.1×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:ECO4	1.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_4$	2.5×10^{5}		Wang et al. (2017)	Q	81, 240
RGMUISDTMIPFQK-UHFFFAOYSA-N	4.2×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:MC5DICARB	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_2$	8.9×10^{2}		Wang et al. (2017)	Q	81, 240
PEBMIJGMJUFNQE-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C4DBM2CO3H	7.8×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_5$	5.1×10^{6}		Wang et al. (2017)	Q	81, 240
OAFSDIWBIPMWQP-UHFFFAOYSA-N	8.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C617CHO	1.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	4.6×10^{2}		Wang et al. (2017)	Q	81, 240
NFXFJRVNKKYMOX-UHFFFAOYSA-N	7.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C617CO3H	2.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	1.2×10^{5}		Wang et al. (2017)	Q	81, 240
GEJLCFNTSCJUHB-UHFFFAOYSA-N	5.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C618CO3H	2.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	1.0×10^{5}		Wang et al. (2017)	Q	81, 240
BCVYZYXNMFZMHQ-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C626CHO	2.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	5.4×10^{4}		Wang et al. (2017)	Q	81, 240
HBIBDTOPQGUCOQ-UHFFFAOYSA-N	2.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C626CO3H	3.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	2.9×10^{6}		Wang et al. (2017)	Q	81, 240
XXGYBOYKTQFTKB-UHFFFAOYSA-N	8.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C6M5CO2OOH	6.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
BPEPZMFTCHTDHQ-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C715CO2OOH	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	5.8×10^{4}		Wang et al. (2017)	Q	81, 240
MXRQCKDWMJYUGS-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C716OOH	1.6×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	8.3×10^{6}		Wang et al. (2017)	Q	81, 240
PDOSKCUHLZEIAA-UHFFFAOYSA-N	2.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C717OOH	1.6×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	4.9×10^{7}		Wang et al. (2017)	Q	81, 240
PIJZITIWWOWVNF-UHFFFAOYSA-N	6.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C718OOH	1.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	2.0×10^{5}		Wang et al. (2017)	Q	81, 240
IUOFUPZPJIEECL-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C731OOH	2.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	4.3×10^{6}		Wang et al. (2017)	Q	81, 240
GGMJSZWHPXYNJN-UHFFFAOYSA-N	4.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C735OOH	1.4×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	8.0×10^{6}		Wang et al. (2017)	Q	81, 240
FKXMDVIITUJJPH-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C736CO	5.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_3$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
XIQVOMVDKSOEBZ-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C736OOH	4.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	1.4×10^{5}		Wang et al. (2017)	Q	81, 240
FLZNSMFAMOSJOT-UHFFFAOYSA-N	4.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C7ADICARB	6.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_2$	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
JOIPXRIQHWMPFU-UHFFFAOYSA-N	8.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C7CO2DBAL	7.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_3$	5.5×10^{4}		Wang et al. (2017)	Q	81, 240
YGMUVGSOGISXBZ-UHFFFAOYSA-N	3.1		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C7CO2DCO3H	9.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_5$	1.8×10^{6}		Wang et al. (2017)	Q	81, 240
GSEZJGCNNFTSDI-UHFFFAOYSA-N	2.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C7CO4DB	5.8×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_6O_4$	1.5×10^{6}		Wang et al. (2017)	Q	81, 240
RYPSCZRULGRFHH-UHFFFAOYSA-N	4.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C7DDICARB	9.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_2$	6.2×10^{2}		Wang et al. (2017)	Q	81, 240
SRVPSCZJUZZLCY-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
MCM:C7DICARB	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_2$	3.7×10^{2}		Wang et al. (2017)	Q	81, 240
GLRVVKVYRCSDLF-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO235C6CHO	1.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_4$	2.6×10^{5}		Wang et al. (2017)	Q	81, 240
DKBJFPXQZAZJBK-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CO25C6CHO	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	2.6×10^{4}		Wang et al. (2017)	Q	81, 240
ZTMYUKBUAYLBJN-UHFFFAOYSA-N	4.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:IC7DICARB	1.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_2$	3.1×10^{2}		Wang et al. (2017)	Q	81, 240
XQQMMKHYZYQABV-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MC6CO2OOH	6.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	6.2×10^{3}		Wang et al. (2017)	Q	81, 240
HBFXSTFRJMUUSF-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C4DBMECO3H	6.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_5$	2.2×10^{6}		Wang et al. (2017)	Q	81, 240
MRKOFGXLZVJMLJ-UHFFFAOYSA-N	6.5×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6CO4M2DB	3.9×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_8O_4$	1.7×10^{6}		Wang et al. (2017)	Q	81, 240
XSTUBABFSAZOJC-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	81, 241
MCM:C6ETCO4DB	4.5×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_8O_4$	8.1×10^{5}		Wang et al. (2017)	Q	81, 240
OAQBTICOMUFUNE-UHFFFAOYSA-N	2.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C718CO3H	1.7×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	2.4×10^{5}		Wang et al. (2017)	Q	81, 240
TVOCFMMHLDKVAZ-UHFFFAOYSA-N	8.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C731CO3H	2.5×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	2.1×10^{6}		Wang et al. (2017)	Q	81, 240
NTZMYPVPFVPPPF-UHFFFAOYSA-N	8.1×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C7M6CO2OOH	5.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	6.6×10^{3}		Wang et al. (2017)	Q	81, 240
SYXNCLOQMRSNCQ-UHFFFAOYSA-N	5.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C7MCO2DBAL	7.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_3$	3.2×10^{4}		Wang et al. (2017)	Q	81, 240
PDQBXAJOXSGWHJ-UHFFFAOYSA-N	1.8		Wang et al. (2017)	Q	81, 241
MCM:C7MCO2OOH	8.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	3.6×10^{4}		Wang et al. (2017)	Q	81, 240
IVJZKSXAPVTQOQ-UHFFFAOYSA-N	7.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C815CO2OOH	7.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	3.2×10^{4}		Wang et al. (2017)	Q	81, 240
BDUHFTDKOJODDX-UHFFFAOYSA-N	6.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C817CO	3.1×10^{5}	12000	Wieser et al. (2023)	Q	439
$C_8H_{12}O_3$	1.7×10^{4}		Wang et al. (2017)	Q	81, 239
WSCYQCAMZDXSLH-UHFFFAOYSA-N	5.8×10^{3}		Wang et al. (2017)	Q	81, 240
	3.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C830CO	5.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_2$	3.8×10^{2}		Wang et al. (2017)	Q	81, 240
MHDCXCKIQVLVLU-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C831CO	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_3$	5.4×10^{3}		Wang et al. (2017)	Q	81, 240
ZUSGUVUFJOBUST-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C86OOH	1.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_4$	3.0×10^{5}		Wang et al. (2017)	Q	81, 240
DHFNMJQLYJIWHS-UHFFFAOYSA-N	3.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C87CO	1.5×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_4$	7.1×10^{4}		Wang et al. (2017)	Q	81, 240
ZGSYEZWRFTZRGE-UHFFFAOYSA-N	2.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C87OOH	1.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	2.8×10^{6}		Wang et al. (2017)	Q	81, 240
ZOZQVMIZJFBYCH-UHFFFAOYSA-N	9.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C8CO2DBAL	6.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_3$	3.9×10^{4}		Wang et al. (2017)	Q	81, 240
WFUAEUZWLUGFPU-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	81, 241
MCM:C8CO2DCO3H	7.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_5$	1.0×10^{6}		Wang et al. (2017)	Q	81, 240
AFZRTBPBEHNFPV-UHFFFAOYSA-N	1.7×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C8CO4DB	3.9×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_8O_4$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
XMBXSFIUGNBAMW-UHFFFAOYSA-N	2.4		Wang et al. (2017)	Q	81, 241
MCM:C8DCO2CO3H	8.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_5$	1.2×10^{6}		Wang et al. (2017)	Q	81, 240
LSJULIYFTAQYGE-UHFFFAOYSA-N	1.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:CO4DBC8	3.9×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_8O_4$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
UUVQUVHMBIAKFN-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	81, 241
MCM:MC7CO2OOH	5.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	3.0×10^{3}		Wang et al. (2017)	Q	81, 240
XEFYLFAPQOHXQI-UHFFFAOYSA-N	9.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C6CO4MEDB	3.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_4$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
KWNUZJFJQSMOTR-UHFFFAOYSA-N	6.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6IPRCO4DB	4.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_4$	8.7×10^{5}		Wang et al. (2017)	Q	81, 240
PHOIWTKCTUWXFI-UHFFFAOYSA-N	1.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6PRCO4DB	3.7×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_4$	9.6×10^{5}		Wang et al. (2017)	Q	81, 240
ZAOQHXFQWRKJIE-UHFFFAOYSA-N	1.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C7CO4EDB	3.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_4$	1.3×10^{6}		Wang et al. (2017)	Q	81, 240
ZLFZFHOVUMHREF-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	81, 241
MCM:C7ECO4DB	3.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_4$	1.3×10^{6}		Wang et al. (2017)	Q	81, 240
AWHQTSPUFRSDOO-UHFFFAOYSA-N	7.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C827CHO	9.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_3$	8.5×10^{3}		Wang et al. (2017)	Q	81, 240
WRGXNTJIWBXAOX-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C828CHO	7.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	5.8×10^{4}		Wang et al. (2017)	Q	81, 240
YZUHPZZEPOWVFM-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C87CO3H	1.5×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_6$	5.3×10^{7}		Wang et al. (2017)	Q	81, 240
AJHPLULEOIFIGV-UHFFFAOYSA-N	2.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C88CHO	3.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	8.9×10^{4}		Wang et al. (2017)	Q	81, 240
NXCXUGLKKPDWEC-UHFFFAOYSA-N	8.5×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C914CO	2.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_4$	1.5×10^{7}		Wang et al. (2017)	Q	81, 240
RDBINALOBQAVHT-UHFFFAOYSA-N	5.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C914OOH	2.6×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	1.6×10^{8}		Wang et al. (2017)	Q	81, 240
ZERYOMDBUHTQAV-UHFFFAOYSA-N	3.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C915OOH	4.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	4.2×10^{6}		Wang et al. (2017)	Q	81, 240
IHUGTHJLMVJZBZ-UHFFFAOYSA-N	2.8×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C916OOH	1.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	4.8×10^{7}		Wang et al. (2017)	Q	81, 240
FURCCROLNKVFJP-UHFFFAOYSA-N	4.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C918OOH	4.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	7.8×10^{5}		Wang et al. (2017)	Q	81, 240
RVRGXPTVZZTPQO-UHFFFAOYSA-N	1.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C919OOH	1.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	4.5×10^{7}		Wang et al. (2017)	Q	81, 240
HGDKSMVLGYFVMB-UHFFFAOYSA-N	2.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C926OOH	7.3×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	5.5×10^{6}		Wang et al. (2017)	Q	81, 240
YGLJXDYJGXWZRQ-UHFFFAOYSA-N	2.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C930OOH	7.3×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	2.6×10^{7}		Wang et al. (2017)	Q	81, 240
UQPOFUKCKANZIY-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:CO4DBC9	2.5×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_4$	1.2×10^{6}		Wang et al. (2017)	Q	81, 240
KCIAXTRCVKQJBW-UHFFFAOYSA-N	7.1		Wang et al. (2017)	Q	81, 241
MCM:LMLKACO	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	8.1×10^{5}		Wang et al. (2017)	Q	81, 240
JZUAMOXWRDMCCH-UHFFFAOYSA-N	8.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:LMLKAOOH	1.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	1.7×10^{7}		Wang et al. (2017)	Q	81, 240
VTXNRXDJNZTEJV-UHFFFAOYSA-N	9.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:LMLKBCO	1.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	5.5×10^{5}		Wang et al. (2017)	Q	81, 240
UMGHNOQMPCKCSD-UHFFFAOYSA-N	6.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:LMLKBOOH	1.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	3.6×10^{7}		Wang et al. (2017)	Q	81, 240
YVDVZIZUYUAKKJ-UHFFFAOYSA-N	3.0×10^{6}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:LMLKET	1.1×10^{6}	13000	Wieser et al. (2023)	Q	439
$C_9H_{14}O_3$	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
CWEQHJLFCKMWEE-UHFFFAOYSA-N	5.4×10^{4}		Wang et al. (2017)	Q	81, 240
	3.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NORLIMAL	6.1×10^{2}	11000	Wieser et al. (2023)	Q	439
$C_9H_{14}O_2$	4.9×10^{1}		Wang et al. (2017)	Q	81, 239
WPNOYHDEEVPEJH-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	81, 240
	9.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NORPINAL	5.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_2$	2.2×10^{2}		Wang et al. (2017)	Q	81, 240
CRBGTXDFEDFKSU-UHFFFAOYSA-N	4.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C1010OOH	2.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_4$	3.8×10^{5}		Wang et al. (2017)	Q	81, 240
PQCOZMUQYGSZBV-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C1012CO	7.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_3$	6.5×10^{4}		Wang et al. (2017)	Q	81, 240
ZTXNVHZVZBDWRG-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C1012OOH	9.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_4$	3.5×10^{5}		Wang et al. (2017)	Q	81, 240
NQAGNHJKHGEOIP-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C106OOH	6.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_5$	3.2×10^{7}		Wang et al. (2017)	Q	81, 240
QENSMPURVPBEBQ-UHFFFAOYSA-N	1.8×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C107OOH	2.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_4$	1.6×10^{4}		Wang et al. (2017)	Q	81, 240
JYIMELQJWXRSLA-UHFFFAOYSA-N	3.2×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C108OOH	6.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_5$	1.7×10^{7}		Wang et al. (2017)	Q	81, 240
AIXQDYAMZUITKH-UHFFFAOYSA-N	2.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C109CO	3.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{14}O_3$	5.6×10^{3}		Wang et al. (2017)	Q	81, 240
GPWOGFGLGKGEOT-UHFFFAOYSA-N	8.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C109OOH	3.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_4$	5.8×10^{4}		Wang et al. (2017)	Q	81, 240
ODTCGEGBAGAWAJ-UHFFFAOYSA-N	5.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:LIMALACO	4.3×10^{4}	13000	Wieser et al. (2023)	Q	439
$C_{10}H_{14}O_3$	2.6×10^{4}		Wang et al. (2017)	Q	81, 239
OXUPJDFJWCMZMO-UHFFFAOYSA-N	2.9×10^{3}		Wang et al. (2017)	Q	81, 240
	3.2×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:LIMALAOOH	2.5×10^{5}	15000	Wieser et al. (2023)	Q	439
$C_{10}H_{16}O_4$	3.5×10^{6}		Wang et al. (2017)	Q	81, 239
DVORBFWFCUOYLW-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
	4.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:LIMALBCO	3.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{14}O_3$	2.0×10^{3}		Wang et al. (2017)	Q	81, 240
OFCYPGCYWHDSNB-UHFFFAOYSA-N	8.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:LIMALBOOH	2.4×10^{5}	15000	Wieser et al. (2023)	Q	439
$C_{10}H_{16}O_4$	2.9×10^{6}		Wang et al. (2017)	Q	81, 239
DCWLKDSHBWMMQU-UHFFFAOYSA-N	2.0×10^{4}		Wang et al. (2017)	Q	81, 240
	1.4×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:LIMAL	4.0×10^{2}	11000	Wieser et al. (2023)	Q	439
$C_{10}H_{16}O_2$	3.8×10^{1}		Wang et al. (2017)	Q	81, 239
OGCGCISRMFSLTC-UHFFFAOYSA-N	7.4×10^{1}		Wang et al. (2017)	Q	81, 240
	2.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PINAL	4.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_2$	2.0×10^{2}		Wang et al. (2017)	Q	81, 240
GCHDWVBHKDJOKU-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:PINALOOH	2.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_4$	1.0×10^{6}		Wang et al. (2017)	Q	81, 240
IKYOAMQPSDRUHL-UHFFFAOYSA-N	5.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C116CO	3.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{16}O_3$	2.0×10^{4}		Wang et al. (2017)	Q	81, 240
XGVKCXDPIYHMTH-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C116OOH	2.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_4$	2.0×10^{6}		Wang et al. (2017)	Q	81, 240
GLQKGYMROFUHSE-UHFFFAOYSA-N	2.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C116CHO	2.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{18}O_3$	1.4×10^{5}		Wang et al. (2017)	Q	81, 240
LCDZSXGLJAAQMI-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C116CO3H	3.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{18}O_5$	2.4×10^{6}		Wang et al. (2017)	Q	81, 240
DYOBAPPYFCSOAS-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C1210OOH	2.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_4$	4.7×10^{6}		Wang et al. (2017)	Q	81, 240
KZRFFJDVJJJBDC-UHFFFAOYSA-N	4.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C129CO	1.9×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{16}O_4$	8.7×10^{5}		Wang et al. (2017)	Q	81, 240
RGVZWLUABXGGBI-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C129OOH	2.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{18}O_5$	1.5×10^{7}		Wang et al. (2017)	Q	81, 240
OVAMHHASBHCMIZ-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C1210CO3H	2.8×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{20}O_5$	1.9×10^{6}		Wang et al. (2017)	Q	81, 240
BXGKTBFSJURUHS-UHFFFAOYSA-N	6.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C131CO	1.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{20}O_3$	2.1×10^{4}		Wang et al. (2017)	Q	81, 240
FDPPFMUIMWYEIX-UHFFFAOYSA-N	3.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:BCLKACO	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{20}O_4$	3.2×10^{6}		Wang et al. (2017)	Q	81, 240
ARRZIWJBJSIOKE-UHFFFAOYSA-N	4.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:BCLKAOOH	1.1×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_5$	1.7×10^{7}		Wang et al. (2017)	Q	81, 240
CKBNEDHFWOQWQD-UHFFFAOYSA-N	2.6×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:BCLKBCO	1.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{20}O_4$	2.9×10^{6}		Wang et al. (2017)	Q	81, 240
NZHCLRCYZNBCMK-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:BCLKBOOH	1.1×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_5$	4.6×10^{7}		Wang et al. (2017)	Q	81, 240
CNYMBWKCKYTSRZ-UHFFFAOYSA-N	1.5×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:BCLKCCO	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{20}O_4$	1.2×10^{6}		Wang et al. (2017)	Q	81, 240
RVZWWCAHYGTHHX-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:BCLKCOOH	1.1×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_5$	1.5×10^{7}		Wang et al. (2017)	Q	81, 240
OVPKMRRDRUAGIL-UHFFFAOYSA-N	6.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:BCLKET	1.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_3$	1.4×10^{5}		Wang et al. (2017)	Q	81, 240
UGDRYISIDBCIAI-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C141CO	4.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_2$	1.6×10^{2}		Wang et al. (2017)	Q	81, 240
LUPUYUXNGLIEMW-UHFFFAOYSA-N	7.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C146CO	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{20}O_4$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
ODTZTSYYOIXMEF-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C146OOH	1.1×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_5$	1.3×10^{7}		Wang et al. (2017)	Q	81, 240
SPXXDEIFDYFSMG-UHFFFAOYSA-N	1.6×10^{5}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:BCALACO	2.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{22}O_3$	3.6×10^{3}		Wang et al. (2017)	Q	81, 240
ULXUQSOGQJAAAV-UHFFFAOYSA-N	4.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:BCALAOOH	3.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{24}O_4$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
CATQWYAHYHBBFL-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:BCALBCO	3.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{22}O_3$	2.9×10^{3}		Wang et al. (2017)	Q	81, 240
DVBAGSYXLVWTHM-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:BCALBOOH	2.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{24}O_4$	3.6×10^{4}		Wang et al. (2017)	Q	81, 240
BXDTVEFUTYSWEH-UHFFFAOYSA-N	1.8×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:BCAL	3.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{24}O_2$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
PJJCDGMFEIUQRZ-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:BCALCCO	2.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{22}O_3$	4.7×10^{3}		Wang et al. (2017)	Q	81, 240
RMGPJKLPPRXORI-UHFFFAOYSA-N	2.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:BCALCOOH	3.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{24}O_4$	1.7×10^{4}		Wang et al. (2017)	Q	81, 240
WQOUANLPJNTVBV-UHFFFAOYSA-N	2.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:PHGLYOX	1.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_6O_2$	8.9×10^{1}		Wang et al. (2017)	Q	81, 240
OJUGVDODNPJEEC-UHFFFAOYSA-N	8.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:MPHGLYOX	1.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_8O_2$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
ILRFLXHICGHRIN-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	81, 241
MCM:DMPHGLYOX	6.5×10^{2}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{10}O_2$	6.6×10^{1}		Wang et al. (2017)	Q	81, 240
COKLAMNWIKZGIN-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	81, 241
MCM:EMPHGLYOX	5.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{12}O_2$	5.3×10^{1}		Wang et al. (2017)	Q	81, 240
LRURTQBJFCJOFP-UHFFFAOYSA-N	8.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:HOCH2COCHO	7.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_4O_3$	4.4×10^{3}		Wang et al. (2017)	Q	81, 240
JLPAWRLRMTZCSF-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	81, 241
MCM:CCOCOCOH	7.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_3$	3.2×10^{3}		Wang et al. (2017)	Q	81, 240
AWMGPEHDHJUMEN-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CO13C4OH	6.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_3$	2.3×10^{4}		Wang et al. (2017)	Q	81, 240
KATSYVMPKZTIRW-UHFFFAOYSA-N	4.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CO2H3CHO	1.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_3$	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
GTYVZUSWKGYETP-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:H13CO2CHO	1.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_4$	4.6×10^{5}		Wang et al. (2017)	Q	81, 240
RAPYKXPBVBNJGC-UHFFFAOYSA-N	3.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:H1CO23CHO	4.7×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_4$	1.2×10^{6}		Wang et al. (2017)	Q	81, 240
XSEYITBSKRUSNL-UHFFFAOYSA-N	3.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO1CO3CHO	1.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_3$	4.0×10^{4}		Wang et al. (2017)	Q	81, 240
CUSSNCHZLYDUPJ-UHFFFAOYSA-N	6.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HOCOC4DIAL	1.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_4$	5.3×10^{5}		Wang et al. (2017)	Q	81, 240
JWBVDBDNUQOADG-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C4MCO2OH	8.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	3.2×10^{3}		Wang et al. (2017)	Q	81, 240
YKNUMNAVGAMCFT-UHFFFAOYSA-N	2.6		Wang et al. (2017)	Q	81, 241
MCM:C512OH	1.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	1.5×10^{5}		Wang et al. (2017)	Q	81, 240
ZSJOVUGBPPFONP-UHFFFAOYSA-N	5.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C5134CO2OH	9.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_4$	4.2×10^{5}		Wang et al. (2017)	Q	81, 240
UFXCMYYHMGNRSQ-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C513CO	7.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_4$	5.9×10^{6}		Wang et al. (2017)	Q	81, 240
GBFAZHBQOBSKET-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C513OH	3.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	8.9×10^{7}		Wang et al. (2017)	Q	81, 240
VLANIYKAIBIISW-UHFFFAOYSA-N	4.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C513OOH	8.9×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	2.5×10^{8}		Wang et al. (2017)	Q	81, 240
FJRVRXOZJCMNIT-UHFFFAOYSA-N	5.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C514CO23OH	4.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	4.5×10^{6}		Wang et al. (2017)	Q	81, 240
JLVNMCMGUWUGCO-UHFFFAOYSA-N	4.3×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C520OH	1.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
BXHDMMHJHUOSNS-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C520OOH	7.1×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	3.0×10^{6}		Wang et al. (2017)	Q	81, 240
BCWSZSNCYSGOQJ-UHFFFAOYSA-N	2.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C5CO3OH	9.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_4$	6.2×10^{5}		Wang et al. (2017)	Q	81, 240
UUUQEQKLOQQXBA-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C5DICAROOH	6.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	1.3×10^{7}		Wang et al. (2017)	Q	81, 240
SXCXUVJXNGWYKY-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:CO3H4CHO	1.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	7.1×10^{3}		Wang et al. (2017)	Q	81, 240
GHHQRUFNLVFZPQ-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	81, 241
MCM:H1C23C4CHO	3.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_4$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
VBLXHDGHHJBCMK-UHFFFAOYSA-N	3.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HMVKBCHO	3.6×10^{5}	11000	Wieser et al. (2023)	Q	439
$C_5H_8O_3$	1.1×10^{5}		Wang et al. (2017)	Q	81, 239
XYGGNMZYIGPNCC-UHFFFAOYSA-N	1.3×10^{5}		Wang et al. (2017)	Q	81, 240
	2.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HO2CO4CHO	1.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	2.5×10^{4}		Wang et al. (2017)	Q	81, 240
NSUJYXKDWVMPFQ-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HOIPRGLYOX	1.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	3.2×10^{4}		Wang et al. (2017)	Q	81, 240
ROKGRLJNHSUEOC-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:IEC2OOH	3.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	2.0×10^{6}		Wang et al. (2017)	Q	81, 240
KGZJHQJCDPZOFG-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MBOCOCO	3.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	6.8×10^{2}		Wang et al. (2017)	Q	81, 240
OCAJTNNCRSVJNU-UHFFFAOYSA-N	8.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C43OHCOCHO	1.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	2.8×10^{4}		Wang et al. (2017)	Q	81, 240
NMZPCKZSNUOBSC-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C517CHO	9.5×10^{2}	13000	Wieser et al. (2023)	Q	439
$C_6H_{10}O_3$	1.0×10^{5}		Wang et al. (2017)	Q	81, 239
JGHPNZFTVGSLKF-UHFFFAOYSA-N	7.8×10^{5}		Wang et al. (2017)	Q	81, 240
	2.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C519CHO	2.8×10^{6}	11000	Wieser et al. (2023)	Q	439
$C_6H_{10}O_3$	1.0×10^{5}		Wang et al. (2017)	Q	81, 239
PVAHQKAVPKMXGV-UHFFFAOYSA-N	2.6×10^{5}		Wang et al. (2017)	Q	81, 240
	6.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C5COOHCO3H	4.7×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_6$	3.2×10^{9}		Wang et al. (2017)	Q	81, 240
DETDOHNNOYOALO-UHFFFAOYSA-N	8.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C5MO132OH	1.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	3.0×10^{3}		Wang et al. (2017)	Q	81, 240
YVTXQDAOLHXGGS-UHFFFAOYSA-N	2.7		Wang et al. (2017)	Q	81, 241
MCM:C6134CO2OH	7.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	1.8×10^{5}		Wang et al. (2017)	Q	81, 240
ZUSWTYLGBZLTMD-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C614CO23OH	3.4×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	3.6×10^{6}		Wang et al. (2017)	Q	81, 240
FTHGMBBEYTXWQT-UHFFFAOYSA-N	1.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C615CO2OH	2.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	1.1×10^{5}		Wang et al. (2017)	Q	81, 240
AEWAJJBQFQHEAB-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C616OH	9.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	7.4×10^{6}		Wang et al. (2017)	Q	81, 240
VJOSQGBCXQMKDE-UHFFFAOYSA-N	8.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C617OH	3.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	4.8×10^{3}		Wang et al. (2017)	Q	81, 240
GSQCYSIEWGMUPC-UHFFFAOYSA-N	7.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C620OH	4.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	9.6×10^{6}		Wang et al. (2017)	Q	81, 240
SMLWDBHBBFROKP-UHFFFAOYSA-N	4.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C628OH	4.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	3.6×10^{7}		Wang et al. (2017)	Q	81, 240
XRZKKMNIWXFNJQ-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C628OOH	6.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	5.4×10^{7}		Wang et al. (2017)	Q	81, 240
BGLCDSUTRBZUMD-UHFFFAOYSA-N	3.5×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C629OH	2.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	1.1×10^{7}		Wang et al. (2017)	Q	81, 240
MIXLBBAGKJLCSO-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C629OOH	4.9×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	2.0×10^{7}		Wang et al. (2017)	Q	81, 240
PARGUUHBZPMBOS-UHFFFAOYSA-N	2.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C630CO	2.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	3.4×10^{5}		Wang et al. (2017)	Q	81, 240
AUMGTZPDEFNUMP-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C65OH	3.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	3.4×10^{4}		Wang et al. (2017)	Q	81, 240
ZWRMEYSYDMGCIE-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C67CHO	3.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	6.2×10^{3}		Wang et al. (2017)	Q	81, 240
BZFZPOBVGBFEBG-UHFFFAOYSA-N	8.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C6CO2M2OH	2.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	4.4×10^{6}		Wang et al. (2017)	Q	81, 240
ZFPKEBYORKZJID-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C6CO2OHOOH	3.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	3.3×10^{6}		Wang et al. (2017)	Q	81, 240
LMEOLDNWXYVMAA-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C6CO3MOH	5.4×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	8.3×10^{4}		Wang et al. (2017)	Q	81, 240
WBLLHOUAAGAGCV-UHFFFAOYSA-N	4.0		Wang et al. (2017)	Q	81, 241
MCM:C6COHOCHO	8.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	4.0×10^{5}		Wang et al. (2017)	Q	81, 240
HJNIDOQIVMJXHS-UHFFFAOYSA-N	2.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C6DICAROOH	5.5×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	9.6×10^{6}		Wang et al. (2017)	Q	81, 240
HIILQMKIFXFEHC-UHFFFAOYSA-N	2.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C6O132OH	1.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	3.6×10^{3}		Wang et al. (2017)	Q	81, 240
GIDOBZXUXDNRDY-UHFFFAOYSA-N	3.0		Wang et al. (2017)	Q	81, 241
MCM:C6TONOHOOH	2.6×10^{11}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_6$	1.1×10^{10}		Wang et al. (2017)	Q	81, 240
CIXJOARRJVNUNZ-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:H2M3CO4CHO	1.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	2.6×10^{4}		Wang et al. (2017)	Q	81, 240
MIIVJRGFVJVTGE-UHFFFAOYSA-N	9.8		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:H3C25C5CHO	3.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	2.0×10^{6}		Wang et al. (2017)	Q	81, 240
CLPDOVMSDUESLY-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HM22COCHO	6.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	1.8×10^{4}		Wang et al. (2017)	Q	81, 240
UTYMQWKKMYQTHJ-UHFFFAOYSA-N	6.0		Wang et al. (2017)	Q	81, 241
MCM:MC52CO2OH	2.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	4.6×10^{6}		Wang et al. (2017)	Q	81, 240
LGFUKTGFFSPNKZ-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MC5COOHOOH	3.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	6.0×10^{6}		Wang et al. (2017)	Q	81, 240
XFHCIPDXRRXAPB-UHFFFAOYSA-N	8.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MIBKHO4CHO	6.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	1.3×10^{4}		Wang et al. (2017)	Q	81, 240
OYDFBAKICJVUQJ-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C61CHO	6.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	1.4×10^{5}		Wang et al. (2017)	Q	81, 240
BDFRSVKDVGXKLG-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C62CHO	7.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	1.3×10^{5}		Wang et al. (2017)	Q	81, 240
QCTBGQUOJXZEIH-UHFFFAOYSA-N	4.3		Wang et al. (2017)	Q	81, 241
MCM:C6COOHCO3H	3.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_6$	2.4×10^{9}		Wang et al. (2017)	Q	81, 240
BNWBZUAKPODUMK-UHFFFAOYSA-N	3.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C6M5CO2OH	1.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	2.2×10^{4}		Wang et al. (2017)	Q	81, 240
YAAUSHWRBSRFSJ-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C715CO2OH	1.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	7.6×10^{4}		Wang et al. (2017)	Q	81, 240
KBBGTWJMXYAKIO-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C716OH	2.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	6.8×10^{6}		Wang et al. (2017)	Q	81, 240
QFGSQPDLKNLDDS-UHFFFAOYSA-N	9.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C717OH	5.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	1.6×10^{7}		Wang et al. (2017)	Q	81, 240
SEENFYUXRUQNHQ-UHFFFAOYSA-N	2.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C718OH	5.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_3$	2.7×10^{4}		Wang et al. (2017)	Q	81, 240
ALYGFZDZOCWXMF-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C731OH	8.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_3$	1.7×10^{6}		Wang et al. (2017)	Q	81, 240
KHEBQEUBDOAJRG-UHFFFAOYSA-N	8.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C733CO	5.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	1.9×10^{7}		Wang et al. (2017)	Q	81, 240
IRSIMXCKMCQRGW-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C733OH	1.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	3.3×10^{8}		Wang et al. (2017)	Q	81, 240
WRHSSXYTISGZIA-UHFFFAOYSA-N	3.7×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C733OOH	7.4×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	7.3×10^{8}		Wang et al. (2017)	Q	81, 240
OWEUBRYSVXGVIC-UHFFFAOYSA-N	2.7×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C735OH	2.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	1.7×10^{7}		Wang et al. (2017)	Q	81, 240
PHOAHMZZKPNPAM-UHFFFAOYSA-N	4.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C736OH	8.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	1.3×10^{5}		Wang et al. (2017)	Q	81, 240
QWXLVLIZAXRZBR-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C7ADCOH	1.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	2.8×10^{6}		Wang et al. (2017)	Q	81, 240
SVQINHOHTZDOCH-UHFFFAOYSA-N	7.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C7ADCOOH	1.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	5.1×10^{6}		Wang et al. (2017)	Q	81, 240
COQUITHNSRNVBJ-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C7CO3OHOOH	3.0×10^{11}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_6$	3.2×10^{8}		Wang et al. (2017)	Q	81, 240
YAEIVOJGWQGWPS-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C7DCOH	2.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	1.9×10^{6}		Wang et al. (2017)	Q	81, 240
VIPBNCDHLKDPDM-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C7DCOOH	4.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	5.1×10^{6}		Wang et al. (2017)	Q	81, 240
AVRZSWZUKXCJRK-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C7DDCOH	1.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	2.6×10^{6}		Wang et al. (2017)	Q	81, 240
HYCGRSOMYJQICU-UHFFFAOYSA-N	6.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C7DDCOOH	3.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	1.4×10^{6}		Wang et al. (2017)	Q	81, 240
VSEOFSAKNXJKSZ-UHFFFAOYSA-N	8.1×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:IC7DCOH	3.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	1.5×10^{6}		Wang et al. (2017)	Q	81, 240
DEDFQTYPJDABTI-UHFFFAOYSA-N	7.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:IC7DCOOH	5.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	5.8×10^{6}		Wang et al. (2017)	Q	81, 240
ZVFWDEWSMKAAIM-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:MC6CO2OH	1.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	1.0×10^{4}		Wang et al. (2017)	Q	81, 240
BNJUZVCUVNAPOM-UHFFFAOYSA-N	3.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C5M2OHCO3H	2.1×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_6$	3.2×10^{9}		Wang et al. (2017)	Q	81, 240
BRIBGOXGRALVGI-UHFFFAOYSA-N	9.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C7M15CO2OH	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_3$	3.0×10^{4}		Wang et al. (2017)	Q	81, 240
OEJDBFGEAKTZGI-UHFFFAOYSA-N	6.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C7M6CO2OH	9.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_3$	1.3×10^{4}		Wang et al. (2017)	Q	81, 240
WXVOVBAGQNBDEE-UHFFFAOYSA-N	4.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C7MO3OHOOH	3.0×10^{11}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_6$	2.2×10^{8}		Wang et al. (2017)	Q	81, 240
UOUKTGYLQYQUAO-UHFFFAOYSA-N	4.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C7OHO2CO3H	2.8×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_6$	1.7×10^{9}		Wang et al. (2017)	Q	81, 240
AOHPTSIBUCEZIY-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C815CO2OH	1.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_3$	3.8×10^{4}		Wang et al. (2017)	Q	81, 240
IPCSMQASRIZASM-UHFFFAOYSA-N	6.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C824CO	1.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_3$	4.6×10^{4}		Wang et al. (2017)	Q	81, 240
BQDQKENHFIFOJZ-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C83COOHOOH	2.7×10^{11}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_6$	2.0×10^{8}		Wang et al. (2017)	Q	81, 240
LBBMWNQOJHPRLQ-UHFFFAOYSA-N	6.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C87OH	2.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	2.1×10^{6}		Wang et al. (2017)	Q	81, 240
DFOLUFIWIMPWQH-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:MC7CO2OH	9.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_3$	6.6×10^{3}		Wang et al. (2017)	Q	81, 240
BSMWBPAKWVVEKL-UHFFFAOYSA-N	1.9×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C5MEJCO3H	1.7×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_6$	2.2×10^{9}		Wang et al. (2017)	Q	81, 240
IZKMPGKTEBWFPK-UHFFFAOYSA-N	5.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C8O2OHCO3H	2.6×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_6$	1.3×10^{9}		Wang et al. (2017)	Q	81, 240
MBOWYQZNYXRQRC-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C8OHO2CO3H	2.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_6$	1.1×10^{9}		Wang et al. (2017)	Q	81, 240
CJLPRBWVJFSMFP-UHFFFAOYSA-N	8.7		Wang et al. (2017)	Q	81, 241
MCM:C914OH	5.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	8.3×10^{7}		Wang et al. (2017)	Q	81, 240
LFDXAZOJHXEEGS-UHFFFAOYSA-N	2.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C915OH	1.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_3$	2.8×10^{6}		Wang et al. (2017)	Q	81, 240
FAAQZCMVHKUUSB-UHFFFAOYSA-N	8.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C916OH	3.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	1.4×10^{7}		Wang et al. (2017)	Q	81, 240
MXDMOPCDPNEDIT-UHFFFAOYSA-N	6.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C918OH	1.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_3$	4.4×10^{5}		Wang et al. (2017)	Q	81, 240
NFJZVEFTUBPOLY-UHFFFAOYSA-N	1.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C919OH	3.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	1.5×10^{7}		Wang et al. (2017)	Q	81, 240
ULXJXURNPDAXQL-UHFFFAOYSA-N	3.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C926OH	1.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	7.3×10^{6}		Wang et al. (2017)	Q	81, 240
DBPGQZSZWKEZHT-UHFFFAOYSA-N	1.2×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C930OH	2.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	5.3×10^{6}		Wang et al. (2017)	Q	81, 240
LNIVXHBNNGOOPM-UHFFFAOYSA-N	3.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:LMLKAOH	2.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	2.6×10^{7}		Wang et al. (2017)	Q	81, 240
XDMVMFNHBSPJDJ-UHFFFAOYSA-N	1.6×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:LMLKBOH	2.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	3.0×10^{7}		Wang et al. (2017)	Q	81, 240
JSAHIYWZESQWRA-UHFFFAOYSA-N	1.1×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:NORLIMOOH	3.8×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{16}O_5$	3.8×10^{8}		Wang et al. (2017)	Q	81, 240
CUMGKBRSRBORIJ-UHFFFAOYSA-N	6.6×10^{4}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C1010OH	6.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_3$	5.3×10^{5}		Wang et al. (2017)	Q	81, 240
NQWGZMQLCPYJCB-UHFFFAOYSA-N	8.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C1012OH	3.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_3$	5.6×10^{5}		Wang et al. (2017)	Q	81, 240
ZSBQFHQMMVQAKS-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C106OH	2.5×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_4$	8.1×10^{6}		Wang et al. (2017)	Q	81, 240
LWIDJJPVYZTGLI-UHFFFAOYSA-N	9.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C107OH	3.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_3$	5.9×10^{4}		Wang et al. (2017)	Q	81, 240
DUMRJPIWTJFZCT-UHFFFAOYSA-N	6.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C108OH	2.5×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_4$	3.2×10^{6}		Wang et al. (2017)	Q	81, 240
ZDBVABFEYYIFLR-UHFFFAOYSA-N	5.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C109OH	6.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_3$	4.3×10^{4}		Wang et al. (2017)	Q	81, 240
PUENXTSKKXKPMK-UHFFFAOYSA-N	2.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:LIMALAOH	3.1×10^{4}	15000	Wieser et al. (2023)	Q	439
$C_{10}H_{16}O_3$	5.8×10^{3}		Wang et al. (2017)	Q	81, 239
VNYSFQVUCPNMDZ-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	81, 240
	1.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:LIMALBOH	5.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_3$	1.8×10^{4}		Wang et al. (2017)	Q	81, 240
SMXSHIIAZMJGAE-UHFFFAOYSA-N	5.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:LIMALOH	2.2×10^{10}	18000	Wieser et al. (2023)	Q	439
$C_{10}H_{18}O_4$	4.2×10^{7}		Wang et al. (2017)	Q	81, 239
ISUQULRVPDSRIP-UHFFFAOYSA-N	2.8×10^{8}		Wang et al. (2017)	Q	81, 240
	9.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:LIMALOOH	4.3×10^{10}	18000	Wieser et al. (2023)	Q	439
$C_{10}H_{18}O_5$	3.5×10^{9}		Wang et al. (2017)	Q	81, 239
OQLBLHLZVAPRGN-UHFFFAOYSA-N	4.0×10^{8}		Wang et al. (2017)	Q	81, 240
	9.6×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PINALOH	8.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_3$	6.0×10^{5}		Wang et al. (2017)	Q	81, 240
NGFXWFWSYUSJMH-UHFFFAOYSA-N	7.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C116OH	9.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_3$	2.6×10^{5}		Wang et al. (2017)	Q	81, 240
JMGXHRKVWURTTA-UHFFFAOYSA-N	5.8×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C117OH	8.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_4$	4.9×10^{8}		Wang et al. (2017)	Q	81, 240
XYBUENVNXDXQKB-UHFFFAOYSA-N	4.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C117OOH	5.4×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_5$	2.0×10^{8}		Wang et al. (2017)	Q	81, 240
NUIUIELMTMWFAB-UHFFFAOYSA-N	5.9×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C118CO	1.3×10^{10}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{16}O_5$	5.6×10^{8}		Wang et al. (2017)	Q	81, 240
QFBAMJSHDLKQRE-UHFFFAOYSA-N	6.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C118OH	6.2×10^{10}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_5$	3.6×10^{10}		Wang et al. (2017)	Q	81, 240
GQNPBTACCNTXDZ-UHFFFAOYSA-N	2.9×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C118OOH	1.6×10^{12}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_6$	3.0×10^{10}		Wang et al. (2017)	Q	81, 240
DZELKNYJHUANPY-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C1210OH	7.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_3$	2.6×10^{6}		Wang et al. (2017)	Q	81, 240
RDCPBXUNBHOYIW-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C1214OH	7.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_4$	4.7×10^{8}		Wang et al. (2017)	Q	81, 240
LBONAAUBRWCFLP-UHFFFAOYSA-N	2.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C1214OOH	4.4×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_5$	1.8×10^{8}		Wang et al. (2017)	Q	81, 240
RDWLNWMMPUJYPV-UHFFFAOYSA-N	8.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C1215CO	1.0×10^{10}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{18}O_5$	3.2×10^{9}		Wang et al. (2017)	Q	81, 240
MFAMPSJMWGSBSP-UHFFFAOYSA-N	2.8×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C1215OH	4.8×10^{10}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_5$	1.1×10^{11}		Wang et al. (2017)	Q	81, 240
ICTVPTJMPURCGE-UHFFFAOYSA-N	3.2×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C1215OOH	1.3×10^{12}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_6$	4.6×10^{10}		Wang et al. (2017)	Q	81, 240
PWIVJRAMQXZVCR-UHFFFAOYSA-N	5.1×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C128CO	3.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{18}O_4$	8.3×10^{7}		Wang et al. (2017)	Q	81, 240
UGSIBTFJEGNWKQ-UHFFFAOYSA-N	6.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C128OH	1.5×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_4$	2.8×10^{9}		Wang et al. (2017)	Q	81, 240
CFXREDIWINSYMD-UHFFFAOYSA-N	1.3×10^{5}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C128OOH	4.7×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_5$	2.6×10^{9}		Wang et al. (2017)	Q	81, 240
UJLXMZVGYRRHNB-UHFFFAOYSA-N	3.3×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C129OH	4.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{18}O_4$	3.8×10^{7}		Wang et al. (2017)	Q	81, 240
LZLVFWPHHNPPPO-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C1312CO	2.9×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{20}O_4$	5.9×10^{7}		Wang et al. (2017)	Q	81, 240
OXGUTNXNCKSGQJ-UHFFFAOYSA-N	6.6×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C1312OH	1.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_4$	1.7×10^{9}		Wang et al. (2017)	Q	81, 240
IOOAKPNHTHIGJB-UHFFFAOYSA-N	2.8×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C1312OOH	3.6×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_5$	6.5×10^{8}		Wang et al. (2017)	Q	81, 240
IMCVJRKOQRMDFG-UHFFFAOYSA-N	3.9×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:BCLKAOH	2.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_4$	4.2×10^{7}		Wang et al. (2017)	Q	81, 240
OIHLYIMTKSRRQE-UHFFFAOYSA-N	5.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:BCLKBOH	1.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_4$	3.0×10^{7}		Wang et al. (2017)	Q	81, 240
LFMWXXSOGPOZAN-UHFFFAOYSA-N	7.4×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:BCLKCOH	2.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_4$	3.6×10^{7}		Wang et al. (2017)	Q	81, 240
WUCWLUFQNHHRAC-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C144OOH	4.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{24}O_5$	6.2×10^{8}		Wang et al. (2017)	Q	81, 240
GLUIAMUUMIPXJY-UHFFFAOYSA-N	5.8×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C146OH	2.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_4$	3.2×10^{7}		Wang et al. (2017)	Q	81, 240
MRXVSIMJFRVVPA-UHFFFAOYSA-N	2.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:BCALAOH	6.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{24}O_3$	3.3×10^{4}		Wang et al. (2017)	Q	81, 240
SOIICZPFVOBBSJ-UHFFFAOYSA-N	6.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:BCALBOH	5.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{24}O_3$	2.1×10^{4}		Wang et al. (2017)	Q	81, 240
WYNIZHBHTSXQQC-UHFFFAOYSA-N	5.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:BCALCOH	6.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{24}O_3$	3.4×10^{4}		Wang et al. (2017)	Q	81, 240
NQPQIVDLCLYNNZ-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241

Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:BCALOH	4.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{26}O_4$	4.2×10^{8}		Wang et al. (2017)	Q	81, 240
MPEWUZJEETZOEB-UHFFFAOYSA-N	5.4×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:BCALOOH	3.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{26}O_5$	8.7×10^{8}		Wang et al. (2017)	Q	81, 240
HSCKVTFOUFPNNB-UHFFFAOYSA-N	3.6×10^{7}		Wang et al. (2017)	Q	81, 241

A3.7 Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH)

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methanoic acid	8.8×10^{1}	6100	Burkholder et al. (2019)	L	
HCOOH	8.8×10^{1}	6100	Burkholder et al. (2015)	L	
(formic acid)	8.8×10^{1}	6100	Sander et al. (2011)	L	
[64-18-6]	8.8×10^{1}	6100	Sander et al. (2006)	L	
BDAGIHXWWSANSR-UHFFFAOYSA-N	6.7×10^{1}	5900	Staudinger and Roberts (2001)	L	
	8.8×10^{1}	6100	Johnson et al. (1996)	M	
	5.4×10^{1}		Khan et al. (1995)	M	
	5.4×10^{1}	5600	Khan and Brimblecombe (1992)	M	
	1.3×10^{2}		Servant et al. (1991)	M	489
	7.3×10^{1}		Johnson (1990)	M	80
	1.5×10^{1}		Hwang et al. (1992)	V	
		5700	Abraham (1984)	V	
		5600	Abraham (1984)	R	490
		5700	Winiwarter et al. (1988)	T	491
	3.7×10^{1}	5700	Jacob (1986)	T	492
	5.5×10^{1}		Keene and Galloway (1986)	T	
	5.9×10^{1}		Gaffney and Senum (1984)	X	391, 493
	5.1×10^{1}		Johnson et al. (1996)	C	
	5.1×10^{1}		Keene et al. (1995)	C	
	5.3×10^{1}		Keene et al. (1995)	C	
	3.7×10^{1}	5700	Lelieveld and Crutzen (1991)	C	
	3.5×10^{1}	5700	Pandis and Seinfeld (1989)	C	
	2.1×10^{2}		Keshavarz et al. (2022)	Q	
	4.0×10^{1}		Duchowicz et al. (2020)	Q	185
	2.2×10^{1}		Wang et al. (2017)	Q	81, 239
	2.5×10^{2}		Wang et al. (2017)	Q	81, 240
	1.0×10^{2}		Wang et al. (2017)	Q	81, 241
	2.3×10^{2}		Hilal et al. (2008)	Q	
	1.2×10^{1}		Modarresi et al. (2007)	Q	68
		5800	Kühne et al. (2005)	Q	
	5.8×10^{1}		Yaffe et al. (2003)	Q	249, 250
	8.6×10^{1}		Abraham (2003)	Q	
	7.7		Katritzky et al. (1998)	Q	
	5.9×10^{1}		Duchowicz et al. (2020)	?	186, 21
		6500	Kühne et al. (2005)	?	
	1.3×10^{1}		Yaws (1999)	?	21
	8.9		Yaws and Yang (1992)	?	21

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethanoic acid	4.0×10^1	6200	Burkholder et al. (2019)	L	
CH_3COOH	4.0×10^1	6200	Burkholder et al. (2015)	L	
(acetic acid)	4.0×10^1	6200	Sander et al. (2011)	L	
[64-19-7]	4.0×10^1	6200	Sander et al. (2006)	L	
QTBSBXVTEAMEQO-UHFFFAOYSA-N	4.6×10^1	6300	Staudinger and Roberts (2001)	L	
	1.4×10^1		von Hartungen et al. (2004)	M	
	4.0×10^1	6300	Johnson et al. (1996)	M	
	5.4×10^1		Khan et al. (1995)	M	
	5.4×10^1	8300	Khan and Brimblecombe (1992)	M	
	9.2×10^1		Servant et al. (1991)	M	489
			Fredenhagen and Liebster (1932)	M	330
	9.1		Hwang et al. (1992)	V	
		6300	Abraham (1984)	V	
		6200	Abraham (1984)	R	490
	4.8×10^1	6400	Plyasunov et al. (2001)	T	
	8.7×10^1	6400	Jacob et al. (1989)	T	
		6400	Winiwarter et al. (1988)	T	491
	8.7×10^1		Keene and Galloway (1986)	T	
	9.7	4900	Goldstein (1982)	X	299
	9.9×10^1		Gaffney and Senum (1984)	X	391, 493
	5.1×10^1		Johnson et al. (1996)	C	
	5.2×10^1		Keene et al. (1995)	C	
	8.5×10^1		Keene et al. (1995)	C	
	1.0×10^2		Keshavarz et al. (2022)	Q	
	3.1×10^1		Duchowicz et al. (2020)	Q	
	1.4×10^1		Wang et al. (2017)	Q	81, 239
	2.9×10^2		Wang et al. (2017)	Q	81, 240
	6.5×10^1		Wang et al. (2017)	Q	81, 241
	3.3×10^1		Li et al. (2014)	Q	242
	2.0×10^1		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^2		Raventos-Duran et al. (2010)	Q	245
	2.0×10^1		Raventos-Duran et al. (2010)	Q	246
	1.3×10^2		Hilal et al. (2008)	Q	
	3.2×10^1		Modarresi et al. (2007)	Q	68
		6100	Kühne et al. (2005)	Q	
	9.9×10^1		Yaffe et al. (2003)	Q	249, 250
	3.1×10^1		Abraham (2003)	Q	
	3.1×10^1		English and Carroll (2001)	Q	231, 232
	1.1×10^1		Katritzky et al. (1998)	Q	
	2.3×10^1		Russell et al. (1992)	Q	280
	3.1×10^1		Suzuki et al. (1992)	Q	233
	3.9×10^1		Nirmalakhandan and Speece (1988)	Q	
	9.9×10^1		Duchowicz et al. (2020)	?	186, 21
	1.1×10^1		Maniere et al. (2011)	?	242, 166
		6200	Kühne et al. (2005)	?	
	8.4		Yaws (1999)	?	21

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.2		Yaws and Yang (1992)	?	21
	3.3×10^{1}		Abraham et al. (1990)	?	
	3.3×10^{1}		Hine and Mookerjee (1975)	?	
acetic anhydride	1.7		Duchowicz et al. (2020)	V	187
$C_4H_6O_3$	3.6		Yaws (2003)	X	238
[108-24-7]	6.3×10^{-1}		Duchowicz et al. (2020)	Q	
WFDIJRYMOXRFFG-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	81, 239
	5.3×10^{1}		Wang et al. (2017)	Q	81, 240
	1.7		Wang et al. (2017)	Q	81, 241
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	3.9		Gharagheizi et al. (2010)	Q	247
	7.1×10^{-1}		Modarresi et al. (2007)	Q	68
	2.3		Yaws (1999)	?	21
propanoic acid	7.1×10^{1}		Kim and Kim (2016)	M	
C_2H_5COOH	1.5×10^{1}		von Hartungen et al. (2004)	M	
(propionic acid)	5.6×10^{1}		Khan et al. (1995)	M	
[79-09-4]	5.5×10^{1}		Khan and Brimblecombe (1992)	M	
XBDQKXXYIPTUBI-UHFFFAOYSA-N	6.1×10^{1}		Servant et al. (1991)	M	489
	2.2×10^{1}		Butler and Ramchandani (1935)	M	
		6800	Abraham (1984)	V	
		6800	Abraham (1984)	R	490
	3.7×10^{1}	6800	Plyasunov et al. (2001)	T	
	2.6×10^{1}		Keshavarz et al. (2022)	Q	
	4.2×10^{1}		Duchowicz et al. (2020)	Q	300
	1.2×10^{1}		Wang et al. (2017)	Q	81, 239
	2.6×10^{2}		Wang et al. (2017)	Q	81, 240
	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	246
	7.0×10^{1}		Hilal et al. (2008)	Q	
	2.8×10^{1}		Modarresi et al. (2007)	Q	68
	2.4×10^{1}		Yaffe et al. (2003)	Q	249, 250
	2.2×10^{1}		Abraham (2003)	Q	
	2.3×10^{1}		English and Carroll (2001)	Q	231, 232
	2.4		Katritzky et al. (1998)	Q	
	5.6		Russell et al. (1992)	Q	360
	2.4×10^{1}		Suzuki et al. (1992)	Q	233
	3.4×10^{1}		Nirmalakhandan and Speece (1988)	Q	
	2.2×10^{1}		Duchowicz et al. (2020)	?	186, 21
	1.1×10^{1}		Yaws (1999)	?	21
	2.2×10^{1}		Abraham et al. (1990)	?	
	2.2×10^{1}		Hine and Mookerjee (1975)	?	

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methoxyacetic acid	1.5×10^{3}		Duchowicz et al. (2020)	V	187
$C_3H_6O_3$	3.0×10^{2}		Duchowicz et al. (2020)	Q	
[625-45-6]	3.0×10^{2}		Wang et al. (2017)	Q	81, 239
RMIODHQZRUFFFF-UHFFFAOYSA-N	6.6×10^{2}		Wang et al. (2017)	Q	81, 240
	1.0×10^{3}		Wang et al. (2017)	Q	81, 241
butanoic acid	4.3×10^{1}		Kim and Kim (2016)	M	
C_3H_7COOH	9.7		von Hartungen et al. (2004)	M	
(butyric acid)	4.7×10^{1}		Khan et al. (1995)	M	
[107-92-6]	4.5×10^{1}		Khan and Brimblecombe (1992)	M	
FERIUCNNQQJTOY-UHFFFAOYSA-N	1.8×10^{1}		Butler and Ramchandani (1935)	M	
	9.4		Hwang et al. (1992)	V	
		7100	Abraham (1984)	V	
		7300	Abraham (1984)	R	490
	2.5×10^{1}		Keshavarz et al. (2022)	Q	
	5.0×10^{1}		Duchowicz et al. (2020)	Q	
	9.1		Wang et al. (2017)	Q	81, 239
	1.3×10^{2}		Wang et al. (2017)	Q	81, 240
	1.4×10^{1}		Wang et al. (2017)	Q	81, 241
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	272, 244
	6.2×10^{1}		Raventos-Duran et al. (2010)	Q	245
	9.9		Raventos-Duran et al. (2010)	Q	246
	4.4×10^{1}		Hilal et al. (2008)	Q	
	2.5×10^{1}		Modarresi et al. (2007)	Q	68
	1.7×10^{1}		Abraham (2003)	Q	
	1.8×10^{1}		English and Carroll (2001)	Q	231, 275
	2.8		Russell et al. (1992)	Q	280
	1.8×10^{1}		Suzuki et al. (1992)	Q	233
	2.7×10^{1}		Nirmalakhandan and Speece (1988)	Q	
	1.8×10^{1}		Duchowicz et al. (2020)	?	186, 21
	1.8×10^{1}		Abraham et al. (1990)	?	
	1.8×10^{1}		Hine and Mookerjee (1975)	?	
2-methylpropanoic acid	4.6×10^{1}		Kim and Kim (2016)	M	
$(CH_3)_2CHCOOH$	9.6		von Hartungen et al. (2004)	M	
(isobutyric acid)	1.1×10^{1}		Khan et al. (1995)	M	
[79-31-2]	1.1×10^{1}		Khan and Brimblecombe (1992)	M	
KQNPFQTWMSNSAP-UHFFFAOYSA-N	5.6×10^{1}		Servant et al. (1991)	M	489
	1.4		Mackay et al. (2006c)	V	
	2.5×10^{1}		Keshavarz et al. (2022)	Q	
	1.9×10^{1}		Duchowicz et al. (2020)	Q	
	1.1×10^{1}		Wang et al. (2017)	Q	81, 239
	6.3×10^{1}		Wang et al. (2017)	Q	81, 240
	1.7×10^{1}		Wang et al. (2017)	Q	81, 241
	2.0×10^{1}		Gharagheizi et al. (2012)	Q	
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	245

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.9		Raventos-Duran et al. (2010)	Q	246
	2.5×10^{1}		Hilal et al. (2008)	Q	
	4.7×10^{1}		Modarresi et al. (2007)	Q	68
	1.1×10^{1}		Duchowicz et al. (2020)	?	186, 21
	1.1×10^{1}		Yaws (1999)	?	21, 12
pentanoic acid	2.3×10^{1}	6900	Staudinger and Roberts (2001)	L	
C_4H_9COOH	2.4×10^{1}		Kim and Kim (2016)	M	
(valeric acid)	1.2×10^{1}		von Hartungen et al. (2004)	M	
[109-52-4]	2.3×10^{1}	6600	Khan et al. (1995)	M	
NQPDZGIKBAWPEJ-UHFFFAOYSA-N	2.1×10^{1}	6900	Khan and Brimblecombe (1992)	M	
	1.2×10^{1}		Mackay et al. (2006c)	V	
	1.2×10^{1}		Mackay et al. (1995)	V	
	1.6×10^{1}		Brimblecombe et al. (1992)	V	
		7500	Abraham (1984)	V	
	1.3×10^{1}		Amoore and Buttery (1978)	V	
		7700	Abraham (1984)	R	490
	7.7		Yaws (2003)	X	238
	1.2×10^{1}		Keshavarz et al. (2022)	Q	
	5.5×10^{1}		Duchowicz et al. (2020)	Q	185
	8.5		Wang et al. (2017)	Q	81, 239
	6.6×10^{1}		Wang et al. (2017)	Q	81, 240
	1.4×10^{1}		Wang et al. (2017)	Q	81, 241
	9.9		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	245
	7.8		Raventos-Duran et al. (2010)	Q	246
	1.6×10^{1}		Gharagheizi et al. (2010)	Q	247
	3.3×10^{1}		Hilal et al. (2008)	Q	
	1.8×10^{1}		Modarresi et al. (2007)	Q	68
		7200	Kühne et al. (2005)	Q	
	1.4×10^{1}		Yaffe et al. (2003)	Q	249, 273
	1.1×10^{1}		Abraham (2003)	Q	
	1.4×10^{1}		English and Carroll (2001)	Q	231, 232
	2.9		Katritzky et al. (1998)	Q	
	2.2×10^{1}		Nirmalakhandan et al. (1997)	Q	
	2.1×10^{1}		Duchowicz et al. (2020)	?	186, 21
		6900	Kühne et al. (2005)	?	
	7.4		Yaws (1999)	?	21
	1.3×10^{1}		Abraham et al. (1990)	?	
2-methylbutanoic acid	6.7		Duchowicz et al. (2020)	V	187
$C_5H_{10}O_2$	4.9		Yaws (2003)	X	238
[116-53-0]	2.1×10^{1}		Duchowicz et al. (2020)	Q	
WLAMNBDJUVNPJU-UHFFFAOYSA-N	8.5		Wang et al. (2017)	Q	81, 239
	3.3×10^{1}		Wang et al. (2017)	Q	81, 240
	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
	8.3		Gharagheizi et al. (2010)	Q	247

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{1}		Hilal et al. (2008)	Q	
	4.4×10^{1}		Modarresi et al. (2007)	Q	68
3-methylbutanoic acid	2.7×10^{1}		Kim and Kim (2016)	M	
$(CH_3)_2CHCH_2COOH$	1.1×10^{1}		von Hartungen et al. (2004)	M	
(isovaleric acid)	1.2×10^{1}		Khan et al. (1995)	M	
[503-74-2]	1.2×10^{1}		Khan and Brimblecombe (1992)	M	
GWYFCOCPABKNJV-UHFFFAOYSA-N	1.2×10^{1}		Amoore and Buttery (1978)	M	
	1.6		Mackay et al. (2006c)	V	
	1.6		Mackay et al. (1995)	V	
	7.3		Amoore and Buttery (1978)	V	
	1.1×10^{1}		Yaws (2003)	X	238, 12
	1.2×10^{1}		Keshavarz et al. (2022)	Q	
	2.1×10^{1}		Duchowicz et al. (2020)	Q	300
	8.5		Wang et al. (2017)	Q	81, 239
	6.8×10^{1}		Wang et al. (2017)	Q	81, 240
	1.7×10^{1}		Wang et al. (2017)	Q	81, 241
	2.2×10^{1}		Gharagheizi et al. (2012)	Q	
	9.9		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	7.8		Raventos-Duran et al. (2010)	Q	246
	8.4		Gharagheizi et al. (2010)	Q	247
	2.8×10^{1}		Hilal et al. (2008)	Q	
	2.0×10^{1}		Modarresi et al. (2007)	Q	68
	4.8×10^{1}		Yao et al. (2002)	Q	230
	1.4×10^{1}		English and Carroll (2001)	Q	231, 232
	1.2×10^{1}		Duchowicz et al. (2020)	?	186, 21
	7.0		Yaws (1999)	?	21, 12
	1.2×10^{1}		Abraham et al. (1990)	?	
2,2-dimethylpropanoic acid	3.5		Khan et al. (1995)	M	
$(CH_3)_3CCOOH$	3.5		Khan and Brimblecombe (1992)	M	
(pivalic acid)	8.4		Yaws (2003)	X	238
[75-98-9]	1.2×10^{1}		Keshavarz et al. (2022)	Q	
IUGYQRQAERSCNH-UHFFFAOYSA-N	9.4		Duchowicz et al. (2020)	Q	
	9.9		Raventos-Duran et al. (2010)	Q	243, 244
	9.9		Raventos-Duran et al. (2010)	Q	245
	7.8		Raventos-Duran et al. (2010)	Q	246
	6.9		Gharagheizi et al. (2010)	Q	247
	1.2×10^{1}		Hilal et al. (2008)	Q	
	1.6×10^{1}		Modarresi et al. (2007)	Q	68
	3.8		Yaffe et al. (2003)	Q	249, 250
	9.0×10^{-1}		Katritzky et al. (1998)	Q	
	3.6		Duchowicz et al. (2020)	?	186, 21

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexanoic acid	1.3×10^1	6100	Staudinger and Roberts (2001)	L	
$C_5H_{11}COOH$	9.9		Kim and Kim (2016)	M	
(caproic acid)	7.5		von Hartungen et al. (2004)	M	
[142-62-1]	1.3×10^1	6300	Khan et al. (1995)	M	
FUZZWVXGSFPDMH-UHFFFAOYSA-N	1.3×10^1	5900	Khan and Brimblecombe (1992)	M	
	1.7×10^1		Mackay et al. (2006c)	V	
	1.7		Mackay et al. (1995)	V	
	1.1×10^1		Brimblecombe et al. (1992)	V	
	2.0×10^1		Hwang et al. (1992)	V	
		8700	Abraham (1984)	V	
		8100	Abraham (1984)	R	490
	2.4×10^1		Yaws (2003)	X	238, 12
	6.1		Keshavarz et al. (2022)	Q	
	5.9×10^1		Duchowicz et al. (2020)	Q	185
	1.7×10^1		Gharagheizi et al. (2012)	Q	
	6.2		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^1		Raventos-Duran et al. (2010)	Q	245
	6.2		Raventos-Duran et al. (2010)	Q	246
	1.4×10^1		Gharagheizi et al. (2010)	Q	247
	2.4×10^1		Hilal et al. (2008)	Q	
	1.7×10^1		Modarresi et al. (2007)	Q	68
		7500	Kühne et al. (2005)	Q	
	1.4×10^1		Yaffe et al. (2003)	Q	249, 250
	8.3		Abraham (2003)	Q	
	3.9×10^1		Yao et al. (2002)	Q	230, 268
	1.1×10^1		English and Carroll (2001)	Q	231, 232
	7.9		Katritzky et al. (1998)	Q	
	1.7×10^1		Nirmalakhandan et al. (1997)	Q	
	1.3×10^1		Duchowicz et al. (2020)	?	186, 21
		7200	Kühne et al. (2005)	?	
	1.5×10^1		Yaws (1999)	?	21, 12
	1.5×10^1		Abraham et al. (1990)	?	
2-methylpentanoic acid	1.1×10^1		Hilal et al. (2008)	Q	
$C_6H_{12}O_2$	3.6×10^1		Modarresi et al. (2007)	Q	68
[97-61-0]					
OVBFMEVBMNZIBR-UHFFFAOYSA-N					
2-ethylbutanoic acid	6.2		Duchowicz et al. (2020)	V	187
$C_6H_{12}O_2$	4.3		Yaws (2003)	X	238
[88-09-5]	2.3×10^1		Duchowicz et al. (2020)	Q	
OXQGTIUCKGYOAA-UHFFFAOYSA-N	8.9		Gharagheizi et al. (2012)	Q	
	6.2		Raventos-Duran et al. (2010)	Q	243, 244
	9.9		Raventos-Duran et al. (2010)	Q	245
	6.2		Raventos-Duran et al. (2010)	Q	246
	7.6		Gharagheizi et al. (2010)	Q	247
	9.0		Hilal et al. (2008)	Q	

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.2×10^{1}		Modarresi et al. (2007)	Q	68
	6.1		Yaffe et al. (2003)	Q	249, 250
	7.9×10^{-1}		Katritzky et al. (1998)	Q	
heptanoic acid	1.5×10^{1}		Kim and Kim (2016)	M	
$C_7H_{14}O_2$	1.5×10^{1}		Duchowicz et al. (2020)	V	187
[111-14-8]	9.6		Brimblecombe et al. (1992)	V	
MNWFXJYAOYHMED-UHFFFAOYSA-N		8500	Abraham (1984)	V	
		8500	Abraham (1984)	R	490
	6.1×10^{1}		Duchowicz et al. (2020)	Q	
	5.5		Wang et al. (2017)	Q	81, 239
	2.9×10^{1}		Wang et al. (2017)	Q	81, 240
	2.0×10^{1}		Wang et al. (2017)	Q	81, 241
	1.0×10^{1}		Gharagheizi et al. (2012)	Q	
	1.7×10^{1}		Hilal et al. (2008)	Q	
	1.6×10^{1}		Modarresi et al. (2007)	Q	68
		7800	Kühne et al. (2005)	Q	
	3.0×10^{1}		Yaffe et al. (2003)	Q	249, 250
	6.4		Abraham (2003)	Q	
	2.9×10^{1}		Yao et al. (2002)	Q	230
	4.3		Katritzky et al. (1998)	Q	
		7900	Kühne et al. (2005)	?	
	2.5×10^{1}		Yaws (1999)	?	21, 12
	1.3×10^{1}		Abraham et al. (1990)	?	
4,4-dimethylpentanoic acid	4.3		Zhang et al. (2010)	Q	288, 289
$C_7H_{14}O_2$	1.4×10^{1}		Zhang et al. (2010)	Q	288, 290
[95823-36-2]	1.6×10^{3}		Zhang et al. (2010)	Q	288, 291
HMMSZUQCCUWXRA-UHFFFAOYSA-N	1.6		Zhang et al. (2010)	Q	288, 292
2-ethyl-2-methylbutanoic acid	4.3		Zhang et al. (2010)	Q	288, 289
$C_7H_{14}O_2$	5.4		Zhang et al. (2010)	Q	288, 290
[19889-37-3]	2.3×10^{2}		Zhang et al. (2010)	Q	288, 291
LHJPKLWGGMAUAN-UHFFFAOYSA-N	1.6		Zhang et al. (2010)	Q	288, 292
octanoic acid	1.1×10^{1}		Duchowicz et al. (2020)	V	187
$C_8H_{16}O_2$	1.5×10^{-1}		Mackay et al. (2006c)	V	
(caprylic acid)	1.5×10^{-1}		Mackay et al. (1995)	V	
[124-07-2]	7.6		Brimblecombe et al. (1992)	V	
WWZKQHOCKIZLMA-UHFFFAOYSA-N		9600	Abraham (1984)	V	
		8900	Abraham (1984)	R	490
	1.9×10^{1}		Yaws (2003)	X	238, 12
	6.4×10^{1}		Duchowicz et al. (2020)	Q	
	6.5		Gharagheizi et al. (2012)	Q	
	1.2×10^{1}		Gharagheizi et al. (2010)	Q	247
	1.3×10^{1}		Hilal et al. (2008)	Q	
	1.2×10^{1}		Modarresi et al. (2007)	Q	68
		8200	Kühne et al. (2005)	Q	

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{1}		Yaffe et al. (2003)	Q	249, 250
	5.7		Abraham (2003)	Q	
	2.7×10^{1}		Yao et al. (2002)	Q	230
	5.8		Katritzky et al. (1998)	Q	
		8400	Kühne et al. (2005)	?	
	1.0×10^{1}		Yaws (1999)	?	21, 12
	1.1×10^{1}		Abraham et al. (1990)	?	
2-ethylhexanoic acid	3.5		HSDB (2015)	V	
$C_8H_{16}O_2$	3.4		Hilal et al. (2008)	Q	
[149-57-5]	2.4×10^{1}		Modarresi et al. (2007)	Q	68
OBETXYAYXDNJHR-UHFFFAOYSA-N					
endothal	2.6×10^{10}		Duchowicz et al. (2020)	V	187
$C_8H_{10}O_5$	1.4×10^{6}		Duchowicz et al. (2020)	Q	
[145-73-3]					
GXEKYRXVRROBEV-UHFFFAOYSA-N					
nonanoic acid	6.1		Duchowicz et al. (2020)	V	187
$C_9H_{18}O_2$	3.8		Brimblecombe et al. (1992)	V	
(pelargic acid)	2.0×10^{1}		Yaws (2003)	X	238, 12
[112-05-0]	6.9		Hilal et al. (2008)	C	
FBUKVWPVBMHYJY-UHFFFAOYSA-N	6.5×10^{1}		Duchowicz et al. (2020)	Q	
	4.0		Gharagheizi et al. (2012)	Q	
	1.3×10^{1}		Gharagheizi et al. (2010)	Q	247
	9.9		Hilal et al. (2008)	Q	
	1.2×10^{1}		Modarresi et al. (2007)	Q	68
	1.2×10^{1}		Yaffe et al. (2003)	Q	249, 273
	4.2		Abraham (2003)	Q	
	2.3×10^{1}		Yao et al. (2002)	Q	230
	5.6		Katritzky et al. (1998)	Q	
	3.0		Maniere et al. (2011)	?	12, 166
	1.1×10^{1}		Yaws (1999)	?	21, 12
decanoic acid	7.4		Duchowicz et al. (2020)	V	187
$C_{10}H_{20}O_2$	6.5		Hilal et al. (2008)	C	
[334-48-5]	6.7×10^{1}		Duchowicz et al. (2020)	Q	
GHVNFZFCNZKVNT-UHFFFAOYSA-N	7.7		Hilal et al. (2008)	Q	
	1.0×10^{1}		Modarresi et al. (2007)	Q	68
	3.0		Abraham (2003)	Q	
	1.9×10^{2}		Yaws (1999)	?	21, 12
3,3,5,5-tetramethylhexanoic acid	1.9		Zhang et al. (2010)	Q	288, 289
$C_{10}H_{20}O_2$	3.5		Zhang et al. (2010)	Q	288, 290
[1135681-77-4]	1.0×10^{3}		Zhang et al. (2010)	Q	288, 291
WRPPDRMFGQJMAR-UHFFFAOYSA-N	6.1×10^{-1}		Zhang et al. (2010)	Q	288, 292

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pinonic acid	6.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_3$	3.0×10^{5}		Wang et al. (2017)	Q	81, 240
[473-72-3]	6.2×10^{5}		Wang et al. (2017)	Q	81, 241
SIZDUQQDBXJXLQ-UHFFFAOYSA-N	5.9×10^{4}		Isaacman-VanWertz et al. (2016)	Q	443
undecanoic acid	7.7		Yaws (2003)	X	238
$C_{11}H_{22}O_2$	1.8×10^{1}		Gharagheizi et al. (2010)	Q	247
[112-37-8]	5.8		Hilal et al. (2008)	Q	
ZDPHROOEEOARMN-UHFFFAOYSA-N	2.2		Abraham (2003)	Q	
dodecanoic acid	4.5		Hilal et al. (2008)	Q	
$C_{12}H_{24}O_2$	1.7		Abraham (2003)	Q	
[143-07-7]	1.7×10^{1}		Yao et al. (2002)	Q	230
POULHZVOKOAJMA-UHFFFAOYSA-N	8.4×10^{1}		Yaws (1999)	?	21, 12
tridecanoic acid	8.0		Yaws (2003)	X	238
$C_{13}H_{26}O_2$	3.8×10^{1}		Gharagheizi et al. (2010)	Q	247
[638-53-9]	1.2		Abraham (2003)	Q	
SZHOJFHSIKHZHA-UHFFFAOYSA-N					
tetradecanoic acid	2.0×10^{1}		Duchowicz et al. (2020)	V	187
$C_{14}H_{28}O_2$	7.1×10^{1}		Duchowicz et al. (2020)	Q	
[544-63-8]	9.4×10^{-1}		Abraham (2003)	Q	
TUNFSRHWOTWDNC-UHFFFAOYSA-N					
pentadecanoic acid	7.1×10^{-1}		Abraham (2003)	Q	
$C_{15}H_{30}O_2$					
[1002-84-2]					
WQEPLUUGTLDZJY-UHFFFAOYSA-N					
hexadecanoic acid	4.9×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{16}H_{32}O_2$	7.2×10^{1}		Duchowicz et al. (2020)	Q	
(palmitic acid)	3.0		Gharagheizi et al. (2012)	Q	
[57-10-3]	5.2×10^{-1}		Abraham (2003)	Q	
IPCSVZSSVZVIGE-UHFFFAOYSA-N					
heptadecanoic acid	3.8×10^{-1}		Abraham (2003)	Q	
$C_{17}H_{34}O_2$					
(margaric acid)					
[506-12-7]					
KEMQGTRYUADPNZ-UHFFFAOYSA-N					
octadecanoic acid	2.1×10^{1}		Duchowicz et al. (2020)	V	187
$C_{18}H_{36}O_2$	2.5×10^{5}		Mackay et al. (1995)	V	
(stearic acid)	7.3×10^{1}		Duchowicz et al. (2020)	Q	
[57-11-4]	8.4×10^{-1}		Hilal et al. (2008)	Q	
QIQXTHQIDYTFRH-UHFFFAOYSA-N	3.5		Modarresi et al. (2007)	Q	68
	3.0×10^{-1}		Abraham (2003)	Q	

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
nonadecanoic acid $C_{19}H_{38}O_2$ [646-30-0] ISYWECDDZWTKFF-UHFFFAOYSA-N	2.3×10^{-1}		Abraham (2003)	Q	
eicosanoic acid $C_{20}H_{40}O_2$ (arachidic acid) [506-30-9] VKOBVWXKNCXXDE-UHFFFAOYSA-N	1.7×10^{-1}		Abraham (2003)	Q	
heneicosanoic acid $C_{21}H_{42}O_2$ [2363-71-5] CKDDRHZIAZRDBW-UHFFFAOYSA-N	1.3×10^{-1}		Abraham (2003)	Q	
docosanoic acid $C_{22}H_{44}O_2$ (behenic acid) [112-85-6] UKMSUNONTOPOIO-UHFFFAOYSA-N	9.5×10^{-2}		Abraham (2003)	Q	
tricosanoic acid $C_{23}H_{46}O_2$ [2433-96-7] XEZVDURJDFGERA-UHFFFAOYSA-N	7.2×10^{-2}		Abraham (2003)	Q	
tetracosanoic acid $C_{24}H_{48}O_2$ (lignoceric acid) [557-59-5] QZZGJDVWLFXDLK-UHFFFAOYSA-N	5.4×10^{-2}		Abraham (2003)	Q	
propenoic acid $C_3H_4O_2$ (acrylic acid) [79-10-7] NIXOWILDQLNWCW-UHFFFAOYSA-N	2.7×10^{1}		Duchowicz et al. (2020)	V	187
	3.1×10^{1}		Lide and Frederikse (1995)	V	
	1.2×10^{2}		Duchowicz et al. (2020)	Q	
	3.3×10^{1}		Wang et al. (2017)	Q	81, 239
	2.2×10^{1}		Wang et al. (2017)	Q	81, 240
	4.6×10^{1}		Wang et al. (2017)	Q	81, 241
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	246
	2.2×10^{1}		Hilal et al. (2008)	Q	
	9.4×10^{2}		Modarresi et al. (2007)	Q	68
	2.4×10^{1}		Yaws (1999)	?	21
	2.4×10^{1}		Yaws and Yang (1992)	?	21

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-butenoic acid	2.3×10^{1}		Duchowicz et al. (2020)	V	187
$C_4H_6O_2$	5.1×10^{1}		Duchowicz et al. (2020)	Q	
(crotonic acid)	4.2×10^{1}		Wang et al. (2017)	Q	81, 239
[3724-65-0]	2.2×10^{1}		Wang et al. (2017)	Q	81, 240
LDHQCZJRKDOVOX-UHFFFAOYSA-N	5.0×10^{1}		Wang et al. (2017)	Q	81, 241
	2.3×10^{1}		Hilal et al. (2008)	Q	
	1.1×10^{2}		Modarresi et al. (2007)	Q	68
(E)-2-butenoic acid	4.1×10^{1}		HSDB (2015)	V	
$C_4H_6O_2$					
(*trans*-crotonic acid)					
[107-93-7]					
LDHQCZJRKDOVOX-NSCUHMNNSA-N					
(Z)-2-butenoic acid	1.5×10^{2}		Duchowicz et al. (2020)	V	187
$C_4H_6O_2$	5.1×10^{1}		Duchowicz et al. (2020)	Q	
(isocrotonic acid)	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
[503-64-0]	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	245
LDHQCZJRKDOVOX-IHWYPQMZSA-N	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	246
	2.3×10^{1}		Hilal et al. (2008)	Q	
	1.1×10^{2}		Modarresi et al. (2007)	Q	68
2-methyl-2-propenoic acid	2.5×10^{1}		Khan et al. (1992)	M	
$C_4H_6O_2$	1.0		Mackay et al. (2006c)	V	
(methacrylic acid)	9.2		Keshavarz et al. (2022)	Q	
[79-41-4]	5.0×10^{1}		Duchowicz et al. (2020)	Q	300
CERQOIWHTDAKMF-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	81, 239
	1.7×10^{1}		Wang et al. (2017)	Q	81, 240
	8.3		Wang et al. (2017)	Q	81, 241
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	246
	1.9×10^{1}		Hilal et al. (2008)	Q	
	1.4×10^{2}		Modarresi et al. (2007)	Q	68
	2.5×10^{1}		Duchowicz et al. (2020)	?	186, 21
methacrylic acid epoxide	1.2×10^{3}		Pye et al. (2013)	Q	494
$C_4H_6O_3$					
CSEUSVYSDPXJAP-UHFFFAOYSA-N					
benzenecarboxylic acid	2.9×10^{2}		Li et al. (2007)	M	
C_6H_5COOH	2.6×10^{2}		Duchowicz et al. (2020)	V	187
(benzoic acid)	2.5×10^{2}		Mackay et al. (2006c)	V	
[65-85-0]	1.4×10^{2}		Lide and Frederikse (1995)	V	
WPYMKLBDIGXBTP-UHFFFAOYSA-N	2.1		Mackay et al. (1995)	V	
	1.7×10^{2}		Meylan and Howard (1991)	V	
	1.4×10^{2}	6500	Goldstein (1982)	X	299
	1.4×10^{2}		Howard (1989)	X	414
	3.1×10^{2}		Duchowicz et al. (2020)	Q	

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.6×10^{2}		Wang et al. (2017)	Q	81, 239
	5.1×10^{2}		Wang et al. (2017)	Q	81, 240
	3.5×10^{2}		Wang et al. (2017)	Q	81, 241
	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	246
	2.4×10^{2}		Hilal et al. (2008)	Q	
		6700	Kühne et al. (2005)	Q	
	9.1×10^{1}		Meylan and Howard (1991)	Q	
	1.5×10^{3}		Maniere et al. (2011)	?	12, 166
		6200	Kühne et al. (2005)	?	
	2.4×10^{2}		Yaws and Yang (1992)	?	21
sorbic acid $C_6H_8O_2$ [110-44-1] WSWCOQWTEOXDQX-MQQKCMAXSA-N	3.3×10^{1}		Abraham et al. (2019)	Q	
	2.0×10^{2}		HSDB (2015)	Q	100
D(-)-isoascorbic acid $C_6H_8O_6$ (erythorbic acid) [89-65-6] CIWBSHSKHKDKBQ-DUZGATOHSA-N	2.4×10^{2}		HSDB (2015)	Q	100
shikimic acid $C_7H_{10}O_5$ [138-59-0] JXOHGGNKMLTUBP-UHFFFAOYSA-N	3.7×10^{8}		HSDB (2015)	Q	100
4-hydroxybenzoic acid $C_7H_6O_3$ [99-96-7] FJKROLUGYXJWQN-UHFFFAOYSA-N	1.4×10^{6}		Duchowicz et al. (2020)	V	187
	1.4×10^{6}		HSDB (2015)	V	
	2.7×10^{6}		Duchowicz et al. (2020)	Q	
3,4,5-trihydroxybenzoic acid $C_7H_6O_5$ (gallic acid) [149-91-7] LNTHITQWFMADLM-UHFFFAOYSA-N	1.2×10^{14}		HSDB (2015)	Q	100
2-methylbenzoic acid $C_8H_8O_2$ (*o*-toluic acid) [118-90-1] ZWLPBLYKEWSWPD-UHFFFAOYSA-N	9.7		Abraham et al. (2019)	Q	
	2.7×10^{2}		Wang et al. (2017)	Q	81, 239
	8.0×10^{1}		Wang et al. (2017)	Q	81, 240
	9.3×10^{1}		Wang et al. (2017)	Q	81, 241
	8.2×10^{1}		Zhang et al. (2010)	Q	288, 289
	3.2×10^{1}		Zhang et al. (2010)	Q	288, 290
	9.9×10^{1}		Zhang et al. (2010)	Q	288, 291
	1.1×10^{2}		Zhang et al. (2010)	Q	288, 292

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methylbenzoic acid	6.6		Mackay et al. (2006c)	V	
$C_8H_8O_2$	1.4×10^{-1}		Mackay et al. (1995)	V	
(*m*-toluic acid)	3.9×10^{1}		Abraham et al. (2019)	Q	
[99-04-7]	2.7×10^{2}		Wang et al. (2017)	Q	81, 239
GPSDUZXPYCFOSQ-UHFFFAOYSA-N	3.7×10^{2}		Wang et al. (2017)	Q	81, 240
	3.6×10^{2}		Wang et al. (2017)	Q	81, 241
	8.2×10^{1}		Zhang et al. (2010)	Q	288, 289
	1.2×10^{2}		Zhang et al. (2010)	Q	288, 290
	5.1×10^{2}		Zhang et al. (2010)	Q	288, 291
	1.1×10^{2}		Zhang et al. (2010)	Q	288, 292
4-methylbenzoic acid	2.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_8O_2$	4.2×10^{2}		Wang et al. (2017)	Q	81, 240
(*p*-toluic acid)	4.7×10^{2}		Wang et al. (2017)	Q	81, 241
[99-94-5]	8.2×10^{1}		Zhang et al. (2010)	Q	288, 289
LPNBBFKOUUSUDB-UHFFFAOYSA-N	1.4×10^{2}		Zhang et al. (2010)	Q	288, 290
	8.8×10^{2}		Zhang et al. (2010)	Q	288, 291
	1.1×10^{2}		Zhang et al. (2010)	Q	288, 292
		7000	Kühne et al. (2005)	Q	
		7500	Kühne et al. (2005)	?	
2-hydroxy-benzoic acid	1.3×10^{3}		Duchowicz et al. (2020)	V	187
$C_7H_6O_3$	8.0×10^{2}		Mackay et al. (2006c)	V	
(salicylic acid)	6.9×10^{2}		Mackay et al. (1995)	V	
[69-72-7]	1.8		Mackay et al. (1995)	V	
YGSDEFSMJLZEOE-UHFFFAOYSA-N	9.0×10^{1}		Yaws (2003)	X	238
	1.5×10^{3}		Duchowicz et al. (2020)	Q	
	1.6×10^{3}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{2}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	246
	8.9×10^{1}		Gharagheizi et al. (2010)	Q	247
benzeneethanoic acid	2.4×10^{2}		Duchowicz et al. (2020)	V	187
$C_8H_8O_2$	1.5×10^{2}		Mackay et al. (2006c)	V	
(phenylacetic acid)	1.8×10^{2}		Mackay et al. (1995)	V	
[103-82-2]	1.4×10^{1}		Mackay et al. (1995)	V	
WLJVXDMOQOGPHL-UHFFFAOYSA-N	3.4×10^{2}		Duchowicz et al. (2020)	Q	
	4.1×10^{2}		Wang et al. (2017)	Q	81, 239
	2.1×10^{3}		Wang et al. (2017)	Q	81, 240
	3.6×10^{3}		Wang et al. (2017)	Q	81, 241
	1.2×10^{3}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{3}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{2}		Raventos-Duran et al. (2010)	Q	246
	9.9×10^{2}		Hilal et al. (2008)	Q	
	3.2×10^{2}		Modarresi et al. (2007)	Q	68
	2.4×10^{2}		Yaffe et al. (2003)	Q	249, 250
	5.1×10^{1}		Katritzky et al. (1998)	Q	

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
phthalic anhydride	6.1×10^{2}		Duchowicz et al. (2020)	V	187
$C_8H_4O_3$	1.6×10^{3}		Lide and Frederikse (1995)	V	
[85-44-9]	1.2×10^{1}		Yaws (2003)	X	238
LGRFSURHDFAFJT-UHFFFAOYSA-N	4.4×10^{1}		Duchowicz et al. (2020)	Q	
	1.2×10^{1}		Gharagheizi et al. (2010)	Q	247
1,2-benzenedicarboxylic acid	4.9×10^{5}		Duchowicz et al. (2020)	V	187
$C_8H_6O_4$	4.9×10^{5}		HSDB (2015)	V	
(phthalic acid)	8.2×10^{6}		Duchowicz et al. (2020)	Q	
[88-99-3]					
XNGIFLGASWRNHJ-UHFFFAOYSA-N					
terephthalic acid	2.5×10^{7}		HSDB (2015)	Q	449
$C_8H_6O_4$	4.8×10^{9}		Gharagheizi et al. (2012)	Q	
[100-21-0]					
KKEYFWRCBNTPAC-UHFFFAOYSA-N					
isophthalic acid	4.0×10^{9}		Yaws (2003)	X	238
$C_8H_6O_4$	7.3×10^{4}		Abraham et al. (2019)	Q	
[121-91-5]	4.5×10^{6}		HSDB (2015)	Q	100
QQVIHTHCMHWDBS-UHFFFAOYSA-N	7.1×10^{8}		Gharagheizi et al. (2012)	Q	
	3.7×10^{9}		Gharagheizi et al. (2010)	Q	247
dehydroacetic acid	2.9×10^{1}		HSDB (2015)	V	
$C_8H_8O_4$					
[520-45-6]					
PGRHXDWITVMQBC-UHFFFAOYSA-N					
2-methoxybenzoic acid	2.5×10^{3}		Abraham et al. (2019)	Q	
$C_8H_8O_3$					
[579-75-9]					
ILUJQPXNXACGAN-UHFFFAOYSA-N					
4-methoxybenzoic acid	1.8×10^{3}		Abraham et al. (2019)	Q	
$C_8H_8O_3$					
[100-09-4]					
ZEYHEAKUIGZSGI-UHFFFAOYSA-N					
caffeic acid	7.0×10^{10}		HSDB (2015)	Q	100
$C_9H_8O_4$					
[331-39-5]					
QAIPRVGONGVQAS-DUXPYHPUSA-N					
4-methylphthalic anhydride	1.4		Zhang et al. (2010)	Q	288, 289
$C_9H_6O_3$	6.4×10^{4}		Zhang et al. (2010)	Q	288, 290
[19438-61-0]	3.5×10^{1}		Zhang et al. (2010)	Q	288, 291
ZOXBWJMCXHTKNU-UHFFFAOYSA-N	3.6×10^{1}		Zhang et al. (2010)	Q	288, 292

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-phenyl-2-propenoic acid	5.8×10^{2}		Duchowicz et al. (2020)	V	187
$C_9H_8O_2$	4.1×10^{2}		Duchowicz et al. (2020)	Q	
(cinnamic acid)	9.9×10^{2}		Raventos-Duran et al. (2010)	Q	243, 244
[621-82-9]	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	245
WBYWAXJHAXSJNI-UHFFFAOYSA-N	7.8×10^{2}		Raventos-Duran et al. (2010)	Q	246
trans-cinnamic acid $C_9H_8O_2$ [140-10-3] WBYWAXJHAXSJNI-VOTSOKGWSA-N	2.8×10^{11}		Abraham et al. (2019)	Q	
p-coumaric acid $C_9H_8O_3$ [501-98-4] NGSWKAQJJWESNS-ZZXKWVIFSA-N	7.2×10^{5}		Abraham et al. (2019)	Q	
3,4-dimethoxybenzoic acid $C_9H_{10}O_4$ (veratric acid) [93-07-2] DAUAQNGYDSHRET-UHFFFAOYSA-N	1.1×10^{5}		Abraham et al. (2019)	Q	
3,4,5-trimethoxybenzoic acid $C_{10}H_{12}O_5$ (eudesmic acid) [118-41-2] SJSOFNCYXJUNBT-UHFFFAOYSA-N	7.3×10^{5}		Abraham et al. (2019)	Q	
1-naphthaleneacetic acid	3.3×10^{2}		Maniere et al. (2011)	?	12, 495, 166
$C_{12}H_{10}O_2$	7.9×10^{3}		Maniere et al. (2011)	?	12, 496, 166
[86-87-3] PRPINYUDVPFIRX-UHFFFAOYSA-N					
2-naphthoxyacetic acid $C_{12}H_{10}O_3$ [120-23-0] RZCJYMOBWVJQGV-UHFFFAOYSA-N	3.5×10^{5}		Ebert et al. (2023)	?	319
p-tert-butylbenzoic acid	3.5×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_{11}H_{14}O_2$	4.5×10^{1}		Zhang et al. (2010)	Q	288, 290
[98-73-7]	3.6×10^{2}		Zhang et al. (2010)	Q	288, 291
KDVYCTOWXSLNNI-UHFFFAOYSA-N	4.2×10^{1}		Zhang et al. (2010)	Q	288, 292
trinexapac $C_{11}H_{12}O_5$ [104273-73-6] DFFWZNDCNBOKDI-UHFFFAOYSA-N	3.9×10^{6} 4.3×10^{8}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benzoic acid, anhydride	7.0		Zhang et al. (2010)	Q	288, 289
$C_{14}H_{10}O_3$	3.7×10^{2}		Zhang et al. (2010)	Q	288, 290
[93-97-0]	6.5×10^{3}		Zhang et al. (2010)	Q	288, 291
CHIHQLCVLOXUJW-UHFFFAOYSA-N	6.4×10^{2}		Zhang et al. (2010)	Q	288, 292
pyromellitic acid	1.6×10^{13}		Yaws (2003)	X	238, 497
$C_{10}H_6O_8$	3.0×10^{13}		Gharagheizi et al. (2012)	Q	
[89-05-4]	1.6×10^{13}		Gharagheizi et al. (2010)	Q	247
CYIDZMCFTVVTJO-UHFFFAOYSA-N					
pyromellitic dianhydride	1.3×10^{3}		HSDB (2015)	Q	100
$C_{10}H_2O_6$	1.3×10^{3}		Zhang et al. (2010)	Q	288, 289
[89-32-7]	1.4×10^{11}		Zhang et al. (2010)	Q	288, 290
ANSXAPJVJOKRDJ-UHFFFAOYSA-N	4.8×10^{4}		Zhang et al. (2010)	Q	288, 291
	9.7×10^{5}		Zhang et al. (2010)	Q	288, 292
naproxen	2.5×10^{5}		Abraham et al. (2019)	Q	
$C_{14}H_{14}O_3$					
[22204-53-1]					
CMWTZPSULFXXJA-VIFPVBQESA-N					
(*Z*,*Z*)-9,12-octadecadienoic acid	4.9×10^{1}		HSDB (2015)	V	
$C_{18}H_{32}O_2$					
(linoleic acid)					
[60-33-3]					
OYHQOLUKZRVURQ-HZJYTTRNSA-N					
rosmarinic acid	3.7×10^{21}		HSDB (2015)	Q	449
$C_{18}H_{16}O_8$					
[537-15-5]					
DOUMFZQKYFQNTF-WUTVXBCWSA-N					
abietic acid	1.5×10^{5}		Yaws (2003)	X	238, 12
$C_{20}H_{30}O_2$	1.7×10^{5}		Gharagheizi et al. (2010)	Q	247
[514-10-3]					
RSWGJHLUYNHPMX-ONCXSQPRSA-N					
ethanedioic acid	6.1×10^{6}		Burkholder et al. (2019)	L	
HOOCCOOH	6.1×10^{6}		Burkholder et al. (2015)	L	
(oxalic acid)	6.1×10^{6}		Compernolle and Müller (2014a)	V	
[144-62-7]	7.1×10^{6}	9800	Clegg et al. (1996)	V	
MUBZPKHOEPUJKR-UHFFFAOYSA-N	3.1×10^{4}	7300	Brimblecombe et al. (1992)	V	
	4.2×10^{5}		Yaws (2003)	X	238, 12
	6.9×10^{4}		Gaffney and Senum (1984)	X	391, 493
	1.6×10^{4}		Keshavarz et al. (2022)	Q	
	1.6×10^{3}		Duchowicz et al. (2020)	Q	
	3.7×10^{7}		Gharagheizi et al. (2012)	Q	
	4.9×10^{4}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{4}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{5}		Raventos-Duran et al. (2010)	Q	246

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.2×10^5		Gharagheizi et al. (2010)	Q	247
	2.4×10^3		Hilal et al. (2008)	Q	
	2.3×10^5		Modarresi et al. (2007)	Q	68
	4.1×10^5		Meylan and Howard (1991)	Q	
	4.9×10^6		Saxena and Hildemann (1996)	E	403
	6.9×10^4		Duchowicz et al. (2020)	?	186, 21
propanedioic acid	2.4×10^8		Burkholder et al. (2019)	L	
$HOOCCH_2COOH$	2.4×10^8		Burkholder et al. (2015)	L	
(malonic acid)	3.7×10^4		Duchowicz et al. (2020)	V	187
[141-82-2]	3.8×10^8	11000	Compernolle and Müller (2014a)	V	
OFOBLEOULBTSOW-UHFFFAOYSA-N	9.3×10^7	14000	Compernolle and Müller (2014a)	V	
	2.1×10^1		Duchowicz et al. (2020)	Q	
	2.5×10^5		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^6		Raventos-Duran et al. (2010)	Q	245
	2.5×10^6		Raventos-Duran et al. (2010)	Q	246
	1.2×10^5		Modarresi et al. (2007)	Q	68
	3.9×10^6		Saxena and Hildemann (1996)	E	403
butanedioic acid	3.1×10^7		Burkholder et al. (2019)	L	
$HOOC(CH_2)_2COOH$	3.1×10^7		Burkholder et al. (2015)	L	
(succinic acid)	2.8×10^7		Duchowicz et al. (2020)	V	187
[110-15-6]	2.7×10^7		HSDB (2015)	V	
KDYFGRWQOYBRFD-UHFFFAOYSA-N	4.1×10^7	11000	Compernolle and Müller (2014a)	V	
	2.0×10^7	12000	Compernolle and Müller (2014a)	V	
	7.2×10^5		Yaws (2003)	X	238
	6.5×10^4		Duchowicz et al. (2020)	Q	
	1.4×10^7		Gharagheizi et al. (2012)	Q	
	4.9×10^6		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^6		Raventos-Duran et al. (2010)	Q	245
	2.0×10^6		Raventos-Duran et al. (2010)	Q	246
	3.2×10^5		Gharagheizi et al. (2010)	Q	247
	3.0×10^6		Saxena and Hildemann (1996)	E	403
pentanedioic acid	3.8×10^7		Burkholder et al. (2019)	L	
$HOOC(CH_2)_3COOH$	3.8×10^7		Burkholder et al. (2015)	L	
(glutaric acid)	1.9×10^7		Mentel et al. (2004)	M	
[110-94-1]	5.1×10^7	12000	Compernolle and Müller (2014a)	V	
JFCQEDHGNNZCLN-UHFFFAOYSA-N	2.4×10^7	13000	Compernolle and Müller (2014a)	V	
	1.0×10^5		Yaws (2003)	X	238, 498
	5.0×10^6		Gharagheizi et al. (2012)	Q	
	4.9×10^6		Raventos-Duran et al. (2010)	Q	272, 244
	3.9×10^7		Raventos-Duran et al. (2010)	Q	245
	1.2×10^6		Raventos-Duran et al. (2010)	Q	246
	3.5×10^5		Gharagheizi et al. (2010)	Q	247
	2.2×10^7		Hilal et al. (2008)	Q	
	2.3×10^5		Modarresi et al. (2007)	Q	68

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.0×10^{6}		Saxena and Hildemann (1996)	E	403
3-hydroxy glutaric acid $C_5H_8O_5$ [638-18-6] ZQHYXNSQOIDNTL-UHFFFAOYSA-N	6.7×10^{8}		Isaacman-VanWertz et al. (2016)	Q	443
hexanedioic acid $HOOC(CH_2)_4COOH$ (adipic acid) [124-04-9] WNLRTRBMVRJNCN-UHFFFAOYSA-N	6.6×10^{7}		Burkholder et al. (2019)	L	
	6.6×10^{7}		Burkholder et al. (2015)	L	
	2.1×10^{6}		Duchowicz et al. (2020)	V	187
	2.1×10^{6}		HSDB (2015)	V	
	6.6×10^{7}	13000	Compernolle and Müller (2014a)	V	
	1.1×10^{1}		Lide and Frederikse (1995)	V	
	1.8×10^{5}	11000	Goldstein (1982)	X	299
	3.3×10^{6}		Duchowicz et al. (2020)	Q	
	2.2×10^{6}		Gharagheizi et al. (2012)	Q	
	3.9×10^{6}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{7}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{5}		Raventos-Duran et al. (2010)	Q	246
	2.5×10^{7}		Hilal et al. (2008)	Q	
	2.5×10^{5}		Modarresi et al. (2007)	Q	68
	2.0×10^{6}		Saxena and Hildemann (1996)	E	403
tricarballylic acid $C_6H_8O_6$ [99-14-9] KQTIIICEAUMSDG-UHFFFAOYSA-N	1.9×10^{9}		Isaacman-VanWertz et al. (2016)	Q	443
heptanedioic acid $C_7H_{12}O_4$ (pimelic acid) [111-16-0] WLJVNTCWHIRURA-UHFFFAOYSA-N	2.6×10^{7}		Duchowicz et al. (2020)	V	187
	8.1×10^{7}	15000	Compernolle and Müller (2014a)	V	
	4.1×10^{6}		Duchowicz et al. (2020)	Q	
3-acetyl pentanedioic acid $C_7H_{10}O_5$ [149474-71-5] TZPGYCKKEMNHRS-UHFFFAOYSA-N	4.5×10^{9}		Isaacman-VanWertz et al. (2016)	Q	443
octanedioic acid $C_8H_{14}O_4$ (suberic acid) [505-48-6] TYFQFVWCELRYAO-UHFFFAOYSA-N	1.8×10^{6}		Duchowicz et al. (2020)	V	187
	7.7×10^{7}	14000	Compernolle and Müller (2014a)	V	
	4.8×10^{6}		Duchowicz et al. (2020)	Q	

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-1,2,3-butanetricarboxylic acid $C_8H_{12}O_6$ [77370-41-3] VMWJGTKDJFMTFZ-UHFFFAOYSA-N	1.9×10^{8}		Isaacman-VanWertz et al. (2016)	Q	443
nonanedioic acid	8.9×10^{7}	17000	Compernolle and Müller (2014a)	V	
$C_9H_{16}O_4$	3.6×10^{6}		Yaws (2003)	X	238, 12
(azelaic acid)	1.9×10^{5}		Gharagheizi et al. (2012)	Q	
[123-99-9]	9.3×10^{5}		Gharagheizi et al. (2010)	Q	247
BDJRBEYXGGNYIS-UHFFFAOYSA-N					
decanedioic acid	7.6×10^{7}		Compernolle and Müller (2014a)	V	
$C_{10}H_{18}O_4$	1.7×10^{6}		Yaws (2003)	X	238, 12
(sebacic acid)	1.6×10^{5}		Gharagheizi et al. (2012)	Q	
[111-20-6]	1.4×10^{6}		Gharagheizi et al. (2010)	Q	247
CXMXRPHRNRROMY-UHFFFAOYSA-N					
dodecanedioic acid $C_{12}H_{22}O_4$ [693-23-2] TVIDDXQYHWJXFK-UHFFFAOYSA-N	9.9×10^{5}		Ebert et al. (2023)	?	317
cis-butenedioic acid	1.4×10^{8}		Lide and Frederikse (1995)	V	
$HOOC(CH)_2COOH$	1.3×10^{6}		Yaws (2003)	X	238
(maleic acid)	6.8×10^{6}		Gharagheizi et al. (2012)	Q	
[110-16-7]	1.3×10^{6}		Gharagheizi et al. (2010)	Q	247
VZCYOOQTPOCHFL-UPHRSURJSA-N	9.9×10^{6}		Saxena and Hildemann (1996)	E	403
citraconic acid	3.6×10^{7}		Yaws (2003)	X	238
$C_5H_6O_4$	4.0×10^{6}		Gharagheizi et al. (2012)	Q	
[498-23-7]	3.7×10^{7}		Gharagheizi et al. (2010)	Q	247
HNEGQIOMVPPMNR-IHWYPQMZSA-N					
itaconic acid	1.3×10^{6}		Yaws (2003)	X	238, 12
$C_5H_6O_4$	1.3×10^{7}		Gharagheizi et al. (2012)	Q	
[97-65-4]	1.3×10^{6}		Gharagheizi et al. (2010)	Q	247
LVHBHZANLOWSRM-UHFFFAOYSA-N					
1,4-cyclohexanedicarboxylic acid	1.1×10^{6}		Yaws (2003)	X	238, 155
$C_8H_{12}O_4$	2.3×10^{6}		Gharagheizi et al. (2012)	Q	
[619-82-9]	1.1×10^{6}		Gharagheizi et al. (2010)	Q	247
PXGZQGDTEZPERC-UHFFFAOYSA-N					
pinic acid	1.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	7.1×10^{7}		Wang et al. (2017)	Q	81, 240
[473-73-4]	3.2×10^{7}		Wang et al. (2017)	Q	81, 241
LEVONNIFUFSRKZ-UHFFFAOYSA-N	1.0×10^{7}		Isaacman-VanWertz et al. (2016)	Q	443

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methanoic peroxyacid	2.9×10^{1}		Sauer (1997)	M	451
HCOOOH	5.2		HSDB (2015)	Q	100
(peroxyformic acid)					
[107-32-4]					
SCKXCAADGDQQCS-UHFFFAOYSA-N					
ethanoic peroxyacid	8.3	5300	Burkholder et al. (2019)	L	
CH_3COOOH	8.3	5300	Burkholder et al. (2015)	L	
(peroxyacetic acid)	8.3	5300	Sander et al. (2011)	L	
[79-21-0]	7.3	5600	Staudinger and Roberts (2001)	L	
KFSLWBXXFJQRDL-UHFFFAOYSA-N	2.4×10^{1}		Sauer (1997)	M	451
	8.3	5300	O'Sullivan et al. (1996)	M	
	6.5	5900	Lind and Kok (1994)	M	53
	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
	9.6		Wang et al. (2017)	Q	81, 240
	1.3×10^{-1}		Wang et al. (2017)	Q	81, 241
	7.8		Raventos-Duran et al. (2010)	Q	243, 244
	2.5		Raventos-Duran et al. (2010)	Q	245
	7.8		Raventos-Duran et al. (2010)	Q	246
	1.8×10^{1}		Hilal et al. (2008)	Q	
	9.3×10^{1}		Modarresi et al. (2007)	Q	68
		6100	Kühne et al. (2005)	Q	
		5300	Kühne et al. (2005)	?	
MCM:M2C43CO2H	8.0		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	1.7×10^{1}		Wang et al. (2017)	Q	81, 240
XFOASZQZPWEJAA-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:M33C3CO2H	4.9		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	1.7×10^{1}		Wang et al. (2017)	Q	81, 240
VUAXHMVRKOTJKP-UHFFFAOYSA-N	9.6		Wang et al. (2017)	Q	81, 241
MCM:C721OOH	1.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	2.8×10^{6}		Wang et al. (2017)	Q	81, 240
ZLURETBBUKLNQX-UHFFFAOYSA-N	6.2×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C721CO3H	1.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	5.5×10^{6}		Wang et al. (2017)	Q	81, 240
HYEGRGIGVZWWFM-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C811OOH	9.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_4$	3.3×10^{6}		Wang et al. (2017)	Q	81, 240
RYDSGVCXHLRTGT-UHFFFAOYSA-N	2.5×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C823OOH	8.7×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_4$	3.0×10^{6}		Wang et al. (2017)	Q	81, 240
KIIRSRLFRXTUMU-UHFFFAOYSA-N	2.9×10^{4}		Wang et al. (2017)	Q	81, 241

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NORPINIC	1.7×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	2.0×10^{7}		Wang et al. (2017)	Q	81, 240
KLGKVMMWRDYKJM-UHFFFAOYSA-N	6.3×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C811CO3H	1.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	3.7×10^{6}		Wang et al. (2017)	Q	81, 240
ZVOGBTSHONFRIW-UHFFFAOYSA-N	2.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C823CO3H	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	1.6×10^{6}		Wang et al. (2017)	Q	81, 240
IESQFENJEQJSTC-UHFFFAOYSA-N	3.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:LIMONIC	1.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	6.6×10^{7}		Wang et al. (2017)	Q	81, 240
JUCWCJYNDRRZKR-UHFFFAOYSA-N	1.8×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C137OOH	8.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_4$	3.7×10^{6}		Wang et al. (2017)	Q	81, 240
RDYPCLKIKFUKHY-UHFFFAOYSA-N	4.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C137CO2H	1.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_4$	1.7×10^{8}		Wang et al. (2017)	Q	81, 240
IYTMEDMFNUDFPT-UHFFFAOYSA-N	1.7×10^{8}		Wang et al. (2017)	Q	81, 241
MCM:C137CO3H	9.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_5$	2.4×10^{6}		Wang et al. (2017)	Q	81, 240
WIBVBPZGNYNCKK-UHFFFAOYSA-N	1.8×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:TM123BCO2H	1.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_2$	9.1×10^{1}		Wang et al. (2017)	Q	81, 240
RIZUCYSQUWMQLX-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:TM124BCO2H	1.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_2$	4.1×10^{2}		Wang et al. (2017)	Q	81, 240
OPVAJFQBSDUNQA-UHFFFAOYSA-N	5.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:TMBCO2H	1.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}O_2$	2.6×10^{2}		Wang et al. (2017)	Q	81, 240
UMVOQQDNEYOJOK-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C2OHOCO2H	2.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_4$	2.0×10^{7}		Wang et al. (2017)	Q	81, 240
RBNPOMFGQQGHHO-UHFFFAOYSA-N	2.1×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:HOC2H4CO2H	3.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_3$	1.1×10^{5}		Wang et al. (2017)	Q	81, 240
ALRHLSYJTWAHJZ-UHFFFAOYSA-N	7.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HC3CO2H	1.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_3$	3.6×10^{5}		Wang et al. (2017)	Q	81, 240
RMQJECWPWQIIPW-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	81, 241

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HMACO2H	6.2×10^4		Wang et al. (2017)	Q	81, 239
$C_4H_6O_3$	8.3×10^2		Wang et al. (2017)	Q	81, 240
AAMTXHVZOHPPQR-UHFFFAOYSA-N	3.6×10^4		Wang et al. (2017)	Q	81, 241
MCM:HO2C3CO2H	3.0×10^4		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	6.9×10^4		Wang et al. (2017)	Q	81, 240
WHBMMWSBFZVSSR-UHFFFAOYSA-N	6.6×10^4		Wang et al. (2017)	Q	81, 241
MCM:HOC3H6CO2H	2.6×10^4		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	1.4×10^5		Wang et al. (2017)	Q	81, 240
SJZRECIVHVDYJC-UHFFFAOYSA-N	1.0×10^6		Wang et al. (2017)	Q	81, 241
MCM:HOIPRCO2H	3.0×10^4		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	4.5×10^4		Wang et al. (2017)	Q	81, 240
DBXBTMSZEOQQDU-UHFFFAOYSA-N	6.9×10^4		Wang et al. (2017)	Q	81, 241
MCM:IPRHOCO2H	9.6×10^2		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	2.3×10^4		Wang et al. (2017)	Q	81, 240
BWLBGMIXKSTLSX-UHFFFAOYSA-N	5.3×10^3		Wang et al. (2017)	Q	81, 241
MCM:C46CO2H	4.9×10^4		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	1.5×10^5		Wang et al. (2017)	Q	81, 240
NJMYQRVWBCSLEU-UHFFFAOYSA-N	5.0×10^4		Wang et al. (2017)	Q	81, 241
MCM:HC4ACO2H	6.9×10^4		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	2.3×10^5		Wang et al. (2017)	Q	81, 240
BERUOTKXCOOJJM-UHFFFAOYSA-N	6.0×10^5		Wang et al. (2017)	Q	81, 241
MCM:HC4CCO2H	6.9×10^4		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	2.0×10^5		Wang et al. (2017)	Q	81, 240
NCQCQZXQBYAHBZ-UHFFFAOYSA-N	6.5×10^5		Wang et al. (2017)	Q	81, 241
MCM:HM22CO2H	1.7×10^4		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	2.1×10^4		Wang et al. (2017)	Q	81, 240
RDFQSFOGKVZWKF-UHFFFAOYSA-N	1.8×10^4		Wang et al. (2017)	Q	81, 241
MCM:HO2C43CO2H	2.8×10^4		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	1.6×10^4		Wang et al. (2017)	Q	81, 240
VEXDRERIMPLZLU-UHFFFAOYSA-N	3.2×10^4		Wang et al. (2017)	Q	81, 241
MCM:HO2C4CO2H	2.3×10^4		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	8.0×10^4		Wang et al. (2017)	Q	81, 240
FMHKPLXYWVCLME-UHFFFAOYSA-N	8.1×10^5		Wang et al. (2017)	Q	81, 241
MCM:HOBUT2CO2H	2.3×10^4		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	3.5×10^4		Wang et al. (2017)	Q	81, 240
JYTYEGKJKIXWOJ-UHFFFAOYSA-N	7.1×10^5		Wang et al. (2017)	Q	81, 241
MCM:C518CO2H	4.6×10^4		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	2.8×10^4		Wang et al. (2017)	Q	81, 240
COPVWTGWHHSRKU-UHFFFAOYSA-N	2.0×10^4		Wang et al. (2017)	Q	81, 241

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:H2M2C4CO2H	1.4×10^4		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	3.0×10^4		Wang et al. (2017)	Q	81, 240
PQJUMPXLDAZULJ-UHFFFAOYSA-N	3.2×10^5		Wang et al. (2017)	Q	81, 241
MCM:H2M3C4CO2H	2.2×10^4		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	2.9×10^4		Wang et al. (2017)	Q	81, 240
BNTHHYUWQILHSA-UHFFFAOYSA-N	2.4×10^5		Wang et al. (2017)	Q	81, 241
MCM:HM22C3CO2H	1.4×10^4		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	2.3×10^4		Wang et al. (2017)	Q	81, 240
WLKUATLKPJGHKX-UHFFFAOYSA-N	1.6×10^5		Wang et al. (2017)	Q	81, 241
MCM:HM2C43CO2H	2.2×10^4		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	2.3×10^4		Wang et al. (2017)	Q	81, 240
QSMSJHRQUBQMKD-UHFFFAOYSA-N	4.7×10^4		Wang et al. (2017)	Q	81, 241
MCM:HM33C3CO2H	1.4×10^4		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.7×10^4		Wang et al. (2017)	Q	81, 240
NGRPJOQCQYDOJX-UHFFFAOYSA-N	6.6×10^5		Wang et al. (2017)	Q	81, 241
MCM:HO2C54CO2H	2.2×10^4		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.6×10^4		Wang et al. (2017)	Q	81, 240
IOXPMKQXROCYFL-UHFFFAOYSA-N	6.3×10^5		Wang et al. (2017)	Q	81, 241
MCM:HO3C5CO2H	2.0×10^4		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	3.7×10^4		Wang et al. (2017)	Q	81, 240
ABIKNKURIGPIRJ-UHFFFAOYSA-N	6.2×10^5		Wang et al. (2017)	Q	81, 241
MCM:C622CO2H	3.6×10^4		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_3$	4.7×10^4		Wang et al. (2017)	Q	81, 240
PHVXTLWKDLVJPT-UHFFFAOYSA-N	2.7×10^5		Wang et al. (2017)	Q	81, 241
MCM:C624CO2H	3.6×10^4		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_3$	3.0×10^4		Wang et al. (2017)	Q	81, 240
IOGKLHPXZHQWIC-UHFFFAOYSA-N	4.3×10^5		Wang et al. (2017)	Q	81, 241
MCM:H3M3C5CO2H	1.1×10^4		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_3$	1.7×10^4		Wang et al. (2017)	Q	81, 240
BHWOTLCMMUBASI-UHFFFAOYSA-N	2.8×10^5		Wang et al. (2017)	Q	81, 241
MCM:C811OH	3.6×10^4		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_3$	1.7×10^6		Wang et al. (2017)	Q	81, 240
UVNHICQQCWWSMK-UHFFFAOYSA-N	9.8×10^5		Wang et al. (2017)	Q	81, 241
MCM:C812OH	3.4×10^6		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_4$	2.9×10^8		Wang et al. (2017)	Q	81, 240
VFUDATRQVLCLSF-UHFFFAOYSA-N	1.2×10^7		Wang et al. (2017)	Q	81, 241
MCM:C812OOH	1.8×10^9		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_5$	4.9×10^8		Wang et al. (2017)	Q	81, 240
TXANCYYWZQZPGK-UHFFFAOYSA-N	1.5×10^8		Wang et al. (2017)	Q	81, 241

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C823OH	3.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_3$	2.0×10^{6}		Wang et al. (2017)	Q	81, 240
HTVBHPNLYICQSI-UHFFFAOYSA-N	9.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C825OH	5.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_4$	3.7×10^{7}		Wang et al. (2017)	Q	81, 240
GZVYHBJSBFFFII-UHFFFAOYSA-N	5.9×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C825OOH	2.8×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_5$	7.8×10^{8}		Wang et al. (2017)	Q	81, 240
XYVJCWMMBMHSFM-UHFFFAOYSA-N	1.8×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C137OH	3.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_3$	1.7×10^{6}		Wang et al. (2017)	Q	81, 240
GRQGZSRLPJOOBF-UHFFFAOYSA-N	2.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C139OH	6.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_4$	7.6×10^{9}		Wang et al. (2017)	Q	81, 240
RQGWJIBQKQBFEC-UHFFFAOYSA-N	1.4×10^{8}		Wang et al. (2017)	Q	81, 241
MCM:C139OOH	1.8×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_5$	1.7×10^{10}		Wang et al. (2017)	Q	81, 240
MQHLLQIJDGKDCT-UHFFFAOYSA-N	9.8×10^{8}		Wang et al. (2017)	Q	81, 241
MCM:C44OOH	7.3×10^{8}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_5$	4.1×10^{7}		Wang et al. (2017)	Q	81, 240
RIVXGQNQRYOWAN-UHFFFAOYSA-N	1.9×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:MALDALCO2H	3.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_3$	6.0×10^{3}		Wang et al. (2017)	Q	81, 240
ZOIRMVZWDRLJPI-UHFFFAOYSA-N	5.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:PRPAL2CO2H	9.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_3$	5.0×10^{3}		Wang et al. (2017)	Q	81, 240
VOKUMXABRRXHAR-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C3MCOCO2H	2.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_3$	9.6×10^{3}		Wang et al. (2017)	Q	81, 240
VXAWORVMCLXEKH-UHFFFAOYSA-N	7.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CO1M22CO2H	5.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
SUMZWDXUXLTFFX-UHFFFAOYSA-N	6.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MC3ODBCO2H	2.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_3$	9.3×10^{3}		Wang et al. (2017)	Q	81, 240
QPFVAKLVWFPTSX-UHFFFAOYSA-N	3.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C3EODBCO2H	2.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	8.3×10^{3}		Wang et al. (2017)	Q	81, 240
XIZBOUDCWHEQCF-UHFFFAOYSA-N	4.6×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C3M2COCO2H	1.6×10^4		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	9.1×10^3		Wang et al. (2017)	Q	81, 240
HLFIROOBCUFLFC-UHFFFAOYSA-N	5.8×10^3		Wang et al. (2017)	Q	81, 241
MCM:C522CO2H	1.3×10^4		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	2.3×10^4		Wang et al. (2017)	Q	81, 240
NSMTVDIDRFOALU-UHFFFAOYSA-N	9.3×10^3		Wang et al. (2017)	Q	81, 241
MCM:RGDCO2H	2.0×10^4		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	8.5×10^3		Wang et al. (2017)	Q	81, 240
HNXWTHGWCGDLKB-UHFFFAOYSA-N	3.0×10^3		Wang et al. (2017)	Q	81, 241
MCM:C615CO2H	3.6×10^6		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	5.4×10^5		Wang et al. (2017)	Q	81, 240
BRDQYLNZHVUNQF-UHFFFAOYSA-N	2.6×10^4		Wang et al. (2017)	Q	81, 241
MCM:C722OOH	3.0×10^8		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	1.6×10^7		Wang et al. (2017)	Q	81, 240
XJSSOLXEKAZFKL-UHFFFAOYSA-N	8.0×10^5		Wang et al. (2017)	Q	81, 241
MCM:IP3ODBCO2H	1.9×10^4		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	4.5×10^3		Wang et al. (2017)	Q	81, 240
HLXOYOZOZOGAJW-UHFFFAOYSA-N	1.1×10^3		Wang et al. (2017)	Q	81, 241
MCM:PC3ODBCO2H	1.7×10^4		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	5.4×10^3		Wang et al. (2017)	Q	81, 240
SHOOYBDWMZRRKO-UHFFFAOYSA-N	2.2×10^3		Wang et al. (2017)	Q	81, 241
MCM:C721CHO	1.2×10^4		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_3$	2.8×10^5		Wang et al. (2017)	Q	81, 240
MQTHUXQLMJSVGN-UHFFFAOYSA-N	2.9×10^4		Wang et al. (2017)	Q	81, 241
MCM:C729CO2H	1.0×10^4		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_3$	1.1×10^5		Wang et al. (2017)	Q	81, 240
NHNJUKWYLMFOQP-UHFFFAOYSA-N	1.7×10^4		Wang et al. (2017)	Q	81, 241
MCM:C823CO	1.0×10^4		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_3$	2.2×10^5		Wang et al. (2017)	Q	81, 240
KUOQBJGRIDTXEZ-UHFFFAOYSA-N	7.1×10^3		Wang et al. (2017)	Q	81, 241
MCM:C822CO2H	4.4×10^4	15000	Wieser et al. (2023)	Q	439
$C_9H_{14}O_3$	8.5×10^3		Wang et al. (2017)	Q	81, 239
ADULCIYKWVJSFE-UHFFFAOYSA-N	9.3×10^4		Wang et al. (2017)	Q	81, 240
	3.0×10^4		Wang et al. (2017)	Q	81, 241
MCM:C830CO2H	9.1×10^3		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_3$	1.9×10^5		Wang et al. (2017)	Q	81, 240
NWNQYPOMHUZLML-UHFFFAOYSA-N	2.3×10^4		Wang et al. (2017)	Q	81, 241

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C89CO2H	9.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_3$	2.0×10^{5}		Wang et al. (2017)	Q	81, 240
RFGXRYLTPBBFIG-UHFFFAOYSA-N	7.4×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C126CO2H	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{20}O_3$	2.4×10^{5}		Wang et al. (2017)	Q	81, 240
FRZAETYQWIEERW-UHFFFAOYSA-N	2.6×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C137CO	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{20}O_3$	2.2×10^{5}		Wang et al. (2017)	Q	81, 240
FQUQDHNCRLRZNB-UHFFFAOYSA-N	7.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C136CO2H	8.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_3$	1.5×10^{5}		Wang et al. (2017)	Q	81, 240
MUFZWTUKICSBHZ-UHFFFAOYSA-N	7.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:COHM2CO2H	2.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_4$	7.1×10^{5}		Wang et al. (2017)	Q	81, 240
DDNPKLYNPFAIEE-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C1H4C5CO2H	1.8×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	3.4×10^{7}		Wang et al. (2017)	Q	81, 240
NIVGPRREFKECGM-UHFFFAOYSA-N	3.2×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:ECOCO2H	7.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_3$	4.1×10^{1}		Wang et al. (2017)	Q	81, 240
TYEYBOSBBBHJIV-UHFFFAOYSA-N	5.8		Wang et al. (2017)	Q	81, 241
MCM:C41CO2H	6.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	4.6×10^{3}		Wang et al. (2017)	Q	81, 240
GCXJINGJZAOJHR-UHFFFAOYSA-N	3.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C5CO14OH	2.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_3$	1.6×10^{4}		Wang et al. (2017)	Q	81, 240
XGTKSWVCNVUVHG-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:CO2C4CO2H	5.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	4.6×10^{5}		Wang et al. (2017)	Q	81, 240
JOOXCMJARBKPKM-UHFFFAOYSA-N	7.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:CO3C4CO2H	5.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	1.5×10^{4}		Wang et al. (2017)	Q	81, 240
FHSUFDYFOHSYHI-UHFFFAOYSA-N	5.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:IPGLYOXOH	6.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	1.7×10^{1}		Wang et al. (2017)	Q	81, 240
QHKABHOOEWYVLI-UHFFFAOYSA-N	5.4		Wang et al. (2017)	Q	81, 241
MCM:PGLYOXOH	5.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	2.0×10^{1}		Wang et al. (2017)	Q	81, 240
KDVFRMMRZOCFLS-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	81, 241

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C51CO2H	5.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	1.6×10^{5}		Wang et al. (2017)	Q	81, 240
NFIWUVRBASXMGK-UHFFFAOYSA-N	1.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C5CODBCO2H	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	1.6×10^{4}		Wang et al. (2017)	Q	81, 240
YUICRCSHEOZHST-UHFFFAOYSA-N	2.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C5DBCOCO2H	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
LRRPKULXSOVRRZ-UHFFFAOYSA-N	2.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C6DCRBBOH	2.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
VUZJJUOKMOGBDH-UHFFFAOYSA-N	4.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:CO2C54CO2H	5.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	8.7×10^{4}		Wang et al. (2017)	Q	81, 240
UZTJTTKEYGHTNM-UHFFFAOYSA-N	3.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:CO2M33CO2H	3.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	8.5×10^{2}		Wang et al. (2017)	Q	81, 240
CBZZWRQRPKSEQI-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:CO3C5CO2H	4.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	2.6×10^{5}		Wang et al. (2017)	Q	81, 240
CLJBDOUIEHLLEN-UHFFFAOYSA-N	3.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C732OOH	3.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	1.8×10^{9}		Wang et al. (2017)	Q	81, 240
ASSSOSHEUJWVOL-UHFFFAOYSA-N	2.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C7ADCCO2H	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	1.3×10^{4}		Wang et al. (2017)	Q	81, 240
GJIWJSZYGQVZNC-UHFFFAOYSA-N	6.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C7CDCCO2H	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	7.8×10^{3}		Wang et al. (2017)	Q	81, 240
OAGXHOMWGVMDLP-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C7DCCO2H	1.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	8.5×10^{3}		Wang et al. (2017)	Q	81, 240
LUXOYEZTEWTGMD-UHFFFAOYSA-N	4.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C7DDCCO2H	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	8.5×10^{3}		Wang et al. (2017)	Q	81, 240
MDDQAVHYGMRQBB-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:CO25C6CO2H	2.7×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	2.2×10^{7}		Wang et al. (2017)	Q	81, 240
WUQQVFQGWWMQLD-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	81, 241

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:IC7DCCO2H	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	6.9×10^{3}		Wang et al. (2017)	Q	81, 240
TZKNMZPMBZQSMV-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C732CO3H	3.6×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_6$	2.2×10^{9}		Wang et al. (2017)	Q	81, 240
IARLEAITRRLVEZ-UHFFFAOYSA-N	2.7×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:KLIMONIC	4.5×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	3.4×10^{10}		Wang et al. (2017)	Q	81, 240
POLIOAJLCGOOTJ-UHFFFAOYSA-N	1.1×10^{9}		Wang et al. (2017)	Q	81, 241
MCM:C827CO2H	1.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	1.3×10^{6}		Wang et al. (2017)	Q	81, 240
UOMMGFNPUVSKTE-UHFFFAOYSA-N	4.9×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C88CO2H	4.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	6.6×10^{7}		Wang et al. (2017)	Q	81, 240
LOFCXTWTTIFNLN-UHFFFAOYSA-N	3.2×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:KLIMONONIC	2.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_4$	5.4×10^{7}		Wang et al. (2017)	Q	81, 240
RRLLKTDJWPIWHS-UHFFFAOYSA-N	8.5×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C928CO2H	1.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_4$	5.6×10^{7}		Wang et al. (2017)	Q	81, 240
SANKOOWGNYBKOU-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:LIMONONIC	5.7×10^{4}	15000	Wieser et al. (2023)	Q	439
$C_{10}H_{16}O_3$	5.8×10^{3}		Wang et al. (2017)	Q	81, 239
NJOIWWRMLFSDTM-UHFFFAOYSA-N	5.9×10^{4}		Wang et al. (2017)	Q	81, 240
	2.4×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C1011CO2H	4.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_3$	1.5×10^{5}		Wang et al. (2017)	Q	81, 240
IUOPXZCJHJMHNP-UHFFFAOYSA-N	2.4×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C1211OOH	3.5×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_5$	1.7×10^{9}		Wang et al. (2017)	Q	81, 240
PTZJPBFCCQIPAZ-UHFFFAOYSA-N	8.1×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C1211CO2H	4.7×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{20}O_5$	9.3×10^{10}		Wang et al. (2017)	Q	81, 240
QUEDJGCZCJPFDA-UHFFFAOYSA-N	2.8×10^{8}		Wang et al. (2017)	Q	81, 241
MCM:C1211CO3H	3.6×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{20}O_6$	4.5×10^{9}		Wang et al. (2017)	Q	81, 240
DVDQWECWXWLOQZ-UHFFFAOYSA-N	8.1×10^{7}		Wang et al. (2017)	Q	81, 241

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C131CO2H	2.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_4$	1.4×10^{8}		Wang et al. (2017)	Q	81, 240
QDUXHZZYSCMHPK-UHFFFAOYSA-N	5.9×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C147CO	1.4×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{20}O_5$	3.2×10^{8}		Wang et al. (2017)	Q	81, 240
MMRJODLWTRWNRH-UHFFFAOYSA-N	2.5×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C147OOH	1.7×10^{11}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_6$	1.0×10^{9}		Wang et al. (2017)	Q	81, 240
MOUQEZQXHGSYER-UHFFFAOYSA-N	3.0×10^{8}		Wang et al. (2017)	Q	81, 241
MCM:C141CO2H	5.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{24}O_3$	2.1×10^{5}		Wang et al. (2017)	Q	81, 240
VGNFSHPHIKPNED-UHFFFAOYSA-N	3.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HOCH2COCO2H	1.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_3H_4O_4$	5.3×10^{2}		Wang et al. (2017)	Q	81, 240
HHDDCCUIIUWNGJ-UHFFFAOYSA-N	4.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:H3C2C4CO2H	8.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	2.0×10^{6}		Wang et al. (2017)	Q	81, 240
IQZHXDCQZNRIRW-UHFFFAOYSA-N	2.8×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:HMVKBCO2H	1.7×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	2.1×10^{6}		Wang et al. (2017)	Q	81, 240
ISMQTZHDOHOVBT-UHFFFAOYSA-N	6.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C517CO2H	1.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	1.3×10^{7}		Wang et al. (2017)	Q	81, 240
APPVMSIJNZFGHP-UHFFFAOYSA-N	2.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C519CO2H	1.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	3.8×10^{6}		Wang et al. (2017)	Q	81, 240
ULHNCRHSCMPZGW-UHFFFAOYSA-N	3.8×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C732OH	1.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	4.7×10^{8}		Wang et al. (2017)	Q	81, 240
PKQMWBHBXJKPID-UHFFFAOYSA-N	4.2×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C734CO	8.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	6.6×10^{7}		Wang et al. (2017)	Q	81, 240
CPJVKYXUMUTCGW-UHFFFAOYSA-N	3.2×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C734OH	1.9×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	8.7×10^{10}		Wang et al. (2017)	Q	81, 240
RDRUHSRUZHRAFB-UHFFFAOYSA-N	4.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C734OOH	1.1×10^{12}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_6$	2.0×10^{11}		Wang et al. (2017)	Q	81, 240
ABEMFUWOTMEDPB-UHFFFAOYSA-N	1.3×10^{8}		Wang et al. (2017)	Q	81, 241

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:H3C25CCO2H	4.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	4.1×10^{9}		Wang et al. (2017)	Q	81, 240
FMZPEVNVWACALO-UHFFFAOYSA-N	2.7×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C813OH	2.1×10^{10}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_5$	6.5×10^{8}		Wang et al. (2017)	Q	81, 240
UHMOZKUUXAVADP-UHFFFAOYSA-N	2.0×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C813OOH	6.2×10^{11}		Wang et al. (2017)	Q	81, 239
$C_8H_{14}O_6$	1.7×10^{8}		Wang et al. (2017)	Q	81, 240
FNGYAHKKJFMZCA-UHFFFAOYSA-N	4.3×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C825CO	2.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	2.6×10^{5}		Wang et al. (2017)	Q	81, 240
PGSQVIJDIYGHPF-UHFFFAOYSA-N	4.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HOPINONIC	8.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_4$	6.0×10^{7}		Wang et al. (2017)	Q	81, 240
MZHKOIVHCBFXJV-UHFFFAOYSA-N	1.0×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C1211OH	1.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_4$	2.7×10^{8}		Wang et al. (2017)	Q	81, 240
JNTJQAWMLAKHDW-UHFFFAOYSA-N	2.8×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C1212OH	1.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_5$	4.7×10^{11}		Wang et al. (2017)	Q	81, 240
OINCQTVJDDDYTJ-UHFFFAOYSA-N	8.9×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C1212OOH	6.5×10^{11}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_6$	1.8×10^{11}		Wang et al. (2017)	Q	81, 240
KZNQDAPBLSOIIR-UHFFFAOYSA-N	1.8×10^{10}		Wang et al. (2017)	Q	81, 241
MCM:C1213CO	1.5×10^{12}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{18}O_6$	3.3×10^{12}		Wang et al. (2017)	Q	81, 240
IKFUCIVDZJUENZ-UHFFFAOYSA-N	2.1×10^{9}		Wang et al. (2017)	Q	81, 241
MCM:C1213OH	7.1×10^{12}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_6$	9.8×10^{11}		Wang et al. (2017)	Q	81, 240
DPGLQQDGNMDAAZ-UHFFFAOYSA-N	1.3×10^{8}		Wang et al. (2017)	Q	81, 241
MCM:C1213OOH	1.9×10^{14}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{20}O_7$	1.3×10^{13}		Wang et al. (2017)	Q	81, 240
ZUGVXCQEOPRNFT-UHFFFAOYSA-N	3.9×10^{8}		Wang et al. (2017)	Q	81, 241
MCM:C1310CO	4.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{20}O_5$	3.9×10^{11}		Wang et al. (2017)	Q	81, 240
NHYXXXJOGAKHPV-UHFFFAOYSA-N	2.6×10^{9}		Wang et al. (2017)	Q	81, 241
MCM:C1310OH	2.0×10^{10}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_5$	1.0×10^{11}		Wang et al. (2017)	Q	81, 240
PXEJSKZGVMTSCR-UHFFFAOYSA-N	1.7×10^{9}		Wang et al. (2017)	Q	81, 241

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C1310OOH	5.4×10^{11}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{22}O_6$	1.1×10^{12}		Wang et al. (2017)	Q	81, 240
HXUMLFGRLLCICH-UHFFFAOYSA-N	5.9×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C147OH	3.3×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_5$	5.6×10^{8}		Wang et al. (2017)	Q	81, 240
IPYASLZXSQHCRG-UHFFFAOYSA-N	7.8×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C151OH	6.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{26}O_5$	2.4×10^{10}		Wang et al. (2017)	Q	81, 240
RRTATIWWWPYIIC-UHFFFAOYSA-N	3.7×10^{9}		Wang et al. (2017)	Q	81, 241
MCM:C151OOH	4.7×10^{11}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{26}O_6$	1.9×10^{11}		Wang et al. (2017)	Q	81, 240
FDHNLWUJMDRLQD-UHFFFAOYSA-N	2.8×10^{10}		Wang et al. (2017)	Q	81, 241
MCM:CO13C3CO2H	6.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_4$	1.5×10^{4}		Wang et al. (2017)	Q	81, 240
YEZSWHPLZBZVLH-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C512CO2H	4.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	6.3×10^{7}		Wang et al. (2017)	Q	81, 240
CGRSCFNOTZUXCX-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C6COALCO2H	4.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	2.3×10^{7}		Wang et al. (2017)	Q	81, 240
TWNJAPRLIZAXHA-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C617CO2H	2.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	9.6×10^{5}		Wang et al. (2017)	Q	81, 240
ZXMACHDUAJJJBQ-UHFFFAOYSA-N	2.4×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C618CO2H	2.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	2.3×10^{5}		Wang et al. (2017)	Q	81, 240
MXMJWVQRGMMLRI-UHFFFAOYSA-N	5.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C626CO2H	3.7×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	8.3×10^{7}		Wang et al. (2017)	Q	81, 240
JCTYMUINHXVDEP-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C732CO	3.7×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	5.0×10^{7}		Wang et al. (2017)	Q	81, 240
ATXVRLJHWCSFDB-UHFFFAOYSA-N	2.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C718CO2H	2.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	1.6×10^{7}		Wang et al. (2017)	Q	81, 240
OBYKYHDGLQUNDK-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C731CO2H	3.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_4$	2.0×10^{8}		Wang et al. (2017)	Q	81, 240
URWVDUFOGQNELZ-UHFFFAOYSA-N	3.8×10^{6}		Wang et al. (2017)	Q	81, 241

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C87CO2H	1.7×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	3.6×10^{8}		Wang et al. (2017)	Q	81, 240
GZPOIVSRXTZTQZ-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C116CO2H	4.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{18}O_4$	1.8×10^{8}		Wang et al. (2017)	Q	81, 240
HWWVGCXKFWUOCT-UHFFFAOYSA-N	1.3×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C1211CO	4.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{18}O_4$	4.2×10^{7}		Wang et al. (2017)	Q	81, 240
VVPUYBXPESADLR-UHFFFAOYSA-N	8.7×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C1210CO2H	3.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{20}O_4$	2.8×10^{8}		Wang et al. (2017)	Q	81, 240
MERIWEKKXYNSHZ-UHFFFAOYSA-N	8.3×10^{5}		Wang et al. (2017)	Q	81, 241

A3.8 Esters (RCOOR)

Table A3.8: Esters (RCOOR)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3-dioxolan-2-one $C_3H_4O_3$ (ethylene carbonate) [96-49-1] KMTRUDSVKNLOMY-UHFFFAOYSA-N	3.6×10^{-2}		HSDB (2015)	Q	100
carbonic acid, dimethyl ester	1.6×10^{-1}	4900	Burkholder et al. (2019)	L	
$C_3H_6O_3$	1.6×10^{-1}	4900	Burkholder et al. (2015)	L	
(dimethyl carbonate)	1.5×10^{-1}	5000	Brockbank (2013)	L	1
[616-38-6]	1.6×10^{-1}	4900	Böhme et al. (2008)	M	
IEJIGPNLZYLLBP-UHFFFAOYSA-N	1.6×10^{-1}	5000	Dohnal et al. (2010)	V	1
	2.5×10^{-1}		Wang et al. (2017)	Q	81, 239
	2.1×10^{-1}		Wang et al. (2017)	Q	81, 240
	2.1×10^{-1}		Wang et al. (2017)	Q	81, 241
	1.6×10^{-2}		HSDB (2015)	Q	100
dimethyl dicarbonate	2.2×10^{-2}		HSDB (2015)	Q	100
$C_4H_6O_5$					
[4525-33-1]					
GZDFHIJNHHMENY-UHFFFAOYSA-N					
carbonic acid, diethyl ester	1.0×10^{-1}	6000	Burkholder et al. (2019)	L	
$C_5H_{10}O_3$	1.0×10^{-1}	6000	Burkholder et al. (2015)	L	
(diethyl carbonate)	1.0×10^{-1}	6400	Brockbank (2013)	L	1
[105-58-8]	1.1×10^{-1}	6100	Böhme et al. (2008)	M	
OIFBSDVPJOWBCH-UHFFFAOYSA-N	1.1×10^{-1}		Duchowicz et al. (2020)	V	187
	1.1×10^{-1}		HSDB (2015)	V	
	1.0×10^{-1}	6100	Dohnal et al. (2010)	V	1
	1.5×10^{-2}		Duchowicz et al. (2020)	Q	
	1.6×10^{-1}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	6.9×10^{-2}		Hilal et al. (2008)	Q	
	2.8×10^{-2}		Modarresi et al. (2007)	Q	68
	1.1×10^{-1}		Yaws (1999)	?	21, 12
methyl methanoate	4.1×10^{-2}	4000	Burkholder et al. (2019)	L	
$HCOOCH_3$	4.1×10^{-2}	4000	Burkholder et al. (2015)	L	
(methyl formate)	4.2×10^{-2}	3800	Brockbank (2013)	L	
[107-31-3]	4.1×10^{-2}	4000	Sander et al. (2011)	L	
TZIHFWKZFHZASV-UHFFFAOYSA-N	4.2×10^{-2}	3900	Plyasunov et al. (2004)	L	
	4.1×10^{-2}	4000	Kutsuna et al. (2005)	M	
	4.6×10^{-2}		Wittig et al. (2001)	M	
	4.1×10^{-2}		Hoff et al. (1993)	M	
	3.9×10^{-2}	4100	Hartkopf and Karger (1973)	M	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.9×10^{-2}		Mackay et al. (2006c)	V	
	4.9×10^{-2}		Mackay et al. (1995)	V	
	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	3.8×10^{-1}		Duchowicz et al. (2020)	Q	
	5.3×10^{-2}		Wang et al. (2017)	Q	81, 239
	1.0×10^{-1}		Wang et al. (2017)	Q	81, 240
	8.7×10^{-2}		Wang et al. (2017)	Q	81, 241
	4.4×10^{-2}		Li et al. (2014)	Q	242
	5.4×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	5.8×10^{-2}		Hilal et al. (2008)	Q	
	5.8×10^{-2}		Modarresi et al. (2007)	Q	68
		4100	Kühne et al. (2005)	Q	
	4.6×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	3.4×10^{-2}		English and Carroll (2001)	Q	231, 232
	2.9×10^{-2}		Katritzky et al. (1998)	Q	
	8.0×10^{-2}		Suzuki et al. (1992)	Q	233
	6.4×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	4.4×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		4200	Kühne et al. (2005)	?	
	5.2×10^{-3}		Yaws (1999)	?	21, 12
	4.4×10^{-2}		Betterton (1992)	?	499
	4.4×10^{-2}		Abraham et al. (1990)	?	
	4.4×10^{-2}		Hine and Mookerjee (1975)	?	499
ethyl methanoate	3.4×10^{-2}	4600	Burkholder et al. (2019)	L	
$HCOOC_2H_5$	3.4×10^{-2}	4600	Burkholder et al. (2015)	L	
(ethyl formate)	3.3×10^{-2}	4000	Brockbank (2013)	L	
[109-94-4]	3.4×10^{-2}	4600	Sander et al. (2011)	L	
WBJINCZRORDGAQ-UHFFFAOYSA-N	3.5×10^{-2}	4600	Plyasunov et al. (2004)	L	
	3.4×10^{-2}	4600	Kutsuna et al. (2005)	M	
	4.0×10^{-2}		Wittig et al. (2001)	M	
	2.3×10^{-2}		Richon et al. (1985)	M	38
	1.9×10^{-3}	4600	Hartkopf and Karger (1973)	M	
	4.9×10^{-2}		Mackay et al. (2006c)	V	
	4.9×10^{-2}		Mackay et al. (1995)	V	
	3.1×10^{-2}		Abraham (1984)	V	
	3.5×10^{-2}		Hine and Mookerjee (1975)	V	
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	1.8×10^{-1}		Duchowicz et al. (2020)	Q	185
	4.1×10^{-2}		Wang et al. (2017)	Q	81, 239
	4.8×10^{-2}		Wang et al. (2017)	Q	81, 240
	5.0×10^{-2}		Wang et al. (2017)	Q	81, 241
	4.7×10^{-2}		Gharagheizi et al. (2012)	Q	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	3.1×10^{-2}		Hilal et al. (2008)	Q	
	5.5×10^{-2}		Modarresi et al. (2007)	Q	68
	2.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.6×10^{-2}		English and Carroll (2001)	Q	231, 232
	3.5×10^{-2}		Katritzky et al. (1998)	Q	
	6.2×10^{-2}		Suzuki et al. (1992)	Q	233
	5.7×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.6×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	4.5×10^{-2}		Yaws (1999)	?	21, 28
	1.7×10^{-2}		Abraham and Weathersby (1994)	?	21
	1.4×10^{-3}		Hoff et al. (1993)	?	21
	3.1×10^{-2}		Abraham et al. (1990)	?	
propyl methanoate	2.6×10^{-2}	5100	Burkholder et al. (2019)	L	
$HCOOC_3H_7$	2.6×10^{-2}	5100	Burkholder et al. (2015)	L	
(propyl formate)	3.1×10^{-2}	4800	Brockbank (2013)	L	
[110-74-7]	2.6×10^{-2}	5100	Sander et al. (2011)	L	
KFNNIILCVOLYIR-UHFFFAOYSA-N	2.8×10^{-2}	4900	Plyasunov et al. (2004)	L	
	2.6×10^{-2}	5100	Kutsuna et al. (2005)	M	
	2.3×10^{-2}		Duchowicz et al. (2020)	V	187
	2.1×10^{-2}		Mackay et al. (2006c)	V	
	2.7×10^{-2}		Hine and Mookerjee (1975)	V	
	2.7×10^{-2}		Yaws (2003)	X	238, 88
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	
	2.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.3×10^{-2}		Hilal et al. (2008)	Q	
	4.5×10^{-2}		Modarresi et al. (2007)	Q	68
	1.3×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	1.9×10^{-2}		English and Carroll (2001)	Q	231, 232
	3.5×10^{-2}		Katritzky et al. (1998)	Q	
	4.7×10^{-2}		Suzuki et al. (1992)	Q	233
	4.4×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.3×10^{-2}		Yaws (1999)	?	21, 88
	2.7×10^{-2}		Abraham et al. (1990)	?	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
isopropyl methanoate	1.9×10^{-2}		Plyasunov et al. (2004)	L	
$HCOOC_3H_7$	1.3×10^{-2}		Duchowicz et al. (2020)	V	187
(isopropyl formate)	1.2×10^{-2}		Hine and Mookerjee (1975)	V	
[625-55-8]	8.2×10^{-2}		Duchowicz et al. (2020)	Q	
RMOUBSOVHSONPZ-UHFFFAOYSA-N	4.4×10^{-2}		Wang et al. (2017)	Q	81, 239
	3.1×10^{-2}		Wang et al. (2017)	Q	81, 240
	7.8×10^{-2}		Wang et al. (2017)	Q	81, 241
	4.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.1×10^{-2}		Hilal et al. (2008)	Q	
	1.3×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.0×10^{-2}		English and Carroll (2001)	Q	231, 275
	3.8×10^{-2}		Katritzky et al. (1998)	Q	
	4.3×10^{-2}		Suzuki et al. (1992)	Q	233
	3.9×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.2×10^{-2}		Abraham et al. (1990)	?	
butyl methanoate	2.6×10^{-2}	3700	Brockbank (2013)	L	
$HCOOC_4H_9$	1.9×10^{-2}		Plyasunov et al. (2004)	L	
(butyl formate)	1.9×10^{-2}		Wittig et al. (2001)	M	
[592-84-7]	1.9×10^{-2}		Duchowicz et al. (2020)	V	187
NMJJFJNHVMGPGM-UHFFFAOYSA-N	1.7×10^{-2}		Yaws (2003)	X	238, 404
	2.3×10^{-1}		Duchowicz et al. (2020)	Q	
	3.0×10^{-2}		Wang et al. (2017)	Q	81, 239
	2.1×10^{-2}		Wang et al. (2017)	Q	81, 240
	3.5×10^{-2}		Wang et al. (2017)	Q	81, 241
	1.4×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
	4.1×10^{-2}		Modarresi et al. (2007)	Q	68
	2.0×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	3.5×10^{-2}		Katritzky et al. (1998)	Q	
	1.9×10^{-2}		Yaws (1999)	?	21, 404
(1-methylpropyl)-methanoate	1.9×10^{-2}		Gharagheizi et al. (2012)	Q	
$C_5H_{10}O_2$					
(*sec*-butyl formate)					
[589-40-2]					
OAEQYDZVVPONKW-UHFFFAOYSA-N					

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(2-methylpropyl)-methanoate	1.6×10^{-2}	5200	Brockbank (2013)	L	
$HCOOC_4H_9$	1.6×10^{-2}	5200	Plyasunov et al. (2004)	L	
(isobutyl formate)	1.9×10^{-2}		Duchowicz et al. (2020)	V	187
[542-55-2]	1.8×10^{-2}		Mackay et al. (2006c)	V	
AVMSWPWPYJVYKY-UHFFFAOYSA-N	1.8×10^{-2}		Mackay et al. (1995)	V	
	1.7×10^{-2}		Hine and Mookerjee (1975)	V	
	1.8×10^{-2}		Yaws (2003)	X	238
	9.1×10^{-2}		Duchowicz et al. (2020)	Q	
	9.5×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.0×10^{-2}		Hilal et al. (2008)	Q	
	3.3×10^{-2}		Modarresi et al. (2007)	Q	68
	2.0×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.5×10^{-2}		English and Carroll (2001)	Q	231, 261
	3.9×10^{-2}		Katritzky et al. (1998)	Q	
	3.3×10^{-2}		Suzuki et al. (1992)	Q	233
	3.1×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	3.3×10^{-2}		Yaws (1999)	?	21
	1.7×10^{-2}		Abraham et al. (1990)	?	
(1,1-dimethylethyl)-methanoate	1.4×10^{-2}	3600	Brockbank (2013)	L	
$HCOOC_4H_9$	1.4×10^{-2}	3600	Arp and Schmidt (2004)	M	
(*tert*-butyl formate; TBF)	2.5×10^{-2}		Yaws (2003)	X	259
[762-75-4]	2.5×10^{-2}		Yaws (2003)	X	238
RUPAXCPQAAOIPB-UHFFFAOYSA-N	7.3×10^{-2}		Dupeux et al. (2022)	Q	260
	2.9×10^{-2}		Keshavarz et al. (2022)	Q	
	4.0×10^{-2}		Duchowicz et al. (2020)	Q	300
	2.3×10^{-2}		Wang et al. (2017)	Q	81, 239
	1.1×10^{-2}		Wang et al. (2017)	Q	81, 240
	6.6×10^{-2}		Wang et al. (2017)	Q	81, 241
	4.5×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
	1.4×10^{-2}		Duchowicz et al. (2020)	?	186, 21
pentyl methanoate	1.7×10^{-2}	6000	Brockbank (2013)	L	1
$C_6H_{12}O_2$	1.6×10^{-2}	5800	Plyasunov et al. (2004)	L	
(pentyl formate)	1.5×10^{-2}		Yaws (2003)	X	238
[638-49-3]	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
DIQMPQMYFZXDAX-UHFFFAOYSA-N	1.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
	1.3×10^{-2}		Hilal et al. (2008)	Q	
	7.5×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	2.8×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	2.5×10^{-2}		Yaws (1999)	?	21

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-pentyl methanoate $C_6H_{12}O_2$ (3-pentyl formate) [58368-67-5] YMJOAYHERILFIM-UHFFFAOYSA-N	1.2×10^{-2}		Gharagheizi et al. (2012)	Q	
1,1-dimethylpropyl methanoate $C_6H_{12}O_2$ (1,1-dimethylpropyl formate) [757-88-0] SVZIJXUUTNJSEJ-UHFFFAOYSA-N	1.7×10^{-2} 3.0×10^{-2} 1.6×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
1,2-dimethylpropyl methanoate $C_6H_{12}O_2$ (1,2-dimethylpropyl formate) [66794-46-5] XEQSPMCNFJQDHU-UHFFFAOYSA-N	1.7×10^{-2} 1.1×10^{-2} 1.7×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
1-methylbutyl methanoate $C_6H_{12}O_2$ (1-methylbutyl formate) [58368-66-4] JNRQSKFTIYCDIP-UHFFFAOYSA-N	1.7×10^{-2} 1.7×10^{-2} 1.5×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
2,2-dimethylpropyl methanoate $C_6H_{12}O_2$ (2,2-dimethylpropyl formate) [23361-67-3] DGMIPKNXUDSQGI-UHFFFAOYSA-N	1.5×10^{-2} 3.1×10^{-3} 1.5×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
2-methylbutyl methanoate $C_6H_{12}O_2$ (2-methylbutyl formate) [35073-27-9] DWORILFBIRYUDC-UHFFFAOYSA-N	1.6×10^{-2} 5.2×10^{-3} 1.4×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
3-methylbutyl methanoate $HCOOC_5H_{11}$ (isoamyl formate) [110-45-2] XKYICAQFSCFURC-UHFFFAOYSA-N	1.2×10^{-2} 1.5×10^{-2} 1.2×10^{-2} 3.9×10^{-2} 9.7×10^{-2} 8.5×10^{-3} 1.5×10^{-2} 1.7×10^{-2} 3.3×10^{-2} 1.6×10^{-2} 1.1×10^{-2} 3.4×10^{-2} 2.5×10^{-2}	5700	Plyasunov et al. (2004) Hine and Mookerjee (1975) Yaws (2003) Keshavarz et al. (2022) Duchowicz et al. (2020) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Yaffe et al. (2003) English and Carroll (2001) Katritzky et al. (1998) Suzuki et al. (1992)	L V X Q Q Q Q Q Q Q Q Q Q	 238 300 247 68 249, 250 231, 232 233

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.4×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.5×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	1.5×10^{-2}		Abraham et al. (1990)	?	
hexyl methanoate	1.0×10^{-2}		Plyasunov et al. (2004)	L	
$C_7H_{14}O_2$	1.0×10^{-2}		Yaws (2003)	X	238
(hexyl formate)	8.0×10^{-3}		Gharagheizi et al. (2012)	Q	
[629-33-4]	8.2×10^{-3}		Gharagheizi et al. (2010)	Q	247
OUGPMNMLWKSBRI-UHFFFAOYSA-N	1.1×10^{-2}		Hilal et al. (2008)	Q	
	1.6×10^{-2}		Nirmalakhandan et al. (1997)	Q	
heptyl methanoate	6.7×10^{-3}		Yaws (2003)	X	238
$C_8H_{16}O_2$	5.9×10^{-3}		Gharagheizi et al. (2012)	Q	
(heptyl formate)	5.2×10^{-3}		Gharagheizi et al. (2010)	Q	247
[112-23-2]					
XEAMDSXSXYAICO-UHFFFAOYSA-N					
octyl methanoate	1.7×10^{-3}		Yaws (2003)	X	238
$C_9H_{18}O_2$	3.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
(octyl formate)	5.1×10^{-3}		Yaws (1999)	?	21
[112-32-3]					
AVBRYQRTMPHARE-UHFFFAOYSA-N					
nonyl methanoate	2.3×10^{-3}		Yaws (2003)	X	238
$C_{10}H_{20}O_2$	3.9×10^{-3}		Gharagheizi et al. (2012)	Q	
(nonyl formate)	2.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
[5451-92-3]					
MOGJOLMSQWGXPA-UHFFFAOYSA-N					
decyl methanoate	1.5×10^{-3}		Yaws (2003)	X	238
$C_{11}H_{22}O_2$	4.8×10^{-3}		Gharagheizi et al. (2012)	Q	
(decyl formate)	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
[5451-52-5]					
BCLJZFLDSCTULJ-UHFFFAOYSA-N					
undecyl methanoate	9.3×10^{-4}		Yaws (2003)	X	238
$C_{12}H_{24}O_2$	6.0×10^{-3}		Gharagheizi et al. (2012)	Q	
(undecyl formate)	9.3×10^{-4}		Gharagheizi et al. (2010)	Q	247
[5454-24-0]					
OASFNORBKVGDRW-UHFFFAOYSA-N					
dodecyl methanoate	6.2×10^{-4}		Yaws (2003)	X	238
$C_{13}H_{26}O_2$	6.6×10^{-4}		Gharagheizi et al. (2010)	Q	247
(dodecyl formate)					
[28303-42-6]					
WPSGFSPBRBRLIQ-UHFFFAOYSA-N					

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
vinyl methanoate	5.2×10^{-2}		Yaws (2003)	X	259
$C_3H_4O_2$	5.2×10^{-2}		Yaws (2003)	X	238
(vinyl formate)	1.2×10^{-2}		Dupeux et al. (2022)	Q	260
[692-45-5]	5.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
GFJVXXWOPWLRNU-UHFFFAOYSA-N					
benzyl methanoate	2.0	7100	Brockbank (2013)	L	
$C_8H_8O_2$					
(benzyl formate)					
[104-57-4]					
UYWQUFXKFGHYNT-UHFFFAOYSA-N					
methyl ethanoate	8.5×10^{-2}	5900	Burkholder et al. (2019)	L	500, 1
CH_3COOCH_3	2.0×10^{-2}	5000	Burkholder et al. (2015)	L	501, 502
(methyl acetate)	8.5×10^{-2}	5900	Brockbank (2013)	L	1
[79-20-9]	8.1×10^{-2}	4800	Plyasunov et al. (2004)	L	
KXKVLQRXCPHEJC-UHFFFAOYSA-N	8.1×10^{-2}	4900	Fenclová et al. (2014)	M	1
	1.2×10^{-1}	7500	Hiatt (2013)	M	
	6.6×10^{-2}	4500	Arp and Schmidt (2004)	M	
	8.3×10^{-2}	4900	Hovorka et al. (2002)	M	
	4.2×10^{-2}		Kaneko et al. (1994)	M	14
	7.7×10^{-2}		Ioffe et al. (1984)	M	
	7.7×10^{-2}	5000	Kieckbusch and King (1979b)	M	503
	8.6×10^{-2}		Buttery et al. (1969)	M	
	1.1×10^{-1}		Butler and Ramchandani (1935)	M	
	8.7×10^{-2}	4800	McKeown and Stowell (1927)	M	
	1.1×10^{-1}		Mackay et al. (2006c)	V	
	1.1×10^{-1}		Mackay et al. (1995)	V	
	4.8×10^{-2}	3300	Djerki and Laub (1988)	V	
	1.1×10^{-1}	4800	Bagno et al. (1991)	T	475
	1.8×10^{-1}		Yaws (2003)	X	259
	9.6×10^{-2}		Dupeux et al. (2022)	Q	260
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	1.7×10^{-1}		Duchowicz et al. (2020)	Q	
	3.4×10^{-2}		Wang et al. (2017)	Q	81, 239
	1.2×10^{-1}		Wang et al. (2017)	Q	81, 240
	2.5×10^{-1}		Wang et al. (2017)	Q	81, 241
	7.3×10^{-2}		Li et al. (2014)	Q	242
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	6.4×10^{-2}		Hilal et al. (2008)	Q	
	6.0×10^{-2}		Modarresi et al. (2007)	Q	68
		4500	Kühne et al. (2005)	Q	
	8.6×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	5.4×10^{-2}		Yao et al. (2002)	Q	230
	7.0×10^{-2}		English and Carroll (2001)	Q	231, 232

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.8×10^{-2}		Katritzky et al. (1998)	Q	
	5.6×10^{-2}		Suzuki et al. (1992)	Q	233
	3.9×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	8.6×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		4900	Kühne et al. (2005)	?	
	1.4×10^{-1}		Yaws (1999)	?	21, 12
	8.0×10^{-2}		Abraham et al. (1990)	?	
ethyl ethanoate	6.5×10^{-2}	5600	Burkholder et al. (2019)	L	504, 1
$CH_3COOC_2H_5$	5.9×10^{-2}	5900	Burkholder et al. (2015)	L	
(ethyl acetate)	6.5×10^{-2}	5600	Brockbank (2013)	L	1
[141-78-6]	5.9×10^{-2}	5900	Sander et al. (2011)	L	
XEKOWRVHYACXOJ-UHFFFAOYSA-N	6.3×10^{-2}	5500	Plyasunov et al. (2004)	L	
	5.9×10^{-2}	5200	Kutsuna and Kaneyasu (2021)	M	
	5.2×10^{-2}	4800	Ammari and Schroen (2019)	M	11
	6.2×10^{-2}	5500	Fenclová et al. (2014)	M	1
	5.1×10^{-2}		Aprea et al. (2007)	M	
	5.9×10^{-2}	5900	Kutsuna et al. (2005)	M	
	3.9×10^{-2}		van Ruth et al. (2002)	M	14
	4.1×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 363
	3.0×10^{-2}		van Ruth et al. (2001)	M	14
			Dewulf et al. (1999)	M	364
	6.6×10^{-2}		Druaux et al. (1998)	M	
	3.4×10^{-2}		Welke et al. (1998)	M	
	5.7×10^{-2}		Landy et al. (1995)	M	
	2.8×10^{-2}		Kaneko et al. (1994)	M	14
	4.4×10^{-2}	3900	Kolb et al. (1992)	M	278
	1.1×10^{-1}		Pividal et al. (1992)	M	81
	4.3×10^{-2}		Guitart et al. (1989)	M	14
	6.2×10^{-2}		Jones et al. (1988)	M	
	4.3×10^{-2}		Richon et al. (1985)	M	38
	1.3×10^{-1}		Ioffe et al. (1984)	M	81
	5.8×10^{-2}	5300	Kieckbusch and King (1979b)	M	503
	5.7×10^{-2}		Nelson and Hoff (1968)	M	298
	7.4×10^{-2}		Butler and Ramchandani (1935)	M	
	7.3×10^{-2}		Mackay et al. (2006c)	V	
	3.1×10^{-2}		Philippe et al. (2003)	V	14
	7.3×10^{-2}		Mackay et al. (1995)	V	
	3.6×10^{-1}		Hwang et al. (1992)	V	
	7.1×10^{-2}		Yaws (2003)	X	259
	4.7×10^{-2}	5700	Janini and Quaddora (1986)	X	299
	3.9×10^{-2}		Nahon et al. (2000)	C	14
	7.8×10^{-2}		Dupeux et al. (2022)	Q	260
	2.2×10^{-2}		Keshavarz et al. (2022)	Q	
	6.9×10^{-2}		Duchowicz et al. (2020)	Q	300
	2.8×10^{-2}		Wang et al. (2017)	Q	81, 239

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.2×10^{-2}		Wang et al. (2017)	Q	81, 240
	2.5×10^{-1}		Wang et al. (2017)	Q	81, 241
	5.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	3.6×10^{-2}		Hilal et al. (2008)	Q	
	4.9×10^{-2}		Modarresi et al. (2007)	Q	68
		4800	Kühne et al. (2005)	Q	
	7.3×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	5.4×10^{-2}		Yao et al. (2002)	Q	230
	5.3×10^{-2}		English and Carroll (2001)	Q	231, 232
	4.5×10^{-2}		Katritzky et al. (1998)	Q	
	1.6×10^{-1}		Russell et al. (1992)	Q	280
	4.3×10^{-2}		Suzuki et al. (1992)	Q	233
	4.1×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	7.4×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		5200	Kühne et al. (2005)	?	
	7.1×10^{-2}		Yaws (1999)	?	21
	8.8×10^{-2}		Hoff et al. (1993)	?	21
	5.8×10^{-2}		Abraham et al. (1990)	?	
ethyl ethanoate-1-13C $CH_3COOC_2H_5$ (ethyl acetate-1-13C) [3424-59-7] XEKOWRVHYACXOJ-AZXPZELESA-N	7.1×10^{-2}	6500	Hiatt (2013)	M	
propyl ethanoate $CH_3COOC_3H_7$ (propyl acetate) [109-60-4] YKYONYBAUNKHLG-UHFFFAOYSA-N	4.4×10^{-2}	6100	Burkholder et al. (2019)	L	505, 1
	4.4×10^{-2}	6000	Brockbank (2013)	L	1
	4.5×10^{-2}	5900	Plyasunov et al. (2004)	L	
	4.5×10^{-2}	5900	Fenclová et al. (2014)	M	1
	3.9×10^{-2}		van Ruth et al. (2002)	M	14
	3.0×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 363
	1.8×10^{-2}		van Ruth et al. (2001)	M	14
	3.7×10^{-2}		Welke et al. (1998)	M	
	2.1×10^{-2}		Kaneko et al. (1994)	M	14
	3.1×10^{-2}		Richon et al. (1985)	M	38
	4.5×10^{-2}	5500	Kieckbusch and King (1979b)	M	503
	4.6×10^{-2}		Mackay et al. (2006c)	V	
	4.6×10^{-2}		Mackay et al. (1995)	V	
	5.0×10^{-2}		Hine and Mookerjee (1975)	V	
	5.0×10^{-2}		Butler and Ramchandani (1935)	V	
	3.7×10^{-2}		Yaws (2003)	X	259
	3.7×10^{-2}		Yaws (2003)	X	238
	4.4×10^{-2}	6000	Janini and Quaddora (1986)	X	299
	5.0×10^{-2}		Dupeux et al. (2022)	Q	260

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.9×10^{-2}		Keshavarz et al. (2022)	Q	
	7.7×10^{-2}		Duchowicz et al. (2020)	Q	
	2.5×10^{-2}		Wang et al. (2017)	Q	81, 239
	3.9×10^{-2}		Wang et al. (2017)	Q	81, 240
	2.1×10^{-1}		Wang et al. (2017)	Q	81, 241
	2.4×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	4.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.9×10^{-2}		Hilal et al. (2008)	Q	
	4.2×10^{-2}		Modarresi et al. (2007)	Q	68
	4.6×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	2.6×10^{-2}		Yao et al. (2002)	Q	230
	4.0×10^{-2}		English and Carroll (2001)	Q	231, 232
	4.1×10^{-2}		Katritzky et al. (1998)	Q	
	9.9×10^{-2}		Russell et al. (1992)	Q	280
	3.3×10^{-2}		Suzuki et al. (1992)	Q	233
	3.3×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	4.5×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	3.4×10^{-2}		Yaws (1999)	?	21
	4.5×10^{-2}		Abraham et al. (1990)	?	
methyl methoxyacetate $C_4H_8O_3$ [6290-49-9] QRMHDGWGLNLHMN-UHFFFAOYSA-N	2.5		Hovorka et al. (2002)	M	38
2-propenyl ethanoate $C_5H_8O_2$ [591-87-7] FWZUNOYOVVKUNF-UHFFFAOYSA-N	7.6×10^{-2}		HSDB (2015)	V	
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	7.0×10^{-2}		Hilal et al. (2008)	Q	
	8.4×10^{-2}		Modarresi et al. (2007)	Q	68
2-propyl ethanoate $CH_3COOC_3H_7$ (isopropyl acetate) [108-21-4] JMMWKPVZQRWMSS-UHFFFAOYSA-N	3.3×10^{-2}	6100	Brockbank (2013)	L	1
	3.3×10^{-2}	5600	Plyasunov et al. (2004)	L	
	1.3×10^{-2}		Kaneko et al. (1994)	M	14
	3.5×10^{-2}		Hine and Mookerjee (1975)	V	
	3.7×10^{-2}		Yaws (2003)	X	259
	2.9×10^{-2}	5500	Janini and Quaddora (1986)	X	299
	4.5×10^{-2}		Dupeux et al. (2022)	Q	260
	2.9×10^{-2}		Keshavarz et al. (2022)	Q	
	3.0×10^{-2}		Duchowicz et al. (2020)	Q	185
	2.6×10^{-2}		Wang et al. (2017)	Q	81, 239
	3.9×10^{-2}		Wang et al. (2017)	Q	81, 240
	1.7×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.0×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-2}		Hilal et al. (2008)	Q	
	2.8×10^{-2}		Modarresi et al. (2007)	Q	68
	4.6×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	3.3×10^{-2}		Yao et al. (2002)	Q	230
	3.9×10^{-2}		English and Carroll (2001)	Q	231, 275
	4.2×10^{-2}		Katritzky et al. (1998)	Q	
	2.9×10^{-2}		Suzuki et al. (1992)	Q	233
	2.9×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	3.6×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	3.6×10^{-2}		Yaws (1999)	?	21
	3.5×10^{-2}		Abraham et al. (1990)	?	
2-methoxyethyl ethanoate $C_5H_{10}O_3$ (methyl cellosolve acetate) [110-49-6] XLLIQLLCWZCATF-UHFFFAOYSA-N	3.0		Hovorka et al. (2002)	M	38
	9.0		HSDB (2015)	V	
glycerol monoacetate $C_5H_{10}O_4$ (acetin) [26446-35-5] KMZHZAAOEWVPSE-UHFFFAOYSA-N	2.4×10^{4}		HSDB (2015)	Q	100
1-propen-2-ol, acetate $C_5H_8O_2$ (isopropenyl acetate) [108-22-5] HETCEOQFVDFGSY-UHFFFAOYSA-N	5.5×10^{-3}		HSDB (2015)	Q	100
butyl ethanoate $CH_3COOC_4H_9$ (butyl acetate) [123-86-4] DKPFZGUDAPQIHT-UHFFFAOYSA-N	3.8×10^{-2}	6300	Brockbank (2013)	L	1
	3.5×10^{-2}	6300	Plyasunov et al. (2004)	L	
	2.4×10^{-2}		Kim and Kim (2014)	M	
	3.5×10^{-2}	6300	Fenclová et al. (2014)	M	1
	2.1×10^{-2}		Helburn et al. (2008)	M	
	2.8×10^{-2}		van Ruth et al. (2002)	M	14
	2.3×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 363
	1.7×10^{-2}		van Ruth et al. (2001)	M	14
	2.7×10^{-2}		Welke et al. (1998)	M	
	1.3×10^{-2}		Kaneko et al. (1994)	M	14
	2.3×10^{-2}	4300	Kolb et al. (1992)	M	278
	3.5×10^{-2}	7100	Ioffe et al. (1984)	M	
	3.5×10^{-2}	6000	Kieckbusch and King (1979b)	M	503
	3.2×10^{-2}		Mackay et al. (2006c)	V	
	3.2×10^{-2}		Mackay et al. (1995)	V	
	2.7×10^{-2}		Hwang et al. (1992)	V	
	3.0×10^{-2}		Hine and Mookerjee (1975)	V	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.2×10^{-2}		Yaws (2003)	X	259
	3.5×10^{-2}	7500	Janini and Quaddora (1986)	X	299
	2.1×10^{-2}	3200	Goldstein (1982)	X	299
	4.3×10^{-2}		Dupeux et al. (2022)	Q	260
	3.9×10^{-2}		Keshavarz et al. (2022)	Q	
	8.2×10^{-2}		Duchowicz et al. (2020)	Q	
	2.0×10^{-2}		Wang et al. (2017)	Q	81, 239
	2.9×10^{-2}		Wang et al. (2017)	Q	81, 240
	1.7×10^{-1}		Wang et al. (2017)	Q	81, 241
	1.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.3×10^{-2}		Hilal et al. (2008)	Q	
	3.0×10^{-2}		Modarresi et al. (2007)	Q	68
		5500	Kühne et al. (2005)	Q	
	3.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.4×10^{-2}		Yao et al. (2002)	Q	230, 268
	3.1×10^{-2}		English and Carroll (2001)	Q	231, 232
	4.1×10^{-2}		Katritzky et al. (1998)	Q	
	5.3×10^{-2}		Russell et al. (1992)	Q	360
	1.6×10^{-2}		Suzuki et al. (1992)	Q	233
	2.6×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	3.5×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		5300	Kühne et al. (2005)	?	
	3.8×10^{-2}		Yaws (1999)	?	21
	3.5×10^{-2}		Abraham et al. (1990)	?	
2-butyl ethanoate	2.3×10^{-2}	6000	Brockbank (2013)	L	1
$C_6H_{12}O_2$	2.3×10^{-2}	6200	Plyasunov et al. (2004)	L	
(*sec*-butyl acetate)	2.3×10^{-2}		HSDB (2015)	V	
[105-46-4]	2.4×10^{-2}		Yaws (2003)	X	259
DCKVNWZUADLDEH-UHFFFAOYSA-N	2.4×10^{-2}		Yaws (2003)	X	238, 12
	2.5×10^{-2}		Dupeux et al. (2022)	Q	260
	2.3×10^{-2}		Wang et al. (2017)	Q	81, 239
	2.6×10^{-2}		Wang et al. (2017)	Q	81, 240
	1.2×10^{-1}		Wang et al. (2017)	Q	81, 241
	2.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.9×10^{-2}		Modarresi et al. (2007)	Q	68
	2.4×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.7×10^{-2}		Yao et al. (2002)	Q	230
			Katritzky et al. (1998)	Q	506
	1.8×10^{-2}		Yaws (1999)	?	21, 12

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1-dimethylethyl ethanoate	1.2×10^{-2}	6100	Brockbank (2013)	L	1
$C_6H_{12}O_2$	1.1×10^{-2}	5600	Plyasunov et al. (2004)	L	
(*tert*-butyl acetate)	1.1×10^{-2}		Duchowicz et al. (2020)	V	187
[540-88-5]	3.2×10^{-2}		Yaws (2003)	X	259
WMOVHXAZOJBABW-UHFFFAOYSA-N	3.2×10^{-2}		Yaws (2003)	X	238
	2.6×10^{-2}		Dupeux et al. (2022)	Q	260
	1.4×10^{-2}		Duchowicz et al. (2020)	Q	
	1.4×10^{-2}		Wang et al. (2017)	Q	81, 239
	1.6×10^{-2}		Wang et al. (2017)	Q	81, 240
	7.4×10^{-2}		Wang et al. (2017)	Q	81, 241
	2.4×10^{-2}		HSDB (2015)	Q	100
	5.8×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.2×10^{-2}		Modarresi et al. (2007)	Q	68
	1.9×10^{-2}		Yao et al. (2002)	Q	230
	2.9×10^{-2}		Yaws (1999)	?	21
2-methylpropyl ethanoate	2.6×10^{-2}	6000	Brockbank (2013)	L	1
$CH_3COOC_4H_9$	2.4×10^{-2}	6200	Plyasunov et al. (2004)	L	
(isobutyl acetate)	1.0×10^{-2}		Kaneko et al. (1994)	M	14
[110-19-0]	1.9×10^{-2}		Mackay et al. (2006c)	V	
GJRQTCIYDGXPES-UHFFFAOYSA-N	1.9×10^{-2}		Mackay et al. (1995)	V	
	2.2×10^{-2}		Hine and Mookerjee (1975)	V	
	3.7×10^{-2}		Yaws (2003)	X	259
	2.3×10^{-2}		Yaws (2003)	X	238
	3.7×10^{-2}		Dupeux et al. (2022)	Q	260
	3.9×10^{-2}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	185
	1.0×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.7×10^{-2}		Hilal et al. (2008)	Q	
	3.2×10^{-2}		Modarresi et al. (2007)	Q	68
		5500	Kühne et al. (2005)	Q	
	1.8×10^{-2}		Yao et al. (2002)	Q	230
	3.1×10^{-2}		English and Carroll (2001)	Q	231, 232
	9.5×10^{-2}		Russell et al. (1992)	Q	280
	2.3×10^{-2}		Suzuki et al. (1992)	Q	233
	2.2×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.2×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		4600	Kühne et al. (2005)	?	
	2.3×10^{-2}		Yaws (1999)	?	21
	2.2×10^{-2}		Abraham et al. (1990)	?	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pentyl ethanoate	2.5×10^{-2}	7200	Brockbank (2013)	L	1
$CH_3COOC_5H_{11}$	2.7×10^{-2}	6700	Plyasunov et al. (2004)	L	
(amyl acetate)	1.3×10^{-1}	5000	Meynier et al. (2003)	M	38
[628-63-7]	9.3×10^{-3}		Kaneko et al. (1994)	M	14
PGMYKACGEOXYJE-UHFFFAOYSA-N	3.4×10^{-2}		Hellmann (1987)	M	88
	2.8×10^{-2}	6500	Kieckbusch and King (1979b)	M	503
	2.4×10^{-2}		Mackay et al. (2006c)	V	
	2.4×10^{-2}		Mackay et al. (1995)	V	
	2.5×10^{-2}		Hine and Mookerjee (1975)	V	
	2.8×10^{-2}		Yaws (2003)	X	259
	2.8×10^{-2}		Yaws (2003)	X	238
	2.5×10^{-2}		Meynier et al. (2003)	C	
	3.3×10^{-2}		Dupeux et al. (2022)	Q	260
	5.3×10^{-2}		Keshavarz et al. (2022)	Q	
	8.6×10^{-2}		Duchowicz et al. (2020)	Q	
	1.4×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.0×10^{-2}		Hilal et al. (2008)	Q	
	2.8×10^{-2}		Modarresi et al. (2007)	Q	68
	2.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.1×10^{-2}		Yao et al. (2002)	Q	230, 268
	2.3×10^{-2}		English and Carroll (2001)	Q	231, 261
	3.8×10^{-2}		Katritzky et al. (1998)	Q	
	2.1×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	2.6×10^{-2}		Russell et al. (1992)	Q	280
	1.9×10^{-2}		Suzuki et al. (1992)	Q	233
	2.1×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.3×10^{-2}		Taft et al. (1985)	Q	
	2.5×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	2.9×10^{-2}		Yaws (1999)	?	21
	2.8×10^{-2}		Abraham et al. (1990)	?	
2-methylbutyl ethanoate	2.8×10^{-2}		Yaws (2003)	X	238
$C_7H_{14}O_2$	7.4×10^{-3}		Gharagheizi et al. (2012)	Q	
(2-methylbutyl acetate)	2.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
[624-41-9]					
XHIUFYZDQBSEMF-UHFFFAOYSA-N					
1,2-dimethylpropyl ethanoate	2.9×10^{-2}		Yaws (2003)	X	238
$C_7H_{14}O_2$	1.2×10^{-2}		Gharagheizi et al. (2012)	Q	
(1,2-dimethylpropyl acetate)	2.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
[5343-96-4]					
ZLSXRPTWWRGMTJ-UHFFFAOYSA-N					

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-ethylpropyl ethanoate $C_7H_{14}O_2$ (1-ethylpropyl acetate) [620-11-1] PBKYSIMDORTIEU-UHFFFAOYSA-N	1.3×10^{-2}		Gharagheizi et al. (2012)	Q	
1,1-dimethylpropyl ethanoate	2.9×10^{-2}		Yaws (2003)	X	259
$C_7H_{14}O_2$	2.9×10^{-2}		Yaws (2003)	X	238
(*tert*-pentyl acetate)	2.0×10^{-2}		Dupeux et al. (2022)	Q	260
[625-16-1]	3.3×10^{-2}		Gharagheizi et al. (2012)	Q	
JCCIFDCPHCKATH-UHFFFAOYSA-N	2.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
2,2-dimethylpropyl ethanoate	2.6×10^{-2}		Yaws (2003)	X	238
$C_7H_{14}O_2$	2.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
(neopentyl acetate) [926-41-0] QLNYTCSELYEEPV-UHFFFAOYSA-N					
1,2-propanediol, diacetate	7.0×10^{1}		HSDB (2015)	Q	100
$C_7H_{12}O_4$ [623-84-7] MLHOXUWWKVQEJB-UHFFFAOYSA-N					
2-pentanol, acetate	1.2×10^{-2}		HSDB (2015)	Q	100
$C_7H_{14}O_2$	1.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[626-38-0] GQKZRWSUJHVIPE-UHFFFAOYSA-N					
3-methylbutyl ethanoate	2.1×10^{-2}	6700	Brockbank (2013)	L	1
$CH_3COOC_5H_{11}$	2.0×10^{-2}	6500	Plyasunov et al. (2004)	L	
(isoamyl acetate)	2.2×10^{-2}	6600	Ammari and Schroen (2019)	M	11
[123-92-2]	8.8×10^{-2}	4300	Meynier et al. (2003)	M	38
MLFHJEHSLIIPHL-UHFFFAOYSA-N	8.8×10^{-3}		Kaneko et al. (1994)	M	14
	2.6×10^{-2}		Mackay et al. (2006c)	V	
	2.6×10^{-2}		Mackay et al. (1995)	V	
	2.1×10^{-2}		Meylan and Howard (1991)	V	
	1.7×10^{-2}		Hine and Mookerjee (1975)	V	
	2.2×10^{-2}		Yaws (2003)	X	238
	2.4×10^{-2}	5000	Goldstein (1982)	X	299
	1.7×10^{-2}		Meynier et al. (2003)	C	
	5.3×10^{-2}		Keshavarz et al. (2022)	Q	
	7.0		Abney (2021)	Q	401
	3.3×10^{-2}		Duchowicz et al. (2020)	Q	300
	1.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.6×10^{-2}		Hilal et al. (2008)	Q	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.2×10^{-2}		Modarresi et al. (2007)	Q	68
	1.8×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.6×10^{-2}		Yao et al. (2002)	Q	230
	2.4×10^{-2}		English and Carroll (2001)	Q	231, 232
	3.8×10^{-2}		Katritzky et al. (1998)	Q	
	1.7×10^{-2}		Suzuki et al. (1992)	Q	233
	1.8×10^{-2}		Meylan and Howard (1991)	Q	
	1.8×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.7×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	2.1×10^{-2}		Yaws (1999)	?	21
	1.7×10^{-2}		Abraham et al. (1990)	?	
hexyl ethanoate	2.0×10^{-2}	7100	Brockbank (2013)	L	1, 507
$CH_3COOC_6H_{13}$	1.7×10^{-2}	7300	Plyasunov et al. (2004)	L	
(hexyl acetate)	1.4×10^{-2}		Souchon et al. (2004)	M	
[142-92-7]	1.5×10^{-2}		Karl et al. (2003)	M	
AOGQPLXWSUTHQB-UHFFFAOYSA-N	5.2×10^{-3}		Mackay et al. (2006c)	V	
	5.2×10^{-3}		Mackay et al. (1995)	V	
	1.8×10^{-2}		Hine and Mookerjee (1975)	V	
	2.0×10^{-2}		Yaws (2003)	X	259
	2.0×10^{-2}		Yaws (2003)	X	238
	3.6×10^{-2}		Dupeux et al. (2022)	Q	260
	7.1×10^{-2}		Keshavarz et al. (2022)	Q	
	8.9×10^{-2}		Duchowicz et al. (2020)	Q	185
	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
	1.4×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	68
	2.0×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.0×10^{-2}		Yao et al. (2002)	Q	230, 268
	1.7×10^{-2}		English and Carroll (2001)	Q	231, 232
	3.6×10^{-2}		Katritzky et al. (1998)	Q	
	9.9×10^{-3}		Russell et al. (1992)	Q	280
	1.5×10^{-2}		Suzuki et al. (1992)	Q	233
	2.2×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	2.0×10^{-2}		Yaws (1999)	?	21
	1.8×10^{-2}		Abraham et al. (1990)	?	
4-methyl-2-pentyl ethanoate	1.7×10^{-2}		HSDB (2015)	V	
$C_8H_{16}O_2$	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
(4-methyl-2-pentyl acetate)	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
[108-84-9]	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
CPIVYSAVIPTCCX-UHFFFAOYSA-N	1.1×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	68
	1.8×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	3.4×10^{-2}		Katritzky et al. (1998)	Q	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyclohexyl ethanoate $C_8H_{14}O_2$ (cyclohexyl acetate) [622-45-7] YYLLIJHXUHJATK-UHFFFAOYSA-N	1.0×10^{-1} 8.2×10^{-2}	7000	Brockbank (2013) HSDB (2015)	L Q	1, 508 100
ethanol, 2-(2-ethoxyethoxy)-, acetate $C_8H_{16}O_4$ (diethylene glycol monoethyl ether acetate) [112-15-2] FPZWZCWUIYYYBU-UHFFFAOYSA-N	4.3×10^{2}		HSDB (2015)	V	
phenyl ethanoate $C_8H_8O_2$ (phenyl acetate) [122-79-2] IPBVNPXQWQGGJP-UHFFFAOYSA-N	1.3 1.5×10^{-1}	7200	Brockbank (2013) HSDB (2015)	L Q	1 100
heptyl ethanoate $C_9H_{18}O_2$ (heptyl acetate) [112-06-1] ZCZSIDMEHXZRLG-UHFFFAOYSA-N	1.2×10^{-2} 1.1×10^{-2} 2.4×10^{-2} 1.1×10^{-2} 1.3×10^{-2}		Yaws (2003) Yaws (2003) Dupeux et al. (2022) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Brockbank (2013)	X X Q Q Q W	259 238 260 247 509
phenylmethyl ethanoate $C_9H_{10}O_2$ (benzyl acetate) [140-11-4] QUKGYYKBILRGFE-UHFFFAOYSA-N	8.5×10^{-1} 8.7×10^{-1} 9.0×10^{-1} 7.6×10^{-1} 5.2×10^{-1} 7.0×10^{-1} 9.2×10^{-1} 5.4×10^{-1}	6800	Brockbank (2013) Duchowicz et al. (2020) HSDB (2015) Dupeux et al. (2022) Duchowicz et al. (2020) Modarresi et al. (2007) Yaffe et al. (2003) Katritzky et al. (1998)	L V V Q Q Q Q Q	 187 260 68 249, 250
octyl ethanoate $CH_3COOC_8H_{17}$ (octyl acetate) [112-14-1] YLYBTZIQSIBWLI-UHFFFAOYSA-N	8.6×10^{-3} 8.6×10^{-3} 1.8×10^{-2} 1.2×10^{-2} 1.0×10^{-2}		Yaws (2003) Yaws (2003) Dupeux et al. (2022) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Brockbank (2013)	X X Q Q Q W	259 238 260 247 510

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-ethylhexyl ethanoate	1.1×10^{-2}		Mackay et al. (2006c)	V	
$C_{10}H_{20}O_2$	1.1×10^{-2}		Mackay et al. (1995)	V	
(2-ethylhexyl acetate)	1.3×10^{-2}		Yaws (2003)	X	238
[103-09-3]	6.6×10^{-3}		HSDB (2015)	Q	100
WOYWLLHHWAMFCB-UHFFFAOYSA-N	2.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
	9.8×10^{-3}		Yao et al. (2002)	Q	230
	1.3×10^{-2}		Yaws (1999)	?	21
nonyl ethanoate	4.1×10^{-2}		Yaws (2003)	X	259
$C_{11}H_{22}O_2$	2.1×10^{-2}		Dupeux et al. (2022)	Q	260
(nonyl acetate)					
[143-13-5]					
GJQIMXVRFNLMTB-UHFFFAOYSA-N					
decyl ethanoate	2.8×10^{-3}		Yaws (2003)	X	259
$C_{12}H_{24}O_2$	1.2×10^{-2}		Dupeux et al. (2022)	Q	260
(decyl acetate)	8.0×10^{-3}		Gharagheizi et al. (2012)	Q	
[112-17-4]					
NUPSHWCALHZGOV-UHFFFAOYSA-N					
undecyl ethanoate	1.5×10^{-2}		Gharagheizi et al. (2012)	Q	
$C_{13}H_{26}O_2$					
(undecyl acetate)					
[1731-81-3]					
CKQGCFFDQIFZFA-UHFFFAOYSA-N					
ethanol,	3.7×10^{7}		HSDB (2015)	Q	100
2,2'-[1,2-ethanediylbis(oxy)]bis-,					
diacetate					
$C_{10}H_{18}O_6$					
(triethylene glycol, diacetate)					
[111-21-7]					
OVOUKWFJRHALDD-UHFFFAOYSA-N					
1-methoxy-2-propyl ethanoate	2.9		Duchowicz et al. (2020)	V	187
$C_6H_{12}O_3$	8.7×10^{-1}		Duchowicz et al. (2020)	Q	
(1-methoxy-2-propyl acetate)	2.5		Raventos-Duran et al. (2010)	Q	243, 244
[108-65-6]	1.6		Raventos-Duran et al. (2010)	Q	245
LLHKCFNBLRBOGN-UHFFFAOYSA-N	2.5		Raventos-Duran et al. (2010)	Q	246
	9.9×10^{-1}		Hilal et al. (2008)	Q	
	6.3×10^{-1}		Modarresi et al. (2007)	Q	68
2-ethoxyethyl ethanoate	3.0		Brockbank (2013)	L	
$C_6H_{12}O_3$	3.0		Hovorka et al. (2002)	M	38
(2-ethoxyethyl acetate)	1.5		Johanson and Dynésius (1988)	M	14
[111-15-9]	3.4		Keshavarz et al. (2022)	Q	
SVONRAPFKPVNKG-UHFFFAOYSA-N	7.5×10^{-1}		Duchowicz et al. (2020)	Q	185
	2.5		Raventos-Duran et al. (2010)	Q	243, 244
	2.5		Raventos-Duran et al. (2010)	Q	245

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.5		Raventos-Duran et al. (2010)	Q	246
	1.9		Hilal et al. (2008)	Q	
	7.2×10^{-1}		Modarresi et al. (2007)	Q	68
	3.1		Duchowicz et al. (2020)	?	186, 21
	7.0		Yaws (1999)	?	21, 12
2-butoxyethyl ethanoate	1.8		Brockbank (2013)	L	
$C_8H_{16}O_3$	1.8	25000	Kim et al. (2000)	M	
(butyl cellosolve acetate)	6.1		Keshavarz et al. (2022)	Q	
[112-07-2]	9.6×10^{-1}		Duchowicz et al. (2020)	Q	300
NQBXSWAWVZHKBZ-UHFFFAOYSA-N	1.2		Raventos-Duran et al. (2010)	Q	243, 244
	1.6		Raventos-Duran et al. (2010)	Q	245
	1.6		Raventos-Duran et al. (2010)	Q	246
	1.3		Hilal et al. (2008)	Q	
	5.2×10^{-1}		Modarresi et al. (2007)	Q	68
	1.8		Duchowicz et al. (2020)	?	186, 21
2-(2-butoxyethoxy)-ethanol, ethanoate	2.8×10^{1}		Duchowicz et al. (2020)	V	187
$C_{10}H_{20}O_4$	2.8×10^{1}		HSDB (2015)	V	
[124-17-4]	1.1×10^{1}		Duchowicz et al. (2020)	Q	
VXQBJTKSVGFQOL-UHFFFAOYSA-N	6.2×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	246
	4.1×10^{1}		Hilal et al. (2008)	Q	
	7.2		Modarresi et al. (2007)	Q	68
1,2-ethanediol, diethanoate	1.2×10^{2}		Duchowicz et al. (2020)	V	187
$C_6H_{10}O_4$	1.2×10^{2}		HSDB (2015)	V	
[111-55-7]	1.3×10^{2}		Yaws (2003)	X	238, 88
JTXMVXSTHSMVQF-UHFFFAOYSA-N	6.4		Duchowicz et al. (2020)	Q	
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	246
	1.4×10^{2}		Gharagheizi et al. (2010)	Q	247
	1.3×10^{1}		Hilal et al. (2008)	Q	
	9.3×10^{1}		Yaws (1999)	?	21, 88
geranyl acetate	4.1×10^{-3}		HSDB (2015)	Q	100
$C_{12}H_{20}O_2$					
[105-87-3]					
HIGQPQRQIQDZMP-DHZHZOJOSA-N					
linalyl acetate	1.8×10^{-2}		Dupeux et al. (2022)	Q	260
$C_{12}H_{20}O_2$	5.8×10^{-3}		HSDB (2015)	Q	100
[115-95-7]					
UWKAYLJWKGQEPM-UHFFFAOYSA-N					

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate $C_{12}H_{22}O_2$ (menthyl acetate) [16409-45-3] XHXUANMFYXWVNG-UHFFFAOYSA-N	1.2×10^{-2}		HSDB (2015)	Q	100
methyl propanoate	5.8×10^{-2}	5700	Brockbank (2013)	L	
$C_2H_5COOCH_3$	5.5×10^{-2}	5400	Plyasunov et al. (2004)	L	
(methyl propionate)	5.2×10^{-2}		Ioffe et al. (1984)	M	
[554-12-1]	5.7×10^{-2}		Buttery et al. (1969)	M	
RJUFJBKOKNCXHH-UHFFFAOYSA-N	6.1×10^{-2}		Mackay et al. (2006c)	V	
	6.1×10^{-2}		Mackay et al. (1995)	V	
	1.3×10^{-1}	3900	Djerki and Laub (1988)	V	
	6.1×10^{-2}		Hine and Mookerjee (1975)	V	
	5.4×10^{-2}	5400	Bagno et al. (1991)	T	475
	2.2×10^{-2}		Keshavarz et al. (2022)	Q	
	2.0×10^{-1}		Duchowicz et al. (2020)	Q	185
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	5.2×10^{-2}		Modarresi et al. (2007)	Q	68
	5.8×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	5.3×10^{-2}		Yao et al. (2002)	Q	230
	5.3×10^{-2}		English and Carroll (2001)	Q	231, 232
	3.9×10^{-2}		Katritzky et al. (1998)	Q	
	4.4×10^{-2}		Suzuki et al. (1992)	Q	233
	4.0×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	5.7×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	5.2×10^{-2}		Yaws (1999)	?	21
	5.8×10^{-2}	5000	Betterton (1992)	?	511
	5.7×10^{-2}		Abraham et al. (1990)	?	
methyl 2-hydroxypropanoate	9.1	5000	Sanz and Gmehling (2005)	M	
$C_4H_8O_3$	4.7		Wang et al. (2017)	Q	81, 239
(methyl lactate)	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
[547-64-8]	1.4×10^{1}		Wang et al. (2017)	Q	81, 241
LPEKGGXMPWTOCB-UHFFFAOYSA-N	1.2×10^{3}		HSDB (2015)	Q	100

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethyl propanoate	3.8×10^{-2}	5900	Brockbank (2013)	L	1
$C_2H_5COOC_2H_5$	4.1×10^{-2}	6000	Plyasunov et al. (2004)	L	
(ethyl propionate)	4.1×10^{-2}	5900	Fenclová et al. (2014)	M	1
[105-37-3]	3.9×10^{-2}		Duchowicz et al. (2020)	V	187
FKRCODPIKNYEAC-UHFFFAOYSA-N	3.9×10^{-2}		HSDB (2015)	V	
	3.8×10^{-2}		Mackay et al. (2006c)	V	
	3.8×10^{-2}		Mackay et al. (1995)	V	
	3.7×10^{-2}		Abraham (1984)	V	
	4.5×10^{-2}		Hine and Mookerjee (1975)	V	
	4.5×10^{-2}		Yaws (2003)	X	259
	4.5×10^{-2}		Yaws (2003)	X	238
	4.1×10^{-2}		Dupeux et al. (2022)	Q	260
	7.7×10^{-2}		Duchowicz et al. (2020)	Q	
	4.5×10^{-2}		Li et al. (2014)	Q	242
	2.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	4.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.6×10^{-2}		Hilal et al. (2008)	Q	
	4.4×10^{-2}		Modarresi et al. (2007)	Q	68
	4.6×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	3.5×10^{-2}		Yao et al. (2002)	Q	230
	4.0×10^{-2}		English and Carroll (2001)	Q	231, 232
	3.9×10^{-2}		Katritzky et al. (1998)	Q	
	3.4×10^{-2}		Suzuki et al. (1992)	Q	233
	3.5×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	4.5×10^{-2}		Yaws (1999)	?	21
	3.8×10^{-2}		Abraham et al. (1990)	?	
propyl propanoate	2.6×10^{-2}	6400	Brockbank (2013)	L	1, 512
$C_2H_5COOC_3H_7$	2.9×10^{-2}	6200	Plyasunov et al. (2004)	L	
(propyl propionate)	2.5×10^{-2}		Duchowicz et al. (2020)	V	187
[106-36-5]	2.5×10^{-2}		Abraham (1984)	V	
MCSINKKTEDDPNK-UHFFFAOYSA-N	2.5×10^{-2}		Hine and Mookerjee (1975)	V	
	8.2×10^{-2}		Duchowicz et al. (2020)	Q	
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.0×10^{-2}		Hilal et al. (2008)	Q	
	3.6×10^{-2}		Modarresi et al. (2007)	Q	68
	2.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.6×10^{-2}		Yao et al. (2002)	Q	230
	3.1×10^{-2}		English and Carroll (2001)	Q	231, 275
	3.9×10^{-2}		Katritzky et al. (1998)	Q	
	2.6×10^{-2}		Suzuki et al. (1992)	Q	233

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.8×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.1×10^{-2}		Yaws (1999)	?	21
	2.5×10^{-2}		Abraham et al. (1990)	?	
isopropyl propanoate	1.8×10^{-2}		Plyasunov et al. (2004)	L	
$C_2H_5COOC_3H_7$	1.7×10^{-2}		Duchowicz et al. (2020)	V	187
(isopropyl propionate)	1.7×10^{-2}		Meylan and Howard (1991)	V	
[637-78-5]	1.7×10^{-2}		Hine and Mookerjee (1975)	V	
IJMWOMHMDSDKGK-UHFFFAOYSA-N	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	1.7×10^{-2}		Hilal et al. (2008)	Q	
	3.1×10^{-2}		Modarresi et al. (2007)	Q	68
	2.3×10^{-2}		Suzuki et al. (1992)	Q	233
	2.4×10^{-2}		Meylan and Howard (1991)	Q	
	2.5×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.7×10^{-2}		Abraham et al. (1990)	?	
butyl propanoate	2.2×10^{-2}	6900	Brockbank (2013)	L	1
$C_7H_{14}O_2$	2.0×10^{-2}	7000	Plyasunov et al. (2004)	L	
(butyl propionate)	2.0×10^{-2}		Duchowicz et al. (2020)	V	187
[590-01-2]	3.3×10^{-2}		Yaws (2003)	X	259
BTMVHUNTONAYDX-UHFFFAOYSA-N	3.3×10^{-2}		Yaws (2003)	X	238, 12
	2.6×10^{-2}		Dupeux et al. (2022)	Q	260
	8.6×10^{-2}		Duchowicz et al. (2020)	Q	
	8.9×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
	3.2×10^{-2}		Modarresi et al. (2007)	Q	68
	6.2×10^{-3}		Yaffe et al. (2003)	Q	249, 273
	2.3×10^{-2}		Yao et al. (2002)	Q	230
	3.7×10^{-2}		Katritzky et al. (1998)	Q	
	1.4×10^{-2}		Yaws (1999)	?	21
(2-methylpropyl)-propanoate	1.5×10^{-2}	6600	Plyasunov et al. (2004)	L	
$C_7H_{14}O_2$	1.5×10^{-2}		Duchowicz et al. (2020)	V	187
(isobutyl propionate)	3.3×10^{-2}		Duchowicz et al. (2020)	Q	
[540-42-1]	1.8×10^{-2}		Hilal et al. (2008)	Q	
FZXRXKLUIMKDEL-UHFFFAOYSA-N		5900	Kühne et al. (2005)	Q	
	6.2×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.9×10^{-2}		Nirmalakhandan et al. (1997)	Q	
		7300	Kühne et al. (2005)	?	
tert-butyl propanoate	7.5×10^{-3}		Ebert et al. (2023)	?	367
$C_7H_{14}O_2$					
[20487-40-5]					
JAELLLITIZHOGQ-UHFFFAOYSA-N					

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pentyl propanoate	1.9×10^{-2}		Plyasunov et al. (2004)	L	
$C_2H_5COOC_5H_{11}$	1.2×10^{-2}		Duchowicz et al. (2020)	V	187
(amyl propionate)	1.4×10^{-2}		Abraham (1984)	V	
[624-54-4]	1.2×10^{-2}		Hine and Mookerjee (1975)	V	
TWSRVQVEYJNFKQ-UHFFFAOYSA-N	8.9×10^{-2}		Duchowicz et al. (2020)	Q	
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	2.6×10^{-2}		Modarresi et al. (2007)	Q	68
	1.2×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.7×10^{-2}		English and Carroll (2001)	Q	231, 232
	3.4×10^{-2}		Katritzky et al. (1998)	Q	
	2.2×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	1.5×10^{-2}		Suzuki et al. (1992)	Q	233
	1.8×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.4×10^{-2}		Abraham et al. (1990)	?	
propanoic acid, 2-hydroxy-, ethyl ester	1.7×10^{1}		Duchowicz et al. (2020)	V	187
$C_5H_{10}O_3$	1.7×10^{1}		HSDB (2015)	V	
(ethyl lactate)	3.1		Duchowicz et al. (2020)	Q	
[97-64-3]					
LZCLXQDLBQLTDK-UHFFFAOYSA-N					
ethyl 3-ethoxypropanoate	1.5×10^{-2}		Yaws (1999)	?	21
$C_7H_{14}O_3$					
(ethyl 3-ethoxypropionate)					
[763-69-9]					
BHXIWUJLHYHGSJ-UHFFFAOYSA-N					
propanoic acid, 2-phenylethyl ester	3.9×10^{-1}		HSDB (2015)	Q	100
$C_{11}H_{14}O_2$					
[122-70-3]					
HVGZQCSMLUDISR-UHFFFAOYSA-N					
methyl butanoate	3.9×10^{-2}	5700	Brockbank (2013)	L	1, 513
$C_3H_7COOCH_3$	4.2×10^{-2}	5700	Plyasunov et al. (2004)	L	
(methyl butyrate)	3.7×10^{-2}		Aprea et al. (2007)	M	
[623-42-7]	3.6×10^{-2}		Ioffe et al. (1984)	M	
UUIQMZJEGPQKFD-UHFFFAOYSA-N	4.8×10^{-2}		Buttery et al. (1969)	M	
	3.6×10^{-1}	4400	Djerki and Laub (1988)	V	
	3.7×10^{-2}		Amoore and Buttery (1978)	V	
		5800	Della Gatta et al. (1981)	T	
	3.5×10^{-2}		Yaws (2003)	X	259
	3.6×10^{-2}		Nahon et al. (2000)	C	14
	4.4×10^{-2}		Dupeux et al. (2022)	Q	260
	2.9×10^{-2}		Keshavarz et al. (2022)	Q	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.3×10^{-1}		Duchowicz et al. (2020)	Q	300
	4.8×10^{-2}		Li et al. (2014)	Q	242
	1.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.8×10^{-2}		Hilal et al. (2008)	Q	
	4.0×10^{-2}		Modarresi et al. (2007)	Q	68
	4.6×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	3.2×10^{-2}		Yao et al. (2002)	Q	230
	4.0×10^{-2}		English and Carroll (2001)	Q	231, 232
	3.9×10^{-2}		Katritzky et al. (1998)	Q	
	1.5×10^{-1}		Russell et al. (1992)	Q	280
	3.4×10^{-2}		Suzuki et al. (1992)	Q	233
	3.2×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	4.8×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	3.5×10^{-2}		Yaws (1999)	?	21
	4.8×10^{-2}		Abraham et al. (1990)	?	
ethyl butanoate	2.5×10^{-2}	6100	Brockbank (2013)	L	1
$C_3H_7COOC_2H_5$	2.9×10^{-2}	6300	Plyasunov et al. (2004)	L	
(ethyl butyrate)	2.9×10^{-2}	6400	Fenclová et al. (2014)	M	1
[105-54-4]	2.4×10^{-2}		Aprea et al. (2007)	M	
OBNCKNCVKJNDBV-UHFFFAOYSA-N	2.6×10^{-2}		Souchon et al. (2004)	M	
	2.1×10^{-2}		van Ruth et al. (2002)	M	14
	2.1×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 363
	1.6×10^{-2}		van Ruth et al. (2001)	M	14
	4.0×10^{-2}		Landy et al. (1996)	M	
	2.4×10^{-2}		Landy et al. (1995)	M	
	2.5×10^{-2}		HSDB (2015)	V	
	2.4×10^{-2}		Mackay et al. (2006c)	V	
	1.2×10^{-2}		Philippe et al. (2003)	V	14
	2.4×10^{-2}		Mackay et al. (1995)	V	
	2.8×10^{-2}		Abraham (1984)	V	
	2.7×10^{-2}		Hine and Mookerjee (1975)	V	
	2.8×10^{-2}		Yaws (2003)	X	259
	2.8×10^{-2}		Yaws (2003)	X	238, 88
	2.7×10^{-2}		Nahon et al. (2000)	C	14
	4.5×10^{-2}		Dupeux et al. (2022)	Q	260
	3.4		Abney (2021)	Q	401
	2.4×10^{-2}		Savary et al. (2014)	Q	
	1.6×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	247

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.0×10^{-2}		Hilal et al. (2008)	Q	
	3.1×10^{-2}		Modarresi et al. (2007)	Q	68
	2.7×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	2.8×10^{-2}		Yao et al. (2002)	Q	230
	3.1×10^{-2}		English and Carroll (2001)	Q	231, 232
	3.9×10^{-2}		Katritzky et al. (1998)	Q	
	2.6×10^{-2}		Suzuki et al. (1992)	Q	233
	2.8×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.4×10^{-2}		Yaws (1999)	?	21, 88
	2.7×10^{-2}		Abraham et al. (1990)	?	
propyl butanoate	1.8×10^{-2}	6400	Brockbank (2013)	L	1
$C_3H_7COOC_3H_7$	2.2×10^{-2}	6600	Plyasunov et al. (2004)	L	
(propyl butyrate)	1.6×10^{-2}		Duchowicz et al. (2020)	V	187
[105-66-8]	1.6×10^{-2}		Meylan and Howard (1991)	V	
HUAZGNHGCJGYNP-UHFFFAOYSA-N	1.9×10^{-2}		Hine and Mookerjee (1975)	V	
	2.6×10^{-2}		Yaws (2003)	X	238, 155
	8.6×10^{-2}		Duchowicz et al. (2020)	Q	
	8.1×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.7×10^{-2}		Gharagheizi et al. (2010)	Q	247
	1.4×10^{-2}		Hilal et al. (2008)	Q	
	2.8×10^{-2}		Modarresi et al. (2007)	Q	68
	2.2×10^{-2}		Yao et al. (2002)	Q	230
	2.3×10^{-2}		English and Carroll (2001)	Q	231, 261
	3.6×10^{-2}		Katritzky et al. (1998)	Q	
	2.0×10^{-2}		Suzuki et al. (1992)	Q	233
	1.8×10^{-2}		Meylan and Howard (1991)	Q	
	2.2×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.6×10^{-2}		Yaws (1999)	?	21, 155
	1.9×10^{-2}		Abraham et al. (1990)	?	
2-propyl butanoate	1.8×10^{-2}		Plyasunov et al. (2004)	L	
$C_7H_{14}O_2$	1.9×10^{-2}		Dupeux et al. (2022)	Q	260
(isopropyl butyrate)					
[638-11-9]					
FFOPEPMHKILNIT-UHFFFAOYSA-N					
butyl butanoate	1.7×10^{-2}	7600	Brockbank (2013)	L	1
$C_8H_{16}O_2$	1.6×10^{-2}	7600	Plyasunov et al. (2004)	L	
(butyl butyrate)	1.4×10^{-2}		Duchowicz et al. (2020)	V	187
[109-21-7]	1.0×10^{-2}		Dupeux et al. (2022)	Q	260
XUPYJHCZDLZNFP-UHFFFAOYSA-N	8.9×10^{-2}		Duchowicz et al. (2020)	Q	
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.3×10^{-2}		Modarresi et al. (2007)	Q	68
	3.4×10^{-2}		Katritzky et al. (1998)	Q	
	1.1×10^{-2}		Yaws (1999)	?	21
2-methylpropyl butanoate $C_8H_{16}O_2$ (2-methylpropyl butyrate) [539-90-2] RGFNRWTWDWVHDD-UHFFFAOYSA-N	1.3×10^{-2}		Hilal et al. (2008)	Q	
2-methylpropyl 2-methylpropanoate $C_8H_{16}O_2$ (isobutyl isobutyrate) [97-85-8] RXGUIWHIADMCFC-UHFFFAOYSA-N	7.4×10^{-3}	6900	Brockbank (2013)	L	1, 514
	7.8×10^{-3}	6700	Plyasunov et al. (2004)	L	
	1.0×10^{-2}		Amoore and Buttery (1978)	M	
	1.2×10^{-2}		Duchowicz et al. (2020)	V	187
	7.2×10^{-3}		Amoore and Buttery (1978)	V	
	1.4×10^{-2}		Duchowicz et al. (2020)	Q	
	1.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	1.0×10^{-2}		Modarresi et al. (2007)	Q	68
	7.5×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.4×10^{-2}		English and Carroll (2001)	Q	231, 232
	1.3×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	6.9×10^{-3}		Yaws (1999)	?	21
	7.0×10^{-3}		Abraham et al. (1990)	?	
pentyl butanoate $C_9H_{18}O_2$ (pentyl butyrate) [540-18-1] CFNJLPHOBMVMNS-UHFFFAOYSA-N	1.7×10^{-2}	6400	Brockbank (2013)	L	
	9.8×10^{-3}		Dupeux et al. (2022)	Q	260
3-methylbutyl butanoate $C_9H_{18}O_2$ (isopentyl butyrate) [106-27-4] PQLMXFQTAMDXIZ-UHFFFAOYSA-N	1.1×10^{-2}	7500	Brockbank (2013)	L	1
methyl 2-methylpropanoate $C_5H_{10}O_2$ (methyl isobutyrate) [547-63-7] BHIWKHZACMWKOJ-UHFFFAOYSA-N	2.6×10^{-2}	5600	Brockbank (2013)	L	1
	2.6×10^{-2}	5500	Plyasunov et al. (2004)	L	
	3.3×10^{-2}	5700	Bagno et al. (1991)	T	475
		5700	Della Gatta et al. (1981)	T	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethyl 2-methylpropanoate	1.5×10^{-2}	6000	Brockbank (2013)	L	1
$C_6H_{12}O_2$	1.7×10^{-2}	6200	Plyasunov et al. (2004)	L	
(ethyl isobutyrate)	2.0×10^{-2}		Hilal et al. (2008)	Q	
[97-62-1]	1.8×10^{-2}		Yao et al. (2002)	Q	230
WDAXFOBOLVPGLV-UHFFFAOYSA-N	2.4×10^{-2}		Yaws (1999)	?	21
hexyl butanoate	1.1×10^{-2}		Dupeux et al. (2022)	Q	260
$C_{10}H_{20}O_2$					
(hexyl butyrate)					
[2639-63-6]					
XAPCMTMQBXLDBB-UHFFFAOYSA-N					
cyclohexyl butanoate		6500	Kühne et al. (2005)	Q	
$C_{10}H_{18}O_2$		5600	Kühne et al. (2005)	?	
(cyclohexyl butyrate)					
[1551-44-6]					
VZHUBBUZNIULNM-UHFFFAOYSA-N					
3-oxobutanoic acid, methyl ester	6.4		Hovorka et al. (2002)	M	38
$C_5H_8O_3$	3.6×10^{1}		Duchowicz et al. (2020)	V	187
(methylacetoacetate)	3.7×10^{1}		HSDB (2015)	V	
[105-45-3]	1.2×10^{1}		Duchowicz et al. (2020)	Q	
WRQNANDWMGAFTP-UHFFFAOYSA-N	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	246
	1.7×10^{1}		Hilal et al. (2008)	Q	
	7.9		Modarresi et al. (2007)	Q	68
3-oxobutanoic acid, ethyl ester	9.0	7200	Brockbank (2013)	L	
$C_6H_{10}O_3$	5.8		Hovorka et al. (2002)	M	38
(ethylacetoacetate)	8.2		Duchowicz et al. (2020)	V	187
[141-97-9]	1.7×10^{1}		Yaws (2003)	X	259
XYIBRDXRRQCHLP-UHFFFAOYSA-N	1.7×10^{1}		Yaws (2003)	X	238, 155
	2.4×10^{1}		Dupeux et al. (2022)	Q	260
	4.5		Duchowicz et al. (2020)	Q	
	7.8		Raventos-Duran et al. (2010)	Q	272, 244
	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{1}		Raventos-Duran et al. (2010)	Q	246
	1.7×10^{1}		Gharagheizi et al. (2010)	Q	247
	1.1×10^{1}		Hilal et al. (2008)	Q	
	5.6		Modarresi et al. (2007)	Q	68
	9.1		Yaws (1999)	?	21, 155

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl pentanoate	3.0×10^{-2}	6100	Plyasunov et al. (2004)	L	
$C_4H_9COOCH_3$	3.1×10^{-2}		Buttery et al. (1969)	M	
(methyl valerate)	9.7×10^{-1}	5000	Djerki and Laub (1988)	V	
[624-24-8]		6200	Della Gatta et al. (1981)	T	
HNBDRPTVWVGKBR-UHFFFAOYSA-N	3.9×10^{-2}		Keshavarz et al. (2022)	Q	
	2.4×10^{-1}		Duchowicz et al. (2020)	Q	300
	2.9×10^{-2}		Li et al. (2014)	Q	242
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.2×10^{-2}		Hilal et al. (2008)	Q	
	3.6×10^{-2}		Modarresi et al. (2007)	Q	68
	3.1×10^{-2}		English and Carroll (2001)	Q	231, 232
	3.8×10^{-2}		Katritzky et al. (1998)	Q	
	2.6×10^{-2}		Suzuki et al. (1992)	Q	233
	2.5×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	3.1×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	3.1×10^{-2}		Abraham et al. (1990)	?	
ethyl pentanoate	2.3×10^{-2}	6800	Plyasunov et al. (2004)	L	
$C_4H_9COOC_2H_5$	1.4×10^{-1}	4800	Meynier et al. (2003)	M	38
(ethyl valerate)	2.7×10^{-2}		Duchowicz et al. (2020)	V	187
[539-82-2]	2.8×10^{-2}		Meylan and Howard (1991)	V	
ICMAFTSLXCXHRK-UHFFFAOYSA-N	2.8×10^{-2}		Abraham (1984)	V	
	2.9×10^{-2}		Hine and Mookerjee (1975)	V	
	2.7×10^{-2}		Meynier et al. (2003)	C	
	8.6×10^{-2}		Duchowicz et al. (2020)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.5×10^{-2}		Hilal et al. (2008)	Q	
	2.6×10^{-2}		Modarresi et al. (2007)	Q	68
	2.3×10^{-2}		English and Carroll (2001)	Q	231, 232
	2.0×10^{-2}		Suzuki et al. (1992)	Q	233
	1.8×10^{-2}		Meylan and Howard (1991)	Q	
	2.2×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.7×10^{-2}		Abraham et al. (1990)	?	
methyl 2,2-dimethylpropanoate	9.5×10^{-3}	5600	Plyasunov et al. (2004)	L	
$C_6H_{12}O_2$	2.3×10^{-2}	6000	Bagno et al. (1991)	T	475
(methyl pivalate)		6000	Della Gatta et al. (1981)	T	
[598-98-1]	3.9×10^{-2}		Keshavarz et al. (2022)	Q	
CNMFHDIDIMZHKY-UHFFFAOYSA-N	4.1×10^{-2}		Duchowicz et al. (2020)	Q	
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.7×10^{-2}		Hilal et al. (2008)	Q	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.7×10^{-2}		Modarresi et al. (2007)	Q	68
	1.8×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	2.3×10^{-2}		English and Carroll (2001)	Q	231, 232
	1.8×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	2.3×10^{-2}		Duchowicz et al. (2020)	?	186, 21
ethyl 2-methylbutanoate $C_7H_{14}O_2$ [7452-79-1] HCRBXQFHJMCTLF-UHFFFAOYSA-N	1.4×10^{-2}	6700	Plyasunov et al. (2004)	L	
	8.9×10^{-3}		Pollien et al. (2003)	M	
	2.7×10^{-2}		Roberts and Pollien (1997)	M	
ethyl 3-methylbutanoate $C_7H_{14}O_2$ (ethyl isovalerate) [108-64-5] PPXUHEORWJQRHJ-UHFFFAOYSA-N	1.4×10^{-2}	6500	Brockbank (2013)	L	1
	1.4×10^{-2}	6700	Plyasunov et al. (2004)	L	
	1.1×10^{-2}	5900	Wieland et al. (2015)	M	515
	1.4×10^{-2}		Duchowicz et al. (2020)	V	187
	2.2×10^{-2}		Dupeux et al. (2022)	Q	260
	3.3×10^{-2}		Duchowicz et al. (2020)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.6×10^{-2}		Hilal et al. (2008)	Q	
	2.8×10^{-2}		Modarresi et al. (2007)	Q	68
	1.5×10^{-2}		Yao et al. (2002)	Q	230
	1.6×10^{-2}		Yaws (1999)	?	21
ethyl 2,2-dimethylpropanoate $C_7H_{14}O_2$ (ethyl pivalate) [3938-95-2] HHEIMYAXCOIQCJ-UHFFFAOYSA-N	6.4×10^{-3}	6700	Brockbank (2013)	L	1
	5.7×10^{-3}	6100	Plyasunov et al. (2004)	L	
butyl pentanoate $C_9H_{18}O_2$ (butyl valerate) [591-68-4] OKJADYKTJJGKDX-UHFFFAOYSA-N	9.8×10^{-3}		Plyasunov et al. (2004)	L	
	2.3×10^{-2}		Dupeux et al. (2022)	Q	260
	2.0×10^{-2}		Yao et al. (2002)	Q	230
	1.5×10^{-2}		Yaws (1999)	?	21
3-methylbutyl 3-methylbutanoate $C_{10}H_{20}O_2$ (isoamyl isovalerate) [659-70-1] XINCECQTMHSORG-UHFFFAOYSA-N	4.0×10^{-3}		Yaws (1999)	?	21

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl hexanoate	2.6×10^{-2}	6600	Plyasunov et al. (2004)	L	
$C_5H_{11}COOCH_3$	1.9×10^{-2}		Aprea et al. (2007)	M	
(methyl caproate)	2.7×10^{-2}		Buttery et al. (1969)	M	
[106-70-7]	2.6	5600	Djerki and Laub (1988)	V	
NUKZAGXMHTUAFE-UHFFFAOYSA-N	5.3×10^{-2}		Keshavarz et al. (2022)	Q	
	2.5×10^{-1}		Duchowicz et al. (2020)	Q	300
	2.7×10^{-2}		Li et al. (2014)	Q	242
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.8×10^{-2}		Hilal et al. (2008)	Q	
	2.9×10^{-2}		Modarresi et al. (2007)	Q	68
	2.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.3×10^{-2}		English and Carroll (2001)	Q	231, 275
	3.6×10^{-2}		Katritzky et al. (1998)	Q	
	2.0×10^{-2}		Suzuki et al. (1992)	Q	233
	2.0×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.7×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	2.7×10^{-2}		Abraham et al. (1990)	?	
ethyl hexanoate	1.9×10^{-2}	7200	Plyasunov et al. (2004)	L	
$C_5H_{11}COOC_2H_5$	1.4×10^{-2}		Aprea et al. (2007)	M	
(ethyl caproate)	1.6×10^{-2}		Landy et al. (1996)	M	
[123-66-0]	9.4×10^{-3}		Landy et al. (1995)	M	
SHZIWNPUGXLXDT-UHFFFAOYSA-N	6.9×10^{-3}		Philippe et al. (2003)	V	14
	1.8×10^{-2}		Abraham (1984)	V	
	3.0		Abney (2021)	Q	401
	1.4×10^{-2}		Savary et al. (2014)	Q	
	1.1×10^{-2}		Hilal et al. (2008)	Q	
	1.7×10^{-2}		English and Carroll (2001)	Q	231, 261
	1.7×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	1.8×10^{-2}		Abraham et al. (1990)	?	
2-ethylbutanoic acid, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester $C_{18}H_{34}O_6$ [95-08-9] JEYLQCXBYFQJRO-UHFFFAOYSA-N	9.9×10^{5}		HSDB (2015)	Q	100
methyl heptanoate $C_8H_{16}O_2$ [106-73-0] XNCNNDVCAUWAIT-UHFFFAOYSA-N	1.8×10^{-2}		Plyasunov et al. (2004)	L	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethyl heptanoate	2.0×10^{-2}		Meylan and Howard (1991)	V	
$C_6H_{13}COOC_2H_5$	2.0×10^{-2}		Abraham (1984)	V	
[106-30-9]	2.0×10^{-2}		Hine and Mookerjee (1975)	V	
TVQGDYNRXLTQAP-UHFFFAOYSA-N	9.6×10^{-2}		Keshavarz et al. (2022)	Q	
	9.1×10^{-2}		Duchowicz et al. (2020)	Q	300
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	9.2×10^{-3}		Hilal et al. (2008)	Q	
	1.9×10^{-2}		Modarresi et al. (2007)	Q	68
	1.2×10^{-2}		Suzuki et al. (1992)	Q	233
	1.0×10^{-2}		Meylan and Howard (1991)	Q	
	2.1×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.0×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	2.0×10^{-2}		Abraham et al. (1990)	?	
methyl octanoate	1.2×10^{-2}		Plyasunov et al. (2004)	L	
$C_6H_{13}COOCH_3$	9.9×10^{-3}		Aprea et al. (2007)	M	
[111-11-5]	1.3×10^{-2}		Buttery et al. (1969)	M	
JGHZJRVDZXSNKQ-UHFFFAOYSA-N	9.6×10^{-2}		Keshavarz et al. (2022)	Q	
	2.7×10^{-1}		Duchowicz et al. (2020)	Q	300
	1.3×10^{-2}		Li et al. (2014)	Q	242
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	68
	4.7×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	1.2×10^{-2}		Suzuki et al. (1992)	Q	233
	1.1×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.3×10^{-2}		Duchowicz et al. (2020)	?	186, 21
ethyl octanoate	1.7×10^{-2}		Plyasunov et al. (2004)	L	
$C_7H_{15}COOC_2H_5$	1.1×10^{-2}		Aprea et al. (2007)	M	
[106-32-1]	1.2×10^{-2}		Abraham (1984)	V	
YYZUSRORWSJGET-UHFFFAOYSA-N	7.8×10^{-3}		Savary et al. (2014)	Q	
octadecanoic acid, 2-methylpropyl ester $C_{22}H_{44}O_2$ (isobutyl stearate) [646-13-9] ORFWYUFLWUWSFM-UHFFFAOYSA-N	2.6×10^{-4}		HSDB (2015)	Q	100

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
octadecanoic acid, butyl ester $C_{22}H_{44}O_2$ [123-95-5] ULBTUVJTXULMLP-UHFFFAOYSA-N	2.6×10^{-4}		HSDB (2015)	Q	100
methyl nonanoate $C_{10}H_{20}O_2$ [1731-84-6] IJXHLVMUNBOGRR-UHFFFAOYSA-N	8.2×10^{-3} 7.0×10^{-3}		Plyasunov et al. (2004) Abraham (1984)	L V	
ethyl nonanoate $C_8H_{17}COOC_2H_5$ [123-29-5] BYEVBITUADOIGY-UHFFFAOYSA-N	1.3×10^{-2}		Abraham (1984)	V	
nonanedioic acid, bis(2-ethylhexyl) ester $C_{25}H_{48}O_4$ (di-2-ethylhexyl azelate) [103-24-2] ZDWGXBPVPXVXMQ-UHFFFAOYSA-N	8.2×10^{-2}		HSDB (2015)	Q	100
methyl decanoate $C_{11}H_{22}O_2$ (methyl caprate) [110-42-9] YRHYCMZPEVDGFQ-UHFFFAOYSA-N	1.1×10^{-2} 4.8×10^{-3} 1.4×10^{-2} 3.2×10^{-3} 2.8×10^{-1} 5.8×10^{-3} 7.7×10^{-3}		Aprea et al. (2007) Duchowicz et al. (2020) Krop et al. (1997) Abraham (1984) Duchowicz et al. (2020) HSDB (2015) Hilal et al. (2008)	M V V V Q Q Q	 187 100
ethyl decanoate $C_9H_{19}COOC_2H_5$ [110-38-3] RGXWDWUGBIJHDO-UHFFFAOYSA-N	1.2×10^{-2} 1.4×10^{-2} 1.7×10^{-2}		Plyasunov et al. (2004) Aprea et al. (2007) Abraham (1984)	L M V	
decanedioic acid, diethyl ester $C_{14}H_{26}O_4$ (diethyl sebacate) [110-40-7] ONKUXPIBXRRIDU-UHFFFAOYSA-N	2.7		Bartelt-Hunt et al. (2008)	?	21
methyl dodecanoate $C_{13}H_{26}O_2$ (methyl laurate) [111-82-0] UQDUPQYQJKYHQI-UHFFFAOYSA-N	8.3×10^{-3} 7.5×10^{-3} 3.3×10^{-3} 4.8×10^{-3}		Krop et al. (1997) Dupeux et al. (2022) HSDB (2015) Hilal et al. (2008)	V Q Q Q	 260 100

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethyl dodecanoate $C_{14}H_{28}O_2$ (ethyl laurate) [106-33-2] MMXKVMNBHPAILY-UHFFFAOYSA-N	7.7×10^{-3} 3.1×10^{-3}		Krop et al. (1997) Hilal et al. (2008)	V Q	
propyl dodecanoate $C_{15}H_{30}O_2$ (propyl laurate) [3681-78-5] FTBUKOLPOATXGV-UHFFFAOYSA-N	7.7×10^{-3} 2.1×10^{-3}		Krop et al. (1997) Hilal et al. (2008)	V Q	
2-hydroxypropyl dodecanoate $C_{15}H_{30}O_3$ [142-55-2] BHIZVZJETFVJMJ-UHFFFAOYSA-N	9.5×10^{-2}		Ebert et al. (2023)	?	319
dodecanoic acid, 2-hydroxy-1-methylethyl ester $C_{15}H_{30}O_3$ [107328-11-0] SVWZGNLBKFWCMV-UHFFFAOYSA-N	2.6×10^{1}		Ebert et al. (2023)	?	319
butyl dodecanoate $C_{16}H_{32}O_2$ (butyl laurate) [106-18-3] NDKYEUQMPZIGFN-UHFFFAOYSA-N	7.1×10^{-3} 1.5×10^{-3}		Krop et al. (1997) Hilal et al. (2008)	V Q	
2-ethylhexyl dodecanoate $C_{20}H_{40}O_2$ (2-ethylhexyl laurate) [20292-08-4] LWLRMRFJCCMNML-UHFFFAOYSA-N	3.0×10^{-3} 8.6×10^{-4}		Krop et al. (1997) Hilal et al. (2008)	V Q	
methyl tetradecanoate $C_{15}H_{30}O_2$ (methyl myristate) [124-10-7] ZAZKJZBWRNNLDS-UHFFFAOYSA-N	5.0×10^{-3} 1.9×10^{-3} 3.1×10^{-3}		Krop et al. (1997) HSDB (2015) Hilal et al. (2008)	V Q Q	 100
methyl hexadecanoate $C_{17}H_{34}O_2$ (methyl palmitate) [112-39-0] FLIACVVOZYBSBS-UHFFFAOYSA-N	2.9×10^{-3} 1.1×10^{-3} 1.8×10^{-3}		Krop et al. (1997) HSDB (2015) Hilal et al. (2008)	V Q Q	 100

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
isopropyl palmitate $C_{19}H_{38}O_2$ [142-91-6] XUGNVMKQXJXZCD-UHFFFAOYSA-N	2.1×10^{-4}		HSDB (2015)	Q	449
ascorbic palmitate $C_{22}H_{38}O_7$ [137-66-6] QAQJMLQRFWZOBN-LAUBAEHRSA-N	7.0×10^{1}		HSDB (2015)	Q	100
methyl octadecanoate $C_{19}H_{38}O_2$ (methyl stearate) [112-61-8] HPEUJPJOZXNMSJ-UHFFFAOYSA-N	1.7×10^{-3} 6.2×10^{-4} 1.1×10^{-3}		Krop et al. (1997) HSDB (2015) Hilal et al. (2008)	V Q Q	 100
methyl eicosanoate $C_{21}H_{42}O_2$ (methyl arachidate) [1120-28-1] QGBRLVONZXHAKJ-UHFFFAOYSA-N	1.0×10^{-3}		Krop et al. (1997)	V	
methyl docosanoate $C_{23}H_{46}O_2$ (methyl behenate) [929-77-1] QSQLTHHMFHEFIY-UHFFFAOYSA-N	5.9×10^{-4}		Krop et al. (1997)	V	
cyclopropanecarboxylic acid, methyl ester $C_5H_8O_2$ [2868-37-3] PKAHQJNJPDVTDP-UHFFFAOYSA-N	4.1×10^{-1} 1.1×10^{-1} 1.4×10^{-1}	6100	Bagno et al. (1991) Hilal et al. (2008) English and Carroll (2001)	T Q Q	475 231, 232
cyclohexanecarboxylic acid, methyl ester $C_6H_{11}COOCH_3$ [4630-82-4] ZQWPRMPSCMSAJU-UHFFFAOYSA-N	1.1×10^{-1} 1.1×10^{-1}	7200	Bagno et al. (1991) English and Carroll (2001)	T Q	475 231, 232
(*Z*,*Z*,*Z*)-9,12,15-octadecatrienoic acid, methyl ester $C_{19}H_{32}O_2$ (methyl linolenate) [301-00-8] DVWSXZIHSUZZKJ-YSTUJMKBSA-N	2.8×10^{-1} 7.2×10^{-3}		Krop et al. (1997) Hilal et al. (2008)	V Q	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(*Z*,*Z*)-9,12-octadecadienoic acid, methyl ester $C_{19}H_{34}O_2$ (methyl linolate) [112-63-0] WTTJVINHCBCLGX-NQLNTKRDSA-N	6.2×10^{-2} 4.8×10^{-3}		Krop et al. (1997) Hilal et al. (2008)	V Q	
(*Z*)-9-octadecenoic acid, methyl ester $C_{19}H_{36}O_2$ (methyl oleate) [112-62-9] QYDYPVFESGNLHU-KHPPLWFESA-N	1.3×10^{-2} 7.0×10^{-4} 2.5×10^{-3}		Krop et al. (1997) HSDB (2015) Hilal et al. (2008)	V Q Q	 100
(*Z*)-13-docosenoic acid, methyl ester $C_{23}H_{44}O_2$ (methyl erucate) [1120-34-9] ZYNDJIBBPLNPOW-KHPPLWFESA-N	5.3×10^{-3} 8.2×10^{-4}		Krop et al. (1997) Hilal et al. (2008)	V Q	
trans-quercus lactone $C_9H_{16}O_2$ (*trans*-whisky lactone) [105119-22-0] WNVCMFHPRIBNCW-SFYZADRCSA-N	3.5×10^{1}		Abney (2021)	Q	401
γ-decalactone $C_{10}H_{18}O_2$ [706-14-9] IFYYFLINQYPWGJ-UHFFFAOYSA-N	5.3×10^{1}		Abney (2021)	Q	401
γ-dodecalactone $C_{12}H_{22}O_2$ [2305-05-7] WGPCZPLRVAWXPW-UHFFFAOYSA-N	3.7×10^{1}		Abney (2021)	Q	401
oxacyclohexadecan-2-one $C_{15}H_{28}O_2$ (pentadecalactone) [106-02-5] FKUPPRZPSYCDRS-UHFFFAOYSA-N	4.0×10^{-3} 7.6×10^{-2}		Amoore and Buttery (1978) Amoore and Buttery (1978)	M V	
2-*tert*-butylcyclohexyl acetate $C_{12}H_{22}O_2$ [88-41-5] FINOAUDUYKVGDS-UHFFFAOYSA-N	9.9×10^{-3} 3.8×10^{-2} 5.3×10^{-1} 7.0×10^{-3}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hedione $C_{13}H_{22}O_3$ [24851-98-7] KVWWIYGFBYDJQC-UHFFFAOYSA-N	7.0×10^{1}		Dupeux et al. (2022)	Q	260
ethylene brassylate $C_{15}H_{26}O_4$ [105-95-3] XRHCAGNSDHCHFJ-UHFFFAOYSA-N	5.3×10^{1}		Dupeux et al. (2022)	Q	260
propyl 3-oxo-2-pentylcyclopentaneacetate $C_{15}H_{26}O_3$ [158474-72-7] IPDFPNNPBMREIF-UHFFFAOYSA-N	1.4×10^{1}		Ebert et al. (2023)	?	319
2-ethyl-3-oxo-butanoic acid, ethyl ester $C_8H_{14}O_3$ [607-97-6] OKANYBNORCUPKZ-UHFFFAOYSA-N	3.4		Hilal et al. (2008)	Q	
2-hydroxypropanoic acid, butyl ester	4.9		HSDB (2015)	V	
$C_7H_{14}O_3$	2.7		Wang et al. (2017)	Q	81, 239
[138-22-7]	2.9×10^{1}		Wang et al. (2017)	Q	81, 240
MRABAEUHTLLEML-UHFFFAOYSA-N	2.6		Wang et al. (2017)	Q	81, 241
	1.6		Raventos-Duran et al. (2010)	Q	272, 244
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	6.4×10^{1}		Hilal et al. (2008)	Q	
	4.3×10^{1}		Modarresi et al. (2007)	Q	68
methyl propenoate	5.0×10^{-2}		Duchowicz et al. (2020)	V	187
$C_4H_6O_2$	4.9×10^{-2}		HSDB (2015)	V	
(methyl acrylate)	5.2×10^{-2}		Mackay et al. (2006c)	V	
[96-33-3]	5.2×10^{-2}		Mackay et al. (1995)	V	
BAPJBEWLBFYGME-UHFFFAOYSA-N	5.8×10^{-2}		Yaws (2003)	X	238, 73
	6.3×10^{-1}		Duchowicz et al. (2020)	Q	
	7.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	6.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
	5.4×10^{-2}		Hilal et al. (2008)	Q	
	7.4×10^{-2}		Modarresi et al. (2007)	Q	68
	5.2×10^{-2}		Yaws (1999)	?	21, 73

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethyl propenoate	3.9×10^{-2}	4400	Brockbank (2013)	L	
$C_5H_8O_2$	2.9×10^{-2}		Duchowicz et al. (2020)	V	187
(ethyl acrylate)	2.9×10^{-2}		HSDB (2015)	V	
[140-88-5]	2.9×10^{-2}		Mackay et al. (2006c)	V	
JIGUQPWFLRLWPJ-UHFFFAOYSA-N	2.9×10^{-2}		Mackay et al. (1995)	V	
	3.9×10^{-2}		Yaws (2003)	X	259
	4.7×10^{-2}		Dupeux et al. (2022)	Q	260
	2.5×10^{-1}		Duchowicz et al. (2020)	Q	
	8.8×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	3.5×10^{-2}		Hilal et al. (2008)	Q	
	5.3×10^{-2}		Modarresi et al. (2007)	Q	68
	8.8×10^{-2}		Yao et al. (2002)	Q	230
	4.0×10^{-2}		Yaws (1999)	?	21
2-propenoic acid, butyl ester	1.5×10^{-2}		Duchowicz et al. (2020)	V	187
$C_7H_{12}O_2$	2.1×10^{-2}		HSDB (2015)	V	
(butyl acrylate)	2.9×10^{-1}		Duchowicz et al. (2020)	Q	
[141-32-2]	2.6×10^{-2}		Gharagheizi et al. (2012)	Q	
CQEYYJKEWSMYFG-UHFFFAOYSA-N	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.0×10^{-2}		Hilal et al. (2008)	Q	
	4.4×10^{-2}		Modarresi et al. (2007)	Q	68
	5.2×10^{-2}		Yao et al. (2002)	Q	230, 268
	1.7×10^{-2}		Yaws (1999)	?	21, 12
2-propenoic acid, 2-methylpropyl ester	1.3×10^{-2}		Duchowicz et al. (2020)	V	187
$C_7H_{12}O_2$	1.6×10^{-2}		HSDB (2015)	V	
(isobutyl acrylate)	1.1×10^{-1}		Duchowicz et al. (2020)	Q	
[106-63-8]	1.4×10^{-2}		Gharagheizi et al. (2012)	Q	
CFVWNXQPGQOHRJ-UHFFFAOYSA-N	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.4×10^{-2}		Hilal et al. (2008)	Q	
	3.4×10^{-2}		Modarresi et al. (2007)	Q	68
	3.9×10^{-2}		Yao et al. (2002)	Q	230
	1.5×10^{-2}		Yaws (1999)	?	21, 73

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-propenoic acid, 2-ethylhexyl ester	2.3×10^{-2}		Duchowicz et al. (2020)	V	187
$C_{11}H_{20}O_2$	2.3×10^{-2}		HSDB (2015)	V	
(2-ethylhexyl acrylate)	2.7×10^{-2}		Yaws (2003)	X	238, 73
[103-11-7]	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
GOXQRTZXKQZDDN-UHFFFAOYSA-N	6.2×10^{-3}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	68
	2.0×10^{-2}		Yao et al. (2002)	Q	230
	2.3×10^{-2}		Yaws (1999)	?	21, 73
2-propenoic acid, 2-hydroxyethyl ester	1.2×10^{3}		HSDB (2015)	V	
$C_5H_8O_3$					
(2-hydroxyethyl acrylate)					
[818-61-1]					
OMIGHNLMNHATMP-UHFFFAOYSA-N					
2-methyl-2-propenoic acid, ethyl ester	1.7×10^{-2}		Duchowicz et al. (2020)	V	187
$C_6H_{10}O_2$	1.7×10^{-2}		HSDB (2015)	V	
[97-63-2]	1.6×10^{-2}		Hilal et al. (2008)	C	
SUPCQIBBMFXVTL-UHFFFAOYSA-N	8.9×10^{-2}		Duchowicz et al. (2020)	Q	
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.9×10^{-2}		Hilal et al. (2008)	Q	
	3.5×10^{-2}		Modarresi et al. (2007)	Q	68
2-methyl-2-propenoic acid, 2-propenyl ester	2.4×10^{-2}		HSDB (2015)	Q	100
$C_7H_{10}O_2$					
(allyl methacrylate)					
[96-05-9]					
FBCQUCJYYPMKRO-UHFFFAOYSA-N					
2-methyl-2-propenoic acid, oxiranylmethyl ester	3.2×10^{1}		HSDB (2015)	Q	100
$C_7H_{10}O_3$					
(glycidyl methacrylate)					
[106-91-2]					
VOZRXNHHFUQHIL-UHFFFAOYSA-N					

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
allyl acetoacetate $C_7H_{10}O_3$ [1118-84-9] AXLMPTNTPOWPLT-UHFFFAOYSA-N	1.2×10^{1}		Ebert et al. (2023)	?	319
2-methyl-2-propenoic acid, propyl ester $C_7H_{12}O_2$ (propyl methacrylate) [2210-28-8] NHARPDSAXCBDDR-UHFFFAOYSA-N	1.8×10^{-2}		HSDB (2015)	Q	100
2-methyl-2-propenoic acid, butyl ester	2.0×10^{-2}		Duchowicz et al. (2020)	V	187
$C_8H_{14}O_2$	2.0×10^{-2}		HSDB (2015)	V	
(butyl methacrylate)	9.9×10^{-2}		Duchowicz et al. (2020)	Q	
[97-88-1]	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
SOGAXMICEFXMKE-UHFFFAOYSA-N	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.8×10^{-2}		Hilal et al. (2008)	Q	
	4.0×10^{-2}		Modarresi et al. (2007)	Q	68
2-methyl-2-propenoic acid, 2-methylpropyl ester	1.9×10^{-2}		Duchowicz et al. (2020)	V	187
$C_8H_{14}O_2$	1.9×10^{-2}		HSDB (2015)	V	
[97-86-9]	3.9×10^{-2}		Duchowicz et al. (2020)	Q	
RUMACXVDVNRZJZ-UHFFFAOYSA-N	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.1×10^{-2}		Hilal et al. (2008)	Q	
	2.7×10^{-2}		Modarresi et al. (2007)	Q	68
2-methyl-2-propenoic acid, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester $C_{14}H_{22}O_6$ [109-16-0] HWSSEYVMGDIFMH-UHFFFAOYSA-N	5.8×10^{6}		HSDB (2015)	Q	100
methyl methacrylate	2.9×10^{-2}	5300	Brockbank (2013)	L	1
$C_5H_8O_2$	4.3×10^{-2}	7700	Hiatt (2013)	M	
[80-62-6]	3.1×10^{-2}		Duchowicz et al. (2020)	V	187
VVQNEPGJFQJSBK-UHFFFAOYSA-N	3.1×10^{-2}		HSDB (2015)	V	
	3.1×10^{-2}	5300	Dohnal et al. (2010)	V	1
	3.1×10^{-2}		Mackay et al. (2006c)	V	
	3.0×10^{-2}		Lide and Frederikse (1995)	V	
	3.1×10^{-2}		Mackay et al. (1995)	V	
	2.4×10^{-1}		Duchowicz et al. (2020)	Q	
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	4.4×10^{-2}		Hilal et al. (2008)	Q	
	3.5×10^{-2}		Modarresi et al. (2007)	Q	68
			Burkholder et al. (2019)	W	516
			Burkholder et al. (2015)	W	517
(*E*)-3-hexenyl ethanoate $C_8H_{14}O_2$ [3681-82-1] NPFVOOAXDOBMCE-SNAWJCMRSA-N	3.3×10^{-2}		Karl et al. (2003)	M	
(*Z*)-3-hexenyl ethanoate $C_8H_{14}O_2$ [3681-71-8] NPFVOOAXDOBMCE-PLNGDYQASA-N	3.1×10^{-2}		Karl et al. (2003)	M	
ethenyl ethanoate $CH_3COOCHCH_2$ (vinyl acetate) [108-05-4] XTXRWKRVRITETP-UHFFFAOYSA-N	2.0×10^{-2}	4500	Burkholder et al. (2019)	L	
	2.0×10^{-2}	4500	Burkholder et al. (2015)	L	
	2.0×10^{-2}	4600	Brockbank (2013)	L	1
	2.0×10^{-2}	4400	Böhme et al. (2008)	M	
	1.9×10^{-2}		HSDB (2015)	V	
	2.0×10^{-2}	4600	Dohnal et al. (2010)	V	1
	1.6×10^{-2}		Mackay et al. (2006c)	V	
	2.0×10^{-2}		Lide and Frederikse (1995)	V	
	1.6×10^{-2}		Mackay et al. (1995)	V	
	2.0×10^{-2}		Yaws (2003)	X	259
	2.0×10^{-2}		Yaws (2003)	X	238
	1.7×10^{-2}		Goldstein (1982)	X	448
	1.7×10^{-2}	2600	Goldstein (1982)	X	299
	1.2×10^{-2}		Dupeux et al. (2022)	Q	260
	5.8×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	2.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
	6.9×10^{-2}		Hilal et al. (2008)	Q	
	6.6×10^{-2}		Modarresi et al. (2007)	Q	68
	2.0×10^{-2}		Yaws (1999)	?	21
(7*E*,9*Z*)-dodecadienyl acetate $C_{14}H_{24}O_2$ [54364-62-4] LLRZUAWETKPZJO-SCFJQAPRSA-N	1.2×10^{-2}		Ebert et al. (2023)	?	319

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(9*Z*,12*E*)-9,12-tetradecadienyl acetate $C_{16}H_{28}O_2$ [30507-70-1] ZZGJZGSVLNSDPG-FDTUMDBZSA-N	1.7×10^{-1}		Ebert et al. (2023)	?	319
isoambrettolide $C_{16}H_{28}O_2$ [28645-51-4] QILMAYXCYBTEDM-IWQZZHSRSA-N	2.5		Dupeux et al. (2022)	Q	260
vetyveryl acetate $C_{17}H_{26}O_2$ [117-98-6] UAVFEMBKDRODDE-UHFFFAOYSA-N	2.2		Dupeux et al. (2022)	Q	260
hydroprene $C_{17}H_{30}O_2$ [41096-46-2] FYQGBXGJFWXIPP-UEVLXMDPSA-N	5.1×10^{-2}		Ebert et al. (2023)	?	317
empenthrin $C_{18}H_{26}O_2$ [54406-48-3] YUGWDVYLFSETPE-UHFFFAOYSA-N	2.9×10^{-2}		Ebert et al. (2023)	?	317
3-(4-methoxyphenyl)-2-propenoic acid, 2-ethylhexyl ester $C_{18}H_{26}O_3$ (octinoxate) [5466-77-3] YBGZDTIWKVFICR-JLHYYAGUSA-N	1.2		HSDB (2015)	Q	449
kinoprene $C_{18}H_{28}O_2$ [42588-37-4] FZRBKIRIBLNOAM-WHVZTFIZSA-N	1.8×10^{-1}		Ebert et al. (2023)	?	317
allethrin $C_{19}H_{26}O_3$ [584-79-2] ZCVAOQKBXKSDMS-UHFFFAOYSA-N	6.0×10^{1}		Ebert et al. (2023)	?	319
S-methoprene $C_{19}H_{34}O_3$ [65733-16-6] NFGXHKASABOEEW-GYMWBFJFSA-N	1.5		Ebert et al. (2023)	?	319

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl benzoate	2.9×10^{-1}	6400	Brockbank (2013)	L	1
$C_6H_5COOCH_3$	3.0×10^{-1}		Duchowicz et al. (2020)	V	187
[93-58-3]	3.0×10^{-1}		HSDB (2015)	V	
QPJVMBTYPHYUOC-UHFFFAOYSA-N	3.0×10^{-1}		Mackay et al. (2006c)	V	
	3.0×10^{-1}		Mackay et al. (1995)	V	
	2.8×10^{-1}		Meylan and Howard (1991)	V	
	5.6×10^{-1}		Hine and Mookerjee (1975)	V	
	3.1×10^{-1}		Abraham et al. (1994a)	R	
	5.8×10^{-1}	6300	Bagno et al. (1991)	T	475
	2.8×10^{-1}		Yaws (2003)	X	259
	2.6×10^{-1}		Dupeux et al. (2022)	Q	260
	1.4		Duchowicz et al. (2020)	Q	
	2.9×10^{-1}		Zhang et al. (2010)	Q	288, 289
	3.6×10^{-1}		Zhang et al. (2010)	Q	288, 290
	9.5×10^{-1}		Zhang et al. (2010)	Q	288, 291
	6.1×10^{-1}		Zhang et al. (2010)	Q	288, 292
	2.9×10^{-1}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Modarresi et al. (2007)	Q	68
		5100	Kühne et al. (2005)	Q	
	3.2×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	6.8×10^{-1}		Yao et al. (2002)	Q	230
	1.1		English and Carroll (2001)	Q	231, 275
	3.0×10^{-1}		Katritzky et al. (1998)	Q	
	5.6×10^{-1}		Suzuki et al. (1992)	Q	233
	2.8×10^{-1}		Meylan and Howard (1991)	Q	
	2.7×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
		3500	Kühne et al. (2005)	?	
	2.8×10^{-1}		Yaws (1999)	?	21
	5.6×10^{-1}		Abraham et al. (1990)	?	
ethyl benzoate	1.7×10^{-1}	6300	Brockbank (2013)	L	1
$C_6H_5COOC_2H_5$	1.3×10^{-1}		Duchowicz et al. (2020)	V	187
[93-89-0]	9.7×10^{-2}		Mackay et al. (2006c)	V	
MTZQAGJQAFMTAQ-UHFFFAOYSA-N	9.7×10^{-2}		Mackay et al. (1995)	V	
	1.9×10^{-1}		Abraham et al. (1994a)	R	
	1.4×10^{-1}		Yaws (2003)	X	259
	1.5×10^{-1}		Dupeux et al. (2022)	Q	260
	5.2×10^{-1}		Duchowicz et al. (2020)	Q	
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	2.1×10^{-1}		Zhang et al. (2010)	Q	288, 289
	2.1×10^{-1}		Zhang et al. (2010)	Q	288, 290
	5.1×10^{-1}		Zhang et al. (2010)	Q	288, 291
	4.8×10^{-1}		Zhang et al. (2010)	Q	288, 292
	1.9×10^{-1}		Hilal et al. (2008)	Q	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{-1}		Modarresi et al. (2007)	Q	68
	1.9×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	6.7×10^{-1}		English and Carroll (2001)	Q	231, 232
	5.1×10^{-1}		Katritzky et al. (1998)	Q	
	2.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.4×10^{-1}		Yaws (1999)	?	21
	1.9×10^{-1}		Abraham et al. (1990)	?	
2-hydroxybenzoic acid methyl ester	1.6	9500	Brockbank (2013)	L	1
$C_8H_8O_3$	3.3×10^{-1}		Karl et al. (2008)	M	
(methyl salicylate)	1.0×10^{-1}		Duchowicz et al. (2020)	V	187
[119-36-8]	1.1×10^{1}		HSDB (2015)	V	
OSWPMRLSEDHDFF-UHFFFAOYSA-N	7.8		Duchowicz et al. (2020)	Q	
	1.8×10^{1}		Hilal et al. (2008)	Q	
	9.3		Modarresi et al. (2007)	Q	68
	1.0×10^{-1}		Bartelt-Hunt et al. (2008)	?	21
	1.0		Yaws (1999)	?	21, 38
benzoic acid, 4-methyl-, methyl ester	2.6×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_9H_{10}O_2$	3.9×10^{-1}		Zhang et al. (2010)	Q	288, 290
[99-75-2]	1.7		Zhang et al. (2010)	Q	288, 291
QSSJZLPUHJDYKF-UHFFFAOYSA-N	3.5×10^{-1}		Zhang et al. (2010)	Q	288, 292
acetylsalicylic acid	7.6×10^{3}		Duchowicz et al. (2020)	V	187
$C_9H_8O_4$	1.5×10^{4}		Duchowicz et al. (2020)	Q	
(aspirin)	1.5×10^{5}		Abraham et al. (2019)	Q	
[50-78-2]	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	272, 244
BSYNRYMUTXBXSQ-UHFFFAOYSA-N	4.9×10^{4}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{3}		Raventos-Duran et al. (2010)	Q	246
1,4-benzenedicarboxylic acid, dimethyl ester	7.4×10^{-2}		Duchowicz et al. (2020)	V	187
$C_{10}H_{10}O_4$	7.6×10^{-2}		HSDB (2015)	V	
[120-61-6]	2.2×10^{2}		Duchowicz et al. (2020)	Q	
WOZVHXUHUFLZGK-UHFFFAOYSA-N	4.4×10^{1}		Zhang et al. (2010)	Q	288, 289
	1.3×10^{2}		Zhang et al. (2010)	Q	288, 290
	5.3×10^{1}		Zhang et al. (2010)	Q	288, 291
	9.2×10^{1}		Zhang et al. (2010)	Q	288, 292
	2.4		Modarresi et al. (2007)	Q	68
butyl benzoate	2.5×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{11}H_{14}O_2$	1.0×10^{-1}		Dupeux et al. (2022)	Q	260
[136-60-7]	5.7×10^{-1}		Duchowicz et al. (2020)	Q	
XSIFPSYPOVKYCO-UHFFFAOYSA-N	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-1}		Zhang et al. (2010)	Q	288, 289

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.0×10^{-1}		Zhang et al. (2010)	Q	288, 290
	5.2×10^{-1}		Zhang et al. (2010)	Q	288, 291
	3.2×10^{-1}		Zhang et al. (2010)	Q	288, 292
	8.3×10^{-2}		Modarresi et al. (2007)	Q	68
diphenyl carbonate	1.2×10^{-1}		HSDB (2015)	Q	100
$C_{13}H_{10}O_3$	1.2×10^{-1}		Zhang et al. (2010)	Q	288, 289
[102-09-0]	1.6×10^{1}		Zhang et al. (2010)	Q	288, 290
ROORDVPLFPIABK-UHFFFAOYSA-N	9.5×10^{-1}		Zhang et al. (2010)	Q	288, 291
	1.2×10^{2}		Zhang et al. (2010)	Q	288, 292
benzyl benzoate	1.8		Mackay et al. (2006c)	V	
$C_{14}H_{12}O_2$	1.8		Mackay et al. (1995)	V	
[120-51-4]	1.7		Dupeux et al. (2022)	Q	260
SESFRYSPDFLNCH-UHFFFAOYSA-N					
trans-ethylcinnamate	2.3		Duchowicz et al. (2020)	V	187
$C_{11}H_{12}O_2$	1.4		Abney (2021)	Q	401
[103-36-6]	6.5×10^{-1}		Duchowicz et al. (2020)	Q	
KBEBGUQPQBELIU-CMDGGOBGSA-N					
dipropylene glycol dibenzoate	7.2×10^{2}		Duchowicz et al. (2020)	V	187
$C_{20}H_{22}O_5$	9.4×10^{2}		Duchowicz et al. (2020)	Q	
[27138-31-4]					
CGLQOIMEUPORRI-UHFFFAOYSA-N					
dimethyl phthalate	5.1×10^{1}	8000	Brockbank (2013)	L	1
$C_{10}H_{10}O_4$	2.3×10^{1}		Chao et al. (2017)	M	
[131-11-3]	5.0×10^{1}		Duchowicz et al. (2020)	V	187
NIQCNGHVCWTJSM-UHFFFAOYSA-N	4.9×10^{1}		HSDB (2015)	V	
	9.3×10^{1}		Mackay et al. (2006c)	V	
	2.0×10^{1}		Saçan et al. (2005)	V	
	1.0×10^{2}		Cousins and Mackay (2000)	V	
	8.1×10^{1}		Staples et al. (1997)	V	
	9.1×10^{1}		Lide and Frederikse (1995)	V	
	9.1×10^{1}		Mackay et al. (1995)	V	
	5.0×10^{1}		Hwang et al. (1992)	V	
	9.0		Wolfe et al. (1980)	V	
	8.8×10^{1}		Yaws (2003)	X	238, 12
	2.9×10^{1}		Goldstein (1982)	X	448
	3.0×10^{1}	5700	Goldstein (1982)	X	299
	2.3×10^{1}		McCarty (1980)	X	370
	5.0×10^{1}		Ryan et al. (1988)	C	
	2.2×10^{2}		Duchowicz et al. (2020)	Q	
	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{2}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	246
	8.2×10^{1}		Gharagheizi et al. (2010)	Q	247
	1.7×10^{2}		Hilal et al. (2008)	Q	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.6		Saçan et al. (2005)	Q	
	5.4×10^{1}		Yaws (1999)	?	21, 12
1,4-cyclohexanedicarboxylic acid, dimethyl ester $C_{10}H_{16}O_4$ (dimethyl hexahydroterephthalate) [94-60-0] LNGAGQAGYITKCW-UHFFFAOYSA-N	1.0×10^{2}		HSDB (2015)	V	
1,3-benzenedicarboxylic acid, dimethyl ester $C_{10}H_{10}O_4$ (dimethyl isophthalate) [1459-93-4] VNGOYPQMJFJDLV-UHFFFAOYSA-N	1.6×10^{2}		HSDB (2015)	Q	100
diethyl phthalate $C_{12}H_{14}O_4$ [84-66-2] FLKPEMZONWLCSK-UHFFFAOYSA-N	6.0×10^{1}	10000	Brockbank (2013)	L	1
	2.2×10^{1}		Chao et al. (2017)	M	
	1.6×10^{1}		Duchowicz et al. (2020)	V	187
	1.6×10^{1}		HSDB (2015)	V	
	2.2×10^{1}		Mackay et al. (2006c)	V	
	4.1×10^{1}		Cousins and Mackay (2000)	V	
	3.7×10^{1}		Staples et al. (1997)	V	
	2.1×10^{1}		Lide and Frederikse (1995)	V	
	1.0×10^{2}		Mackay et al. (1995)	V	
	4.9×10^{2}		Wolfe et al. (1980)	V	
	6.9×10^{1}		Yaws (2003)	X	238
	1.2×10^{1}		Goldstein (1982)	X	448
	1.2×10^{1}	5600	Goldstein (1982)	X	299
	2.1×10^{-1}		Ryan et al. (1988)	C	
	5.8×10^{-1}		Petrasek et al. (1983)	C	
	3.4×10^{1}		Duchowicz et al. (2020)	Q	
	1.5×10^{1}		Gharagheizi et al. (2012)	Q	
	2.5×10^{1}		Zhang et al. (2010)	Q	288, 289
	1.5×10^{2}		Zhang et al. (2010)	Q	288, 290
	2.7×10^{2}		Zhang et al. (2010)	Q	288, 291
	5.6×10^{1}		Zhang et al. (2010)	Q	288, 292
	6.5×10^{1}		Gharagheizi et al. (2010)	Q	247
	7.7×10^{1}		Hilal et al. (2008)	Q	
		12000	Kühne et al. (2005)	Q	
	5.8		Saçan et al. (2005)	Q	
	2.1×10^{1}		Yao et al. (2002)	Q	230
	1.6×10^{1}		Bartelt-Hunt et al. (2008)	?	21
		12000	Kühne et al. (2005)	?	
	6.9×10^{1}		Yaws (1999)	?	21

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dipropyl phthalate	2.2×10^{1}		Brockbank (2013)	L	
$C_{14}H_{18}O_4$	2.4×10^{1}		Duchowicz et al. (2020)	V	187
[131-16-8]	1.8×10^{1}		Cousins and Mackay (2000)	V	518
MQHNKCZKNAJROC-UHFFFAOYSA-N	3.3		Cousins and Mackay (2000)	V	518
	3.2×10^{1}		Staples et al. (1997)	V	
	4.1×10^{1}		Duchowicz et al. (2020)	Q	
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	272, 244
	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	246
	2.4×10^{1}		Saçan et al. (2005)	Q	
diallyl phthalate	3.5×10^{1}		Saçan et al. (2005)	V	
$C_{14}H_{14}O_4$	2.3×10^{1}		Cousins and Mackay (2000)	V	
[131-17-9]	3.5×10^{1}		Staples et al. (1997)	V	
QUDWYFHPNIMBFC-UHFFFAOYSA-N	2.5×10^{1}		HSDB (2015)	Q	100
	1.7×10^{1}		Saçan et al. (2005)	Q	
bis(2-methoxyethyl) phthalate	2.3×10^{1}		Fishbein and Albro (1972)	V	12
$C_{14}H_{18}O_5$	3.5×10^{7}		HSDB (2015)	Q	100
[117-82-8]					
HSUIVCLOAAJSRE-UHFFFAOYSA-N					
dibutyl phthalate	1.1×10^{1}	12000	Brockbank (2013)	L	1, 519
$C_{16}H_{22}O_4$	9.3		Lee et al. (2012)	M	
[84-74-2]	5.5		Atlas et al. (1983)	M	73
DOIRQSBPFJWKBE-UHFFFAOYSA-N	2.2×10^{1}		Mackay et al. (2006c)	V	
	2.7×10^{1}		Saçan et al. (2005)	V	
	7.5		Cousins and Mackay (2000)	V	
	1.1×10^{1}		Staples et al. (1997)	V	
	2.2×10^{1}		Lide and Frederikse (1995)	V	
	2.0×10^{1}		Mackay et al. (1995)	V	
	2.6×10^{2}		Hwang et al. (1992)	V	
	7.6		Wolfe et al. (1980)	V	
	5.6×10^{1}		Yaws (2003)	X	238, 12
	1.6×10^{-1}		McCarty (1980)	X	370
	3.4×10^{1}		Ryan et al. (1988)	C	
	5.6×10^{1}		Gharagheizi et al. (2010)	Q	247
	2.9×10^{1}		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	68
		14000	Kühne et al. (2005)	Q	
	3.7×10^{1}		Saçan et al. (2005)	Q	
		13000	Kühne et al. (2005)	?	
	2.7×10^{1}		Yaws (1999)	?	21, 12
diisobutyl phthalate	3.5		HSDB (2015)	V	
$C_{16}H_{22}O_4$	7.5		Cousins and Mackay (2000)	V	
[84-69-5]	5.4×10^{1}		Staples et al. (1997)	V	
MGWAVDBGNNKXQV-UHFFFAOYSA-N	3.1×10^{1}		Saçan et al. (2005)	Q	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-benzenedicarboxylic acid, butyl cyclohexyl ester $C_{18}H_{24}O_4$ (butyl cyclohexyl phthalate) [84-64-0] BHKLONWXRPJNAE-UHFFFAOYSA-N	1.0×10^{1}		HSDB (2015)	Q	100
butyl glycolyl butyl phthalate $C_{18}H_{24}O_6$ [85-70-1] GOJCZVPJCKEBQV-UHFFFAOYSA-N	4.7×10^{2}		HSDB (2015)	Q	100
diamyl phthalate $C_{18}H_{26}O_4$ [131-18-0] IPKKHRVROFYTEK-UHFFFAOYSA-N	1.1×10^{1}		HSDB (2015)	Q	100
butyl benzyl phthalate	1.0×10^{2}		Lee et al. (2012)	M	
$C_{19}H_{20}O_4$	7.8		Duchowicz et al. (2020)	V	187
[85-68-7]	7.6		HSDB (2015)	V	
IRIAEXORFWYRCZ-UHFFFAOYSA-N	7.5		Mackay et al. (2006c)	V	
	1.9×10^{1}		Saçan et al. (2005)	V	
	4.9		Cousins and Mackay (2000)	V	
	1.3×10^{1}		Staples et al. (1997)	V	
	7.8		Mackay et al. (1995)	V	
	9.6		Ryan et al. (1988)	C	
	2.9×10^{2}		Duchowicz et al. (2020)	Q	
	3.2×10^{1}		Saçan et al. (2005)	Q	
	>9.9		Petrasek et al. (1983)	E	
dihexyl phthalate	8.3		Brockbank (2013)	L	
$C_{20}H_{30}O_4$	3.8×10^{-1}		Duchowicz et al. (2020)	V	187
[84-75-3]	3.8×10^{-1}		HSDB (2015)	V	
KCXZNSGUUQJJTR-UHFFFAOYSA-N	1.4		Cousins and Mackay (2000)	V	
	2.2×10^{-1}		Staples et al. (1997)	V	
	5.5×10^{1}		Duchowicz et al. (2020)	Q	
	1.6×10^{1}		Saçan et al. (2005)	Q	
butyl 2-ethylhexyl phthalate	2.1		Cousins and Mackay (2000)	V	
$C_{20}H_{30}O_4$	2.5×10^{1}		Staples et al. (1997)	V	
[85-69-8]	4.7		HSDB (2015)	Q	100
AVOLBYOSCILFLL-UHFFFAOYSA-N	6.9×10^{1}		Saçan et al. (2005)	Q	
diphenyl terephthalate	3.2×10^{2}		Zhang et al. (2010)	Q	288, 289
$C_{20}H_{14}O_4$	4.3×10^{4}		Zhang et al. (2010)	Q	288, 290
[1539-04-4]	2.7×10^{4}		Zhang et al. (2010)	Q	288, 291
HPGJOUYGWKFYQW-UHFFFAOYSA-N	7.7×10^{4}		Zhang et al. (2010)	Q	288, 292

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dicyclohexyl phthalate	9.9×10^{1}		Duchowicz et al. (2020)	V	187
$C_{20}H_{26}O_4$	9.9×10^{1}		HSDB (2015)	V	
[84-61-7]	4.8×10^{2}		Duchowicz et al. (2020)	Q	
VOWAEIGWURALJQ-UHFFFAOYSA-N					
bis(2-butoxyethyl) phthalate	4.9×10^{6}		HSDB (2015)	Q	100
$C_{20}H_{30}O_6$					
[117-83-9]					
CMCJNODIWQEOAI-UHFFFAOYSA-N					
diheptyl phthalate	5.9×10^{-1}		Cousins and Mackay (2000)	V	
$C_{22}H_{34}O_4$	2.8		HSDB (2015)	Q	100
[3648-21-3]	8.9×10^{-1}		Saçan et al. (2005)	Q	
JQCXWCOOWVGKMT-UHFFFAOYSA-N					
dioctyl phthalate	3.8		Duchowicz et al. (2020)	V	187
$C_{24}H_{38}O_4$	3.8		HSDB (2015)	V	
[117-84-0]	9.6×10^{-2}		Mackay et al. (2006c)	V	
MQIUGAXCHLFZKX-UHFFFAOYSA-N	2.5×10^{-1}		Cousins and Mackay (2000)	V	
	9.6×10^{-2}		Staples et al. (1997)	V	
	1.8		Mackay et al. (1995)	V	
	1.8		Wolfe et al. (1980)	V	
	8.9×10^{1}		Yaws (2003)	X	238, 80
	3.4×10^{1}		Ryan et al. (1988)	C	
	6.2×10^{1}		Duchowicz et al. (2020)	Q	
	7.2×10^{1}		Gharagheizi et al. (2010)	Q	247
	6.4		Saçan et al. (2005)	Q	
	>9.9		Petrasek et al. (1983)	E	
	7.6×10^{1}		Yaws (1999)	?	21, 80
diisooctyl phthalate	3.1×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{24}H_{38}O_4$	3.2×10^{-1}		HSDB (2015)	V	
[27554-26-3]	2.5×10^{-1}		Cousins and Mackay (2000)	V	
IJFPVINAQGWBRJ-UHFFFAOYSA-N	9.5		Duchowicz et al. (2020)	Q	
	1.5×10^{2}		Saçan et al. (2005)	Q	
decyl hexyl phthalate	1.6×10^{2}		Saçan et al. (2005)	Q	
$C_{24}H_{38}O_4$					
[25724-58-7]					
OMQBXAQAHHFSST-UHFFFAOYSA-N					
bis(2-ethylhexyl)-phthalate	3.7×10^{1}		Duchowicz et al. (2020)	V	187
$C_{24}H_{38}O_4$	3.7×10^{1}		HSDB (2015)	V	
(DEHP)	5.8×10^{-1}		Mackay et al. (2006c)	V	
[117-81-7]	1.4×10^{1}		Saçan et al. (2005)	V	
BJQHLKABXJIVAM-UHFFFAOYSA-N	2.5×10^{-1}		Cousins and Mackay (2000)	V	
	5.8×10^{-1}		Staples et al. (1997)	V	
	3.7×10^{1}		Mackay et al. (1995)	V	
	6.7×10^{-1}		Meylan and Howard (1991)	V	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.4×10^{-2}		Riederer (1990)	V	
	2.2×10^{1}		Wolfe et al. (1980)	V	
	3.4×10^{1}		Ryan et al. (1988)	C	
	8.2×10^{1}		Petrasek et al. (1983)	C	
	9.5		Duchowicz et al. (2020)	Q	
	2.5×10^{1}		Saçan et al. (2005)	Q	
	8.4×10^{-1}		Meylan and Howard (1991)	Q	
	3.7×10^{1}		Bartelt-Hunt et al. (2008)	?	21
bis(2-ethylhexyl) terephthalate $C_{24}H_{38}O_4$ [6422-86-2] RWPICVVBGZBXNA-UHFFFAOYSA-N	9.9×10^{-1}		HSDB (2015)	Q	100
dinonyl phthalate $C_{26}H_{42}O_4$ [84-76-4] DROMNWUQASBTFM-UHFFFAOYSA-N	1.1×10^{-1}		Cousins and Mackay (2000)	V	
	7.0×10^{-1}		HSDB (2015)	Q	100
	3.0×10^{1}		Saçan et al. (2005)	Q	
diisononyl phthalate $C_{26}H_{42}O_4$ [28553-12-0] HBGGXOJOCNVPFY-UHFFFAOYSA-N	6.6		Duchowicz et al. (2020)	V	187
	6.6		HSDB (2015)	V	
	1.1×10^{-1}		Cousins and Mackay (2000)	V	
	9.9		Duchowicz et al. (2020)	Q	
	3.3×10^{1}		Saçan et al. (2005)	Q	
didecyl phthalate $C_{28}H_{46}O_4$ [84-77-5] PGIBJVOPLXHHGS-UHFFFAOYSA-N	4.6×10^{-2}		Cousins and Mackay (2000)	V	
	3.5×10^{-1}		HSDB (2015)	Q	100
diisodecyl phthalate $C_{28}H_{46}O_4$ [26761-40-0] ZVFDTKUVRCTHQE-UHFFFAOYSA-N	8.9		Duchowicz et al. (2020)	V	187
	9.0		HSDB (2015)	V	
	3.8×10^{1}		Saçan et al. (2005)	V	
	4.6×10^{-2}		Cousins and Mackay (2000)	V	
	1.1×10^{1}		Yaws (2003)	X	238, 80
	1.0×10^{1}		Duchowicz et al. (2020)	Q	
	1.3×10^{1}		Gharagheizi et al. (2010)	Q	247
	2.4×10^{1}		Saçan et al. (2005)	Q	
	8.9		Yaws (1999)	?	21, 80
diundecyl phthalate $C_{30}H_{50}O_4$ [3648-20-2] QQVHEQUEHCEAKS-UHFFFAOYSA-N	3.3×10^{1}		Saçan et al. (2005)	V	
	2.0×10^{-2}		Cousins and Mackay (2000)	V	
	1.8×10^{-1}		HSDB (2015)	Q	100
	1.4×10^{1}		Saçan et al. (2005)	Q	
ditridecyl phthalate $C_{34}H_{58}O_4$ [119-06-2] YCZJVRCZIPDYHH-UHFFFAOYSA-N	3.6×10^{-3}		Cousins and Mackay (2000)	V	
	4.5×10^{-2}		HSDB (2015)	Q	100
	7.9×10^{1}		Saçan et al. (2005)	Q	

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethanedioic acid, dimethyl ester	3.4		Duchowicz et al. (2020)	V	187
$C_4H_6O_4$	2.6×10^{1}		Duchowicz et al. (2020)	Q	
(dimethyl oxalate)	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
[553-90-2]	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	245
LOMVENUNSWAXEN-UHFFFAOYSA-N	3.9		Raventos-Duran et al. (2010)	Q	246
	6.9		Hilal et al. (2008)	Q	
	4.6×10^{-1}		Modarresi et al. (2007)	Q	68
ethanedioic acid, diethyl ester	4.5		Duchowicz et al. (2020)	V	187
$C_6H_{10}O_4$	6.4		Duchowicz et al. (2020)	Q	
[95-92-1]					
WYACBZDAHNBPPB-UHFFFAOYSA-N					
propanedioic acid, dimethyl ester	3.8×10^{1}	11000	Katrib et al. (2003)	M	
$C_5H_8O_4$					
(dimethyl malonate)					
[108-59-8]					
BEPAFCGSDWSTEL-UHFFFAOYSA-N					
propanedioic acid, diethyl ester	3.9	7500	Brockbank (2013)	L	1
$C_7H_{12}O_4$	4.7		Duchowicz et al. (2020)	V	187
(diethyl malonate)	7.9		Duchowicz et al. (2020)	Q	
[105-53-3]	2.0		Raventos-Duran et al. (2010)	Q	243, 244
IYXGSMUGOJNHAZ-UHFFFAOYSA-N	4.9		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	246
	3.9		Hilal et al. (2008)	Q	
	5.0×10^{-1}		Modarresi et al. (2007)	Q	68
		5900	Kühne et al. (2005)	Q	
	4.2		Bartelt-Hunt et al. (2008)	?	21
		6400	Kühne et al. (2005)	?	
	4.1		Yaws (1999)	?	21, 14
butanedioic acid, dimethyl ester	3.0×10^{1}	8500	Katrib et al. (2003)	M	
$C_6H_{10}O_4$	1.5×10^{2}		HSDB (2015)	Q	100
(dimethyl succinate)		7100	Kühne et al. (2005)	Q	
[106-65-0]		7000	Kühne et al. (2005)	?	
MUXOBHXGJLMRAB-UHFFFAOYSA-N					
diethyl succinate	1.9×10^{1}		Duchowicz et al. (2020)	V	187
$C_8H_{14}O_4$	9.3		Duchowicz et al. (2020)	Q	
[123-25-1]	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
DKMROQRQHGEIOW-UHFFFAOYSA-N	4.9		Raventos-Duran et al. (2010)	Q	245
	9.9		Raventos-Duran et al. (2010)	Q	246
	4.0		Hilal et al. (2008)	Q	
	1.3		Modarresi et al. (2007)	Q	68

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(Z)-2-butenedioic acid dimethyl ester	1.4×10^{1}		Duchowicz et al. (2020)	V	187
$C_6H_8O_4$	5.2×10^{1}		Duchowicz et al. (2020)	Q	
(dimethyl maleate)	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	272, 244
[624-48-6]	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
LDCRTTXIJACKKU-ARJAWSKDSA-N	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	246
	2.3×10^{1}		Hilal et al. (2008)	Q	
	1.6		Modarresi et al. (2007)	Q	68
(E)-2-butenedioic acid dimethyl ester	1.4×10^{1}		HSDB (2015)	Q	100
$C_6H_8O_4$					
(dimethyl fumarate)					
[624-49-7]					
LDCRTTXIJACKKU-ONEGZZNKSA-N					
pentanedioic acid, dimethyl ester	1.5×10^{1}		Duchowicz et al. (2020)	V	187
$C_7H_{12}O_4$	6.9×10^{1}		Duchowicz et al. (2020)	Q	
[1119-40-0]					
XTDYIOOONNVFMA-UHFFFAOYSA-N					
diethyl glutarate	1.7×10^{1}		Ebert et al. (2023)	?	317
$C_9H_{16}O_4$					
[818-38-2]					
OUWSNHWQZPEFEX-UHFFFAOYSA-N					
diethyl pimelate	2.2×10^{1}		Duchowicz et al. (2020)	V	187
$C_{11}H_{20}O_4$	1.3×10^{1}		Duchowicz et al. (2020)	Q	
[2050-20-6]	1.5		Hilal et al. (2008)	Q	
LKKOGZVQGQUVHF-UHFFFAOYSA-N	8.6×10^{-1}		Modarresi et al. (2007)	Q	68
	2.2×10^{1}		Bartelt-Hunt et al. (2008)	?	21
1,3-benzenedicarboxylic acid, diethyl ester	2.5×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_{14}O_4$	1.9×10^{1}		Zhang et al. (2010)	Q	288, 290
[636-53-3]	2.9×10^{7}		Zhang et al. (2010)	Q	288, 291
JLVWYWVLMFVCDI-UHFFFAOYSA-N	5.6×10^{1}		Zhang et al. (2010)	Q	288, 292
dibutyl maleate	2.6×10^{1}		Duchowicz et al. (2020)	V	187
$C_{12}H_{20}O_4$	1.5×10^{1}		Duchowicz et al. (2020)	Q	
[105-76-0]	2.5		Raventos-Duran et al. (2010)	Q	272, 244
JBSLOWBPDRZSMB-FPLPWBNLSA-N	4.9		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	246
dimethyl sebacate	1.8×10^{1}		Ebert et al. (2023)	?	317
$C_{12}H_{22}O_4$					
(decanedioic acid, dimethyl ester)					
[106-79-6]					
ALOUNLDAKADEEB-UHFFFAOYSA-N					

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,6-naphthalenedicarboxylic acid, dimethyl ester	4.5×10^{2}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_{12}O_4$	2.5×10^{3}		Zhang et al. (2010)	Q	288, 290
[840-65-3]	2.6×10^{7}		Zhang et al. (2010)	Q	288, 291
GYUVMLBYMPKZAZ-UHFFFAOYSA-N	1.3×10^{3}		Zhang et al. (2010)	Q	288, 292
diisooctyl adipate	1.9×10^{-1}		HSDB (2015)	Q	100
$C_{22}H_{42}O_4$					
[1330-86-5]					
CJFLBOQMPJCWLR-UHFFFAOYSA-N					
di-(2-ethylhexyl)-adipate	2.3×10^{1}		Felder et al. (1986)	M	88
$C_{22}H_{42}O_4$	4.3×10^{-1}		Hilal et al. (2008)	Q	
[103-23-1]	4.0×10^{-1}		Modarresi et al. (2007)	Q	68
SAOKZLXYCUGLFA-UHFFFAOYSA-N					
peroxybenzoic acid, *tert*-butyl ester	4.7×10^{-2}		HSDB (2015)	Q	100
$C_{11}H_{14}O_3$	4.7×10^{-2}		Zhang et al. (2010)	Q	288, 289
[614-45-9]	1.8×10^{-1}		Zhang et al. (2010)	Q	288, 290
GJBRNHKUVLOCEB-UHFFFAOYSA-N	8.2		Zhang et al. (2010)	Q	288, 291
	5.4		Zhang et al. (2010)	Q	288, 292
neodecaneperoxoic acid, 1,1-dimethylethyl ester	9.9×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_{28}O_3$	4.7×10^{-3}		Zhang et al. (2010)	Q	288, 290
[26748-41-4]	1.2×10^{-1}		Zhang et al. (2010)	Q	288, 291
NMOALOSNPWTWRH-UHFFFAOYSA-N	2.3×10^{-2}		Zhang et al. (2010)	Q	288, 292
neoheptaneperoxoic acid, 1-methyl-1-phenylethyl ester	3.8×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_{24}O_3$	9.0×10^{-2}		Zhang et al. (2010)	Q	288, 290
[130097-36-8]	2.5		Zhang et al. (2010)	Q	288, 291
WFAUFYAGXAXBEG-UHFFFAOYSA-N	1.3		Zhang et al. (2010)	Q	288, 292
hydroxypropyl acrylate	5.8×10^{3}		HSDB (2015)	Q	100
$C_6H_{10}O_3$					
[25584-83-2]					
AYEFIAVHMUFQPZ-UHFFFAOYSA-N					
2-hydroxyethyl methacrylate	4.6×10^{1}		Duchowicz et al. (2020)	V	187
$C_6H_{10}O_3$	6.6×10^{1}		Duchowicz et al. (2020)	Q	
[868-77-9]	2.1×10^{3}		HSDB (2015)	Q	100
WOBHKFSMXKNTIM-UHFFFAOYSA-N					
2-hydroxypropyl acrylate	1.6×10^{3}		HSDB (2015)	Q	100
$C_6H_{10}O_3$					
[999-61-1]					
GWZMWHWAWHPNHN-UHFFFAOYSA-N					

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexanedioic acid, dimethyl ester	4.3		Duchowicz et al. (2020)	V	187
$C_8H_{14}O_4$	8.1×10^1		Duchowicz et al. (2020)	Q	
(dimethyl adipate)	1.0×10^1		HSDB (2015)	Q	100
[627-93-0]	6.0		Bartelt-Hunt et al. (2008)	?	21
UDSFAEKRVUSQDD-UHFFFAOYSA-N					
methyl 4-hydroxybenzoate	4.5×10^3		HSDB (2015)	Q	100
$C_8H_8O_3$					
(methylparaben)					
[99-76-3]					
LXCFILQKKLGQFO-UHFFFAOYSA-N					
diethyl fumarate	4.1×10^2		HSDB (2015)	Q	100
$C_8H_{12}O_4$					
[623-91-6]					
IEPRKVQEAMIZSS-AATRIKPKSA-N					
diethyl adipate	2.7		Duchowicz et al. (2020)	V	187
$C_{10}H_{18}O_4$	2.7		HSDB (2015)	V	
[141-28-6]	1.2×10^1		Duchowicz et al. (2020)	Q	
VIZORQUEIQEFRT-UHFFFAOYSA-N	3.7		Bartelt-Hunt et al. (2008)	?	21
propyl 4-hydroxybenzoate	1.5×10^3		HSDB (2015)	Q	100
$C_{10}H_{12}O_3$					
(propylparaben)					
[94-13-3]					
QELSKZZBTMNZEB-UHFFFAOYSA-N					
diethylene glycol diacrylate	1.0×10^4		HSDB (2015)	Q	100
$C_{10}H_{14}O_5$					
[4074-88-8]					
LEJBBGNFPAFPKQ-UHFFFAOYSA-N					
(2,2-dimethyl-3-prop-2-enoyloxypropyl) prop-2-enoate	2.7×10^1		HSDB (2015)	Q	449
$C_{11}H_{16}O_4$					
(2,2-dimethyltrimethylene acrylate)					
[2223-82-7]					
MXFQRSUWYYSPOC-UHFFFAOYSA-N					
methyl jasmonate	5.0×10^1		Karl et al. (2008)	M	
$C_{13}H_{20}O_3$	7.0×10^2		HSDB (2015)	Q	100
[1211-29-6]					
GEWDNTWNSAZUDX-NNOMMRTBSA-N					

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cinoxate $C_{14}H_{18}O_4$ [104-28-9] CMDKPGRTAQVGFQ-RMKNXTFCSA-N	1.9×10^{3}		HSDB (2015)	Q	449
trimethylolpropane triacrylate $C_{15}H_{20}O_6$ [15625-89-5] DAKWPKUUDNSNPN-UHFFFAOYSA-N	1.6×10^{4}		HSDB (2015)	Q	449
benzyl cinnamate $C_{16}H_{14}O_2$ [103-41-3] NGHOLYJTSCBCGC-VAWYXSNFSA-N	3.0×10^{1}		HSDB (2015)	Q	100
2,2,4-trimethyl-1,3-pentanediol diisobutyrate $C_{16}H_{30}O_4$ [6846-50-0] OMVSWZDEEGIJJI-UHFFFAOYSA-N	9.0×10^{-1}		HSDB (2015)	Q	100
nonanedioic acid, dibutyl ester $C_{17}H_{32}O_4$ (dibutyl azelate) [2917-73-9] RISLXYINQFKFRL-UHFFFAOYSA-N	8.2×10^{-1}		HSDB (2015)	Q	100
isopropyl myristate $C_{17}H_{34}O_2$ [110-27-0] AXISYYRBXTVTFY-UHFFFAOYSA-N	4.2×10^{-4}		HSDB (2015)	Q	100
decanedioic acid, dibutyl ester $C_{18}H_{34}O_4$ [109-43-3] PYGXAGIECVVIOZ-UHFFFAOYSA-N	2.0×10^{2} 2.1×10^{2} 1.8×10^{1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
diethylene glycol dibenzoate $C_{18}H_{18}O_5$ [120-55-8] NXQMCAOPTPLPRL-UHFFFAOYSA-N	3.3×10^{6}		HSDB (2015)	Q	100
12-hydroxy-9-octadecenoic acid, methyl ester $C_{19}H_{36}O_3$ (ricinoleic acid, methyl ester) [141-24-2] XKGDWZQXVZSXAO-RAXLEYEMSA-N	6.7×10^{1}		HSDB (2015)	Q	100

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chrysanthemumic acid 2,4-dimethylbenzyl ester $C_{19}H_{26}O_2$ (dimethrin) [70-38-2] FHNKBSDJERHDHZ-UHFFFAOYSA-N	1.3×10^{-1}		HSDB (2015)	Q	100
tributyl acetylcitrate $C_{20}H_{34}O_8$ (acetyl tributyl citrate) [77-90-7] QZCLKYGREBVARF-UHFFFAOYSA-N	2.6×10^{4}		HSDB (2015)	Q	100
hexanedioic acid, bis[2-(2-butoxyethoxy)ethyl] ester $C_{22}H_{42}O_8$ (bis(2-(2-butoxyethoxy)ethyl) adipate) [141-17-3] SCABKEBYDRTODC-UHFFFAOYSA-N	3.2×10^{7}		HSDB (2015)	Q	100
1,2-benzenedicarboxylic acid, decyl octyl ester $C_{26}H_{42}O_4$ [119-07-3] LVAGMBHLXLZJKZ-UHFFFAOYSA-N	4.7×10^{-1}		HSDB (2015)	Q	100
phthalic acid, isodecyl octyl ester $C_{26}H_{42}O_4$ [1330-96-7] UXLBXTIBYMXRNX-UHFFFAOYSA-N	4.7×10^{-1}		HSDB (2015)	Q	100
diisononyl hexahydrophthalate $C_{26}H_{48}O_4$ [166412-78-8] HORIEOQXBKUKGQ-UHFFFAOYSA-N	1.4×10^{-1}		HSDB (2015)	Q	100
decanedioic acid, bis(2-ethylhexyl) ester $C_{26}H_{50}O_4$ (bis(2-ethylhexyl) sebacate) [122-62-3] VJHINFRRDQUWOJ-UHFFFAOYSA-N	1.2×10^{-1}		HSDB (2015)	Q	100
glycerol tricaprylate $C_{27}H_{50}O_6$ (tricaprylin) [538-23-8] VLPFTAMPNXLGLX-UHFFFAOYSA-N	3.9×10^{2}		HSDB (2015)	Q	100

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tris(2-ethylhexyl) trimellitate $C_{33}H_{54}O_6$ [3319-31-1] KRADHMIOFJQKEZ-UHFFFAOYSA-N	2.2×10^{1}		HSDB (2015)	Q	100
MCM:CHOOCH2OOH	3.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_2H_4O_4$	7.4×10^{2}		Wang et al. (2017)	Q	81, 240
RHCLSHTZJFAXOU-UHFFFAOYSA-N	6.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CHOOCHO	3.3		Wang et al. (2017)	Q	81, 239
$C_2H_2O_3$	2.5×10^{1}		Wang et al. (2017)	Q	81, 240
VGGRCVDNFAQIKO-UHFFFAOYSA-N	1.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:CHOOMCO3H	4.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_3H_4O_5$	2.0×10^{3}		Wang et al. (2017)	Q	81, 240
NYMJKVCDMUPZFI-UHFFFAOYSA-N	3.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ETHFORMOOH	3.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_4$	2.9×10^{2}		Wang et al. (2017)	Q	81, 240
DJECRZORXDSOEF-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MECOFOROOH	1.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_3H_4O_5$	3.6×10^{4}		Wang et al. (2017)	Q	81, 240
TUWVUCWHUYJQAO-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:METACETHO	2.2		Wang et al. (2017)	Q	81, 239
$C_3H_4O_3$	4.4×10^{1}		Wang et al. (2017)	Q	81, 240
ORWKVZNEPHTCQE-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:METACETO2H	2.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_4$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
AIBRVUZTVKELQP-UHFFFAOYSA-N	4.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MMCF	1.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_3H_4O_4$	7.8×10^{1}		Wang et al. (2017)	Q	81, 240
IIHOUWJOSQHHHH-UHFFFAOYSA-N	3.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:MMCFOOH	1.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_3H_4O_6$	5.9×10^{5}		Wang et al. (2017)	Q	81, 240
LQGPNTLGGGGYKM-UHFFFAOYSA-N	4.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MOCOCH2OOH	2.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_4$	2.5×10^{2}		Wang et al. (2017)	Q	81, 240
OQIIXPHPHGKJRP-UHFFFAOYSA-N	5.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ACEC2H4OOH	2.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	2.0×10^{3}		Wang et al. (2017)	Q	81, 240
JNHNRXKAKFYQGM-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:ACETMECO3H	3.2×10^4		Wang et al. (2017)	Q	81, 239
$C_4H_6O_5$	3.5×10^3		Wang et al. (2017)	Q	81, 240
UCKKJLQTXHILBL-UHFFFAOYSA-N	7.8×10^1		Wang et al. (2017)	Q	81, 241
MCM:COO2C3CO3H	3.2×10^4		Wang et al. (2017)	Q	81, 239
$C_4H_6O_5$	2.9×10^3		Wang et al. (2017)	Q	81, 240
CKNWOSHDVKEZAO-UHFFFAOYSA-N	2.0×10^1		Wang et al. (2017)	Q	81, 241
MCM:COO2C4OOH	2.1×10^3		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	1.6×10^3		Wang et al. (2017)	Q	81, 240
KATJWBCCJXQUDM-UHFFFAOYSA-N	4.4×10^2		Wang et al. (2017)	Q	81, 241
MCM:EOCOCH2OOH	2.1×10^3		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	1.1×10^2		Wang et al. (2017)	Q	81, 240
ZDXGLRBKCRTGQP-UHFFFAOYSA-N	3.3×10^1		Wang et al. (2017)	Q	81, 241
MCM:ETHACETOOH	2.4×10^3		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	2.7×10^2		Wang et al. (2017)	Q	81, 240
FITNUWWXWGTMFO-UHFFFAOYSA-N	2.8×10^1		Wang et al. (2017)	Q	81, 241
MCM:IPRFORMOOH	2.0×10^3		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	5.1×10^1		Wang et al. (2017)	Q	81, 240
DHNDYBGDIQCRQB-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	81, 241
maleic anhydride	1.9×10^1		Wang et al. (2017)	Q	81, 239
$C_4H_2O_3$	1.2×10^5		Wang et al. (2017)	Q	81, 240
(MCM:MALANHY)	9.6		Wang et al. (2017)	Q	81, 241
[108-31-6]					
FPYJFEHAWHCUMM-UHFFFAOYSA-N					
MCM:MECOACEOOH	1.1×10^5		Wang et al. (2017)	Q	81, 239
$C_4H_6O_5$	6.6×10^4		Wang et al. (2017)	Q	81, 240
ZCPJTWSQAFRVMG-UHFFFAOYSA-N	5.3×10^2		Wang et al. (2017)	Q	81, 241
MCM:ACCOETOOH	8.7×10^4		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	5.8×10^5		Wang et al. (2017)	Q	81, 240
MRPVYADEHOUTJI-UHFFFAOYSA-N	8.1×10^3		Wang et al. (2017)	Q	81, 241
MCM:ACCOMECO3H	1.3×10^6		Wang et al. (2017)	Q	81, 239
$C_5H_6O_6$	8.5×10^5		Wang et al. (2017)	Q	81, 240
OSZJUWKUAMKWAM-UHFFFAOYSA-N	1.3×10^3		Wang et al. (2017)	Q	81, 241
MCM:ACETC2CO3H	2.5×10^4		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	3.2×10^3		Wang et al. (2017)	Q	81, 240
LEMDJBHCHPODAJ-UHFFFAOYSA-N	5.0×10^1		Wang et al. (2017)	Q	81, 241
MCM:ACETCOC2H5	1.2		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	2.5×10^1		Wang et al. (2017)	Q	81, 240
KLUDQUOLAFVLOL-UHFFFAOYSA-N	2.4		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:BUFORMOOH	2.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	9.8×10^{1}		Wang et al. (2017)	Q	81, 240
HTFWPRQCJNWCFL-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:COO2C4CO3H	2.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	2.5×10^{3}		Wang et al. (2017)	Q	81, 240
XFYUESMQFXHHIL-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:IPRACBCO3H	2.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	6.9×10^{2}		Wang et al. (2017)	Q	81, 240
IEXBKLGSFAHQBW-UHFFFAOYSA-N	6.6		Wang et al. (2017)	Q	81, 241
MCM:IPRACBOOH	1.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	7.3×10^{2}		Wang et al. (2017)	Q	81, 240
HJBGHGSQOFAQDB-UHFFFAOYSA-N	5.3		Wang et al. (2017)	Q	81, 241
MCM:IPRACOOH	1.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	5.9×10^{1}		Wang et al. (2017)	Q	81, 240
UMMAXRSQAGVERV-UHFFFAOYSA-N	1.8		Wang et al. (2017)	Q	81, 241
MCM:MMALANHY	1.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_4O_3$	2.1×10^{5}		Wang et al. (2017)	Q	81, 240
AYKYXWQEBUNJCN-UHFFFAOYSA-N	8.7		Wang et al. (2017)	Q	81, 241
MCM:MTBEAALOOH	1.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	2.3×10^{2}		Wang et al. (2017)	Q	81, 240
OJPAWJIXAIXDOD-UHFFFAOYSA-N	5.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MTBEALCO3H	2.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
GVHAIIVWIJOUAR-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NPRACAOOH	1.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	7.4×10^{2}		Wang et al. (2017)	Q	81, 240
BAISPQOWBPLMQI-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NPRACBOOH	1.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	1.5×10^{2}		Wang et al. (2017)	Q	81, 240
KUTULJFZWKOEBJ-UHFFFAOYSA-N	9.8		Wang et al. (2017)	Q	81, 241
MCM:NPRACCOOH	1.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	1.0×10^{3}		Wang et al. (2017)	Q	81, 240
GYDFEBDSBUDYEN-UHFFFAOYSA-N	5.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PRCOFORM	1.6		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	1.4×10^{1}		Wang et al. (2017)	Q	81, 240
JKMPLJUAEDQBOK-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:PRCOFOROOH	1.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	2.4×10^{5}		Wang et al. (2017)	Q	81, 240
VVRRHCGIFBEYON-UHFFFAOYSA-N	9.1×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PRCOOMOOH	1.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	4.9×10^{2}		Wang et al. (2017)	Q	81, 240
JALZRJAYIBRIKJ-UHFFFAOYSA-N	2.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:TLFUONE	3.2×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_2$	1.4×10^{2}		Wang et al. (2017)	Q	81, 240
BGLUXFNVVSVEET-UHFFFAOYSA-N	8.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:ACCOPROOH	8.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	2.1×10^{5}		Wang et al. (2017)	Q	81, 240
HNMHVARGKGGINS-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:ACETCOC3H7	1.0		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	1.3×10^{1}		Wang et al. (2017)	Q	81, 240
BVQHHUQLZPXYAQ-UHFFFAOYSA-N	2.4		Wang et al. (2017)	Q	81, 241
MCM:BOCOCH2OOH	1.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	3.5×10^{1}		Wang et al. (2017)	Q	81, 240
DQCMTBDKSIDVDF-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DMMALANHY	8.1		Wang et al. (2017)	Q	81, 239
$C_6H_6O_3$	1.7×10^{5}		Wang et al. (2017)	Q	81, 240
MFGALGYVFGDXIX-UHFFFAOYSA-N	8.7		Wang et al. (2017)	Q	81, 241
MCM:EBFUONE	3.0×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_2$	7.8×10^{1}		Wang et al. (2017)	Q	81, 240
GOUILHYTHSOMQJ-UHFFFAOYSA-N	4.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:EMALANHY	1.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_3$	1.1×10^{5}		Wang et al. (2017)	Q	81, 240
AXGOOCLYBPQWNG-UHFFFAOYSA-N	5.8		Wang et al. (2017)	Q	81, 241
MCM:MCOOTBOOH	1.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	2.8×10^{2}		Wang et al. (2017)	Q	81, 240
GZZAVFPVGHHZEL-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MXYFUONE	2.2×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_2$	9.1×10^{1}		Wang et al. (2017)	Q	81, 240
SAXRUMLUKZBSTO-UHFFFAOYSA-N	3.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NBUACAOOH	1.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	5.9×10^{2}		Wang et al. (2017)	Q	81, 240
VUJYCIVMLKMZJB-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NBUACBOOH	1.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	4.4×10^{2}		Wang et al. (2017)	Q	81, 240
ZDNJENJHBNLWSZ-UHFFFAOYSA-N	6.9		Wang et al. (2017)	Q	81, 241
MCM:NBUACCOOH	1.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
CCXFYGGLIMLVCI-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PRCOOMCO3H	2.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	8.7×10^{2}		Wang et al. (2017)	Q	81, 240
NIESGQMUWIIUQP-UHFFFAOYSA-N	2.1		Wang et al. (2017)	Q	81, 241
MCM:SBUACAOOH	1.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	3.6×10^{1}		Wang et al. (2017)	Q	81, 240
XEFYSNUZBIEBQZ-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	81, 241
MCM:SBUACBOOH	1.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	3.6×10^{2}		Wang et al. (2017)	Q	81, 240
SHPWQWOSZRJPCY-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:TBUACCO3H	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	1.2×10^{2}		Wang et al. (2017)	Q	81, 240
CTLNPRHGCLAPPZ-UHFFFAOYSA-N	2.7		Wang et al. (2017)	Q	81, 241
MCM:TMB1FUONE	2.2×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_2$	1.3×10^{2}		Wang et al. (2017)	Q	81, 240
GLCOTRLUPUIAFI-UHFFFAOYSA-N	3.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:IPBFUONE	2.8×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_2$	6.9×10^{1}		Wang et al. (2017)	Q	81, 240
LWFKYUIZWLTJCA-UHFFFAOYSA-N	4.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:IPMALANHY	9.3		Wang et al. (2017)	Q	81, 239
$C_7H_8O_3$	6.3×10^{4}		Wang et al. (2017)	Q	81, 240
QSWLSAYLEATCSH-UHFFFAOYSA-N	2.8		Wang et al. (2017)	Q	81, 241
MCM:MEBFUONE	2.0×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_2$	5.4×10^{1}		Wang et al. (2017)	Q	81, 240
UVERQUDHQJYTIT-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PBFUONE	2.3×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_2$	5.5×10^{1}		Wang et al. (2017)	Q	81, 240
CLCLZCBNFSGUOD-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PMALANHY	8.7		Wang et al. (2017)	Q	81, 239
$C_7H_8O_3$	6.0×10^{4}		Wang et al. (2017)	Q	81, 240
LPFJFXRQANKTRA-UHFFFAOYSA-N	4.2		Wang et al. (2017)	Q	81, 241
MCM:TMB2FUONE	1.5×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_2$	9.1×10^{1}		Wang et al. (2017)	Q	81, 240
OSFZDFIHIYXIEL-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C1013OOH	2.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_4$	9.8×10^{2}		Wang et al. (2017)	Q	81, 240
BQYOGPDLQGPEQM-UHFFFAOYSA-N	2.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C1013CO3H	2.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_5$	6.3×10^{2}		Wang et al. (2017)	Q	81, 240
ZWRGNVXICSEPNH-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PXYFUONE	2.3×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_2$	3.0×10^{2}		Wang et al. (2017)	Q	81, 240
VGHBEMPMIVEGJP-UHFFFAOYSA-N	4.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:OXYFUONE	1.6×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_2$	2.8×10^{2}		Wang et al. (2017)	Q	81, 240
QHQDWCHELGHSTO-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:CHOOCH2OH	1.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_4O_3$	6.5×10^{1}		Wang et al. (2017)	Q	81, 240
APUQIHKCZFWODD-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ETHFORMOH	1.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_3$	6.2×10^{1}		Wang et al. (2017)	Q	81, 240
JRUKHAIVAGVYRP-UHFFFAOYSA-N	7.3		Wang et al. (2017)	Q	81, 241
MCM:ETOHOCHO	1.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_3$	3.3×10^{2}		Wang et al. (2017)	Q	81, 240
UKQJDWBNQNAJHB-UHFFFAOYSA-N	2.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:METACETOH	9.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_3$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
JYVNDCLJHKQUHE-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MMCFOH	4.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_3H_4O_5$	1.4×10^{5}		Wang et al. (2017)	Q	81, 240
XDYLYGBFMHJJOW-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MOXCOCH2OH	5.0		Wang et al. (2017)	Q	81, 239
$C_3H_6O_3$	1.5×10^{2}		Wang et al. (2017)	Q	81, 240
GSJFXBNYJCXDGI-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ACEETOHOOH	8.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_5$	2.9×10^{4}		Wang et al. (2017)	Q	81, 240
QQYYYRFGUJQKRH-UHFFFAOYSA-N	2.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:BZFUOH	4.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_4$	3.3×10^{7}		Wang et al. (2017)	Q	81, 240
SGMJBNSHAZVGMC-UHFFFAOYSA-N	1.7×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:BZFUOOH	7.8×10^{9}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_5$	8.9×10^{7}		Wang et al. (2017)	Q	81, 240
LZJWYIKGTDPLAQ-UHFFFAOYSA-N	3.2×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:EOX2COMEOH	4.0		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	7.1×10^{1}		Wang et al. (2017)	Q	81, 240
ZANNOFHADGWOLI-UHFFFAOYSA-N	1.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ETACETOH	9.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	3.6×10^{2}		Wang et al. (2017)	Q	81, 240
HXDLWJWIAHWIKI-UHFFFAOYSA-N	3.4×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:ETHACETOH	8.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	7.1×10^{1}		Wang et al. (2017)	Q	81, 240
MLAFRLBDNVSLPE-UHFFFAOYSA-N	7.4		Wang et al. (2017)	Q	81, 241
MCM:HOACETEOOH	3.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_5$	5.6×10^{5}		Wang et al. (2017)	Q	81, 240
QWYGOSGRTMPWCI-UHFFFAOYSA-N	5.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:IPRFORMOH	7.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	3.2×10^{1}		Wang et al. (2017)	Q	81, 240
SVJMGLNDGCVDIT-UHFFFAOYSA-N	2.9		Wang et al. (2017)	Q	81, 241
MCM:MALANHY2OH	7.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_5$	4.8×10^{8}		Wang et al. (2017)	Q	81, 240
BOGVTNYNTGOONP-UHFFFAOYSA-N	3.9×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:MALANHYOOH	1.2×10^{12}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_6$	1.0×10^{9}		Wang et al. (2017)	Q	81, 240
UPSCPEYLZZUIND-UHFFFAOYSA-N	1.3×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:PROL2FORM	1.5×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	2.6×10^{2}		Wang et al. (2017)	Q	81, 240
CRMUFGZQBODVGS-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:BUOHFORM	8.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	3.0×10^{1}		Wang et al. (2017)	Q	81, 240
KIZCCPGSHHAFRX-UHFFFAOYSA-N	4.6		Wang et al. (2017)	Q	81, 241
MCM:IPRACBOH	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	2.0×10^{2}		Wang et al. (2017)	Q	81, 240
YJNKLTDJZSXVHQ-UHFFFAOYSA-N	2.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:IPRACOH	5.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	4.1×10^{1}		Wang et al. (2017)	Q	81, 240
MYOAZFOMGTTYOD-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	81, 241
MCM:MMALNHY2OH	3.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_5$	6.8×10^{8}		Wang et al. (2017)	Q	81, 240
DGWWNMWYNUWPBC-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:MMALNHYOOH	6.3×10^{11}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_6$	6.8×10^{8}		Wang et al. (2017)	Q	81, 240
JNCHKPBVXWMPAJ-UHFFFAOYSA-N	7.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:MTBEACHOHO	8.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	7.6×10^{1}		Wang et al. (2017)	Q	81, 240
GQMJADBSHHFADW-UHFFFAOYSA-N	8.3		Wang et al. (2017)	Q	81, 241
MCM:NPRACAOH	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	3.2×10^{2}		Wang et al. (2017)	Q	81, 240
PPPFYBPQAPISCT-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NPRACBOH	7.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	4.7×10^{1}		Wang et al. (2017)	Q	81, 240
VEGXEWGKYMMJKP-UHFFFAOYSA-N	3.2		Wang et al. (2017)	Q	81, 241
MCM:NPRACCOH	6.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	6.3×10^{2}		Wang et al. (2017)	Q	81, 240
DOUBAFNWVFAWEC-UHFFFAOYSA-N	9.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PXYFUOH	2.7×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	4.3×10^{7}		Wang et al. (2017)	Q	81, 240
OHTGZAWPVDWARE-UHFFFAOYSA-N	3.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:PXYFUOOH	4.5×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	4.9×10^{7}		Wang et al. (2017)	Q	81, 240
IEFDVDGOIVKGRZ-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:TLFUOH	4.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	3.7×10^{7}		Wang et al. (2017)	Q	81, 240
JYHWQRJRDKSSIF-UHFFFAOYSA-N	7.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:TLFUOOH	7.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	1.0×10^{8}		Wang et al. (2017)	Q	81, 240
GNXADMJANDYCAE-UHFFFAOYSA-N	2.9×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:BOX2COMOH	2.9		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	2.9×10^{1}		Wang et al. (2017)	Q	81, 240
VFGRALUHHHDIQI-UHFFFAOYSA-N	9.8		Wang et al. (2017)	Q	81, 241
MCM:DMMALYOH	2.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	1.2×10^{9}		Wang et al. (2017)	Q	81, 240
KIOPGGAGDHZEGB-UHFFFAOYSA-N	4.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:DMMALYOOH	3.5×10^{11}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_6$	8.9×10^{8}		Wang et al. (2017)	Q	81, 240
VRKLPKITGMCVQP-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:EBFUOH	4.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	3.5×10^{7}		Wang et al. (2017)	Q	81, 240
AQSJHOPJZAKOAP-UHFFFAOYSA-N	3.7×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:EBFUOOH	6.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	8.5×10^{7}		Wang et al. (2017)	Q	81, 240
KIZOVCBYCQGADC-UHFFFAOYSA-N	7.6×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:EMALNHY2OH	3.6×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	8.3×10^{8}		Wang et al. (2017)	Q	81, 240
GPJQUVLKFIAXFZ-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:EMALNHYOOH	5.0×10^{11}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_6$	8.5×10^{8}		Wang et al. (2017)	Q	81, 240
LSSHMOINJMVLHQ-UHFFFAOYSA-N	6.3×10^{5}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MXYFUOH	2.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	3.7×10^{7}		Wang et al. (2017)	Q	81, 240
WCMYKJKBZGIGND-UHFFFAOYSA-N	3.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:MXYFUOOH	4.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	2.8×10^{7}		Wang et al. (2017)	Q	81, 240
WCIMCWKIICZLLM-UHFFFAOYSA-N	3.6×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:NBUACAOH	5.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	6.5×10^{2}		Wang et al. (2017)	Q	81, 240
KLUHZXMBIDAHSJ-UHFFFAOYSA-N	6.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NBUACBOH	8.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	2.1×10^{2}		Wang et al. (2017)	Q	81, 240
BZLQSYFOTWOIDC-UHFFFAOYSA-N	5.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NBUACCOH	5.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	3.6×10^{1}		Wang et al. (2017)	Q	81, 240
BMNRJWUOBYYCRX-UHFFFAOYSA-N	2.7		Wang et al. (2017)	Q	81, 241
MCM:OXYFUOH	1.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	3.2×10^{7}		Wang et al. (2017)	Q	81, 240
GZKXVWYDQQSODI-UHFFFAOYSA-N	1.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:OXYFUOOH	2.4×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	2.3×10^{7}		Wang et al. (2017)	Q	81, 240
DHHFHIZBMAEZJT-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:PRCOOETOH	6.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.3×10^{2}		Wang et al. (2017)	Q	81, 240
GIOCILWWMFZESP-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:SBUACAOH	4.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	3.2×10^{1}		Wang et al. (2017)	Q	81, 240
WAXXMBOGFVJIHX-UHFFFAOYSA-N	7.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:SBUACBOH	9.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.7×10^{2}		Wang et al. (2017)	Q	81, 240
BCWWODMTUXMSAB-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:TBOCOCH2OH	2.0		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.7×10^{1}		Wang et al. (2017)	Q	81, 240
WINGEFIITRDOLJ-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	81, 241
MCM:TBUACOH	4.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	9.1×10^{1}		Wang et al. (2017)	Q	81, 240
GWOKHTMCBUZSOP-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:TMB1FUOH	2.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	2.2×10^{7}		Wang et al. (2017)	Q	81, 240
AUTABLFJFWRKGZ-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:TMB1FUOOH	1.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	7.4×10^{7}		Wang et al. (2017)	Q	81, 240
NFODFJMABSYJFC-UHFFFAOYSA-N	4.2×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:BOXCOOLOOH	2.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_5$	2.4×10^{5}		Wang et al. (2017)	Q	81, 240
PDOIGHDIMNJPNL-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:IPBFUOH	3.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	3.0×10^{7}		Wang et al. (2017)	Q	81, 240
ZIPHTXAVHSYMQR-UHFFFAOYSA-N	5.3×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:IPBFUOOH	5.4×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	7.8×10^{7}		Wang et al. (2017)	Q	81, 240
HVQWCSPFZPPNOE-UHFFFAOYSA-N	2.1×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:IPMLNHY2OH	3.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	1.2×10^{9}		Wang et al. (2017)	Q	81, 240
RBIJYTIBBLMIRU-UHFFFAOYSA-N	4.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:IPMLNHYOOH	4.7×10^{11}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_6$	1.1×10^{9}		Wang et al. (2017)	Q	81, 240
LGGLTRMSNOIPLU-UHFFFAOYSA-N	9.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:MEBFUOH	2.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	2.2×10^{7}		Wang et al. (2017)	Q	81, 240
SYHJYGJIPQZFIO-UHFFFAOYSA-N	1.6×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:MEBFUOOH	3.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	1.7×10^{7}		Wang et al. (2017)	Q	81, 240
VRHMFTJWRSNJLN-UHFFFAOYSA-N	2.2×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:PBFUOH	3.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	2.4×10^{7}		Wang et al. (2017)	Q	81, 240
DMMDFVMQHRHVSU-UHFFFAOYSA-N	5.6×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:PBFUOOH	5.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	6.2×10^{7}		Wang et al. (2017)	Q	81, 240
KAMUACRVJWJEFX-UHFFFAOYSA-N	6.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PMALNHY2OH	2.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	8.9×10^{8}		Wang et al. (2017)	Q	81, 240
PVDNZCIFUUKKBS-UHFFFAOYSA-N	1.3×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:PMALNHYOOH	4.1×10^{11}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_6$	8.0×10^{8}		Wang et al. (2017)	Q	81, 240
VKSMRBCXNQEUFP-UHFFFAOYSA-N	4.4×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PRCOOPROL	6.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_3$	1.3×10^{2}		Wang et al. (2017)	Q	81, 240
QXXGFEMAULVMST-UHFFFAOYSA-N	4.5×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:TMB2FUOH	1.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_4$	1.8×10^{7}		Wang et al. (2017)	Q	81, 240
YEQCQVSGZKCWAA-UHFFFAOYSA-N	1.3×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:TMB2FUOOH	2.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	1.2×10^{7}		Wang et al. (2017)	Q	81, 240
MINPHQZFUPUEBD-UHFFFAOYSA-N	3.6×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C1013OH	7.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_3$	5.4×10^{2}		Wang et al. (2017)	Q	81, 240
OYGVMQZTRRRABW-UHFFFAOYSA-N	3.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ALCOMOXOOH	2.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_3H_4O_5$	1.6×10^{5}		Wang et al. (2017)	Q	81, 240
DRQRCDXSDDWNEU-UHFFFAOYSA-N	9.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DFC	1.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_2O_5$	6.9×10^{3}		Wang et al. (2017)	Q	81, 240
DOMHJQJKOPZSOM-UHFFFAOYSA-N	1.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:MOXY2CHO	3.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_3H_4O_3$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
MFRMAQFRVTUENW-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MOXYCOCHO	3.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_3H_4O_3$	3.2×10^{1}		Wang et al. (2017)	Q	81, 240
KFKXSMSQHIOMSO-UHFFFAOYSA-N	6.5×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:ACETETCHO	2.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_3$	1.8×10^{2}		Wang et al. (2017)	Q	81, 240
GUPGZURVZDIQPM-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO14O3CHO	2.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_4$	1.2×10^{4}		Wang et al. (2017)	Q	81, 240
ZFWWLKBCHQUFEJ-UHFFFAOYSA-N	8.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:COO2C3CHO	2.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_3$	5.4×10^{1}		Wang et al. (2017)	Q	81, 240
AGADEVQOWQDDFX-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:EOCOCHO	2.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_3$	1.7×10^{1}		Wang et al. (2017)	Q	81, 240
DBPFRRFGLYGEJI-UHFFFAOYSA-N	8.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:ACCOMECHO	1.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_4$	1.6×10^{4}		Wang et al. (2017)	Q	81, 240
GRUDDVNYUQQBCU-UHFFFAOYSA-N	9.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ACEC2CHO	2.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	1.7×10^{2}		Wang et al. (2017)	Q	81, 240
PRSPLAWXBFRHKV-UHFFFAOYSA-N	7.4×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:COO2C4CHO	2.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	1.3×10^{2}		Wang et al. (2017)	Q	81, 240
DLZVZNAPRCRXEG-UHFFFAOYSA-N	3.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:IPRACBCHO	2.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	3.9×10^{1}		Wang et al. (2017)	Q	81, 240
FXPPNKAYSGWCQG-UHFFFAOYSA-N	5.0		Wang et al. (2017)	Q	81, 241
MCM:MTBEACHO13	1.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	5.8		Wang et al. (2017)	Q	81, 240
MDWWHOIDIKOPHH-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	81, 241
MCM:BOXCOALOOH	1.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	2.0×10^{4}		Wang et al. (2017)	Q	81, 240
MZUJTBRWESAMQA-UHFFFAOYSA-N	4.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:BOXCOCHO	1.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	6.0		Wang et al. (2017)	Q	81, 240
NRYDRJHYTRBBEA-UHFFFAOYSA-N	1.5×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C14O3ECHO	1.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	3.3×10^{3}		Wang et al. (2017)	Q	81, 240
FVLOJCOPOCRBFF-UHFFFAOYSA-N	5.6		Wang et al. (2017)	Q	81, 241
MCM:PRCOOMCHO	1.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	4.7×10^{1}		Wang et al. (2017)	Q	81, 240
YEBNSRBQIIWQQC-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:TBOCOCHO	1.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	3.6		Wang et al. (2017)	Q	81, 240
WDPZTIFGRQKSEN-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:TBUACCO	1.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	6.6		Wang et al. (2017)	Q	81, 240
BYYPPVMBDPUHHR-UHFFFAOYSA-N	5.5		Wang et al. (2017)	Q	81, 241
MCM:C14O3IPCHO	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	2.3×10^{3}		Wang et al. (2017)	Q	81, 240
NPPWDFRKAMDHMM-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	81, 241
MCM:C14O3PCHO	1.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	2.1×10^{3}		Wang et al. (2017)	Q	81, 240
GNODSIBUYMXKGR-UHFFFAOYSA-N	3.6		Wang et al. (2017)	Q	81, 241
MCM:C1014OOH	5.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_5$	8.3×10^{4}		Wang et al. (2017)	Q	81, 240
REYZAYCUYYNPLJ-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:BCALBOC	2.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{24}O_3$	3.0×10^{1}		Wang et al. (2017)	Q	81, 240
FEPYZLRQFOQWRK-UHFFFAOYSA-N	8.5×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CHOOMCO2H	4.7×10^{5}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_4$	1.9×10^{5}		Wang et al. (2017)	Q	81, 240
CBNAABWGSNQFTA-UHFFFAOYSA-N	8.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C1014OH	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{18}O_4$	2.1×10^{5}		Wang et al. (2017)	Q	81, 240
IJPJFXOOJHUBTK-UHFFFAOYSA-N	9.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C152OH	2.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{26}O_5$	1.0×10^{8}		Wang et al. (2017)	Q	81, 240
XZXFZFZFZSKVDT-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C152OOH	2.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{26}O_6$	2.2×10^{8}		Wang et al. (2017)	Q	81, 240
PKQOWOPWICZSPN-UHFFFAOYSA-N	5.1×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C23O3CHO	1.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_4$	7.3×10^{3}		Wang et al. (2017)	Q	81, 240
RULCSXTUAHNYHJ-UHFFFAOYSA-N	6.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:MCOCOMOOOH	1.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_5$	2.5×10^{5}		Wang et al. (2017)	Q	81, 240
BJTKGFWDIAZUGI-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:MCOCOMOX	2.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_3$	3.0×10^{1}		Wang et al. (2017)	Q	81, 240
CWKLZLBVOJRSOM-UHFFFAOYSA-N	4.3		Wang et al. (2017)	Q	81, 241
MCM:PRNFORMOOH	2.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_5$	5.4×10^{3}		Wang et al. (2017)	Q	81, 240
LIFMXPSJWIBAGH-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PRONFORM	2.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_6O_3$	1.5×10^{2}		Wang et al. (2017)	Q	81, 240
WNVAJGCMEDTLIE-UHFFFAOYSA-N	3.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ACCOCOMOOH	6.8×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_6$	3.2×10^{6}		Wang et al. (2017)	Q	81, 240
WKJHUBLAYZIBAJ-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:ACECOCOCH3	8.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_4$	9.1×10^{3}		Wang et al. (2017)	Q	81, 240
OBTVATRSWTWNGS-UHFFFAOYSA-N	8.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:ACEPROPONE	1.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	1.8×10^{2}		Wang et al. (2017)	Q	81, 240
DBERHVIZRVGDFO-UHFFFAOYSA-N	8.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ACPRONEOOH	1.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	5.5×10^{3}		Wang et al. (2017)	Q	81, 240
FOWIMBLOPIOWII-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C23O3CCO3H	1.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_6$	5.5×10^{5}		Wang et al. (2017)	Q	81, 240
SPYAIQASSDQEIX-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C23O3MCOOH	1.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	6.6×10^{4}		Wang et al. (2017)	Q	81, 240
RVGUYYZMHBERKG-UHFFFAOYSA-N	6.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PRNOCOMOOH	1.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	2.2×10^{5}		Wang et al. (2017)	Q	81, 240
GJTAOZDAMDVHTP-UHFFFAOYSA-N	8.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:ACBUOAOOH	1.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	1.1×10^{5}		Wang et al. (2017)	Q	81, 240
BDHJVYCZNHBETI-UHFFFAOYSA-N	3.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:ACBUONBOOH	1.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	2.5×10^{3}		Wang et al. (2017)	Q	81, 240
RISONYRIGLPILV-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:ACCOCOC2H5	6.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	4.7×10^{3}		Wang et al. (2017)	Q	81, 240
WZGYRWNUCYXCFD-UHFFFAOYSA-N	3.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:ACCOCOEOOH	6.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_6$	1.5×10^{6}		Wang et al. (2017)	Q	81, 240
RKPSGJVLERUIIG-UHFFFAOYSA-N	2.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:ACCOPRONE	6.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	1.6×10^{4}		Wang et al. (2017)	Q	81, 240
RYLHMXPGTMYTTF-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:ACEBUTBONE	1.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	8.1×10^{1}		Wang et al. (2017)	Q	81, 240
LHGWJCBYBIICPP-UHFFFAOYSA-N	4.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ACEBUTONE	1.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	1.8×10^{2}		Wang et al. (2017)	Q	81, 240
NWCYECXHIYEBJE-UHFFFAOYSA-N	5.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:ACOMCOMOOH	5.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_6$	5.4×10^{6}		Wang et al. (2017)	Q	81, 240
NKXSSYAJYGYQPN-UHFFFAOYSA-N	4.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C23O3ECOOH	1.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	3.0×10^{4}		Wang et al. (2017)	Q	81, 240
NLYPTRYHUBHKKI-UHFFFAOYSA-N	4.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C23O3EHO	6.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	4.6×10^{3}		Wang et al. (2017)	Q	81, 240
AIDIMUPPUNPUTI-UHFFFAOYSA-N	3.7×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C23O3MCO3H	1.5×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_6$	1.1×10^{5}		Wang et al. (2017)	Q	81, 240
FIPISRZHVPVVNA-UHFFFAOYSA-N	9.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C6O4KETOOH	3.6×10^{10}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_7$	3.8×10^{8}		Wang et al. (2017)	Q	81, 240
LLKUMVBDCSCXDR-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C6OTKETCO	5.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_5$	1.0×10^{6}		Wang et al. (2017)	Q	81, 240
GAPVBMQBWAUBHC-UHFFFAOYSA-N	3.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6OTKETOOH	7.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_6$	8.3×10^{5}		Wang et al. (2017)	Q	81, 240
USMDUVUWRKQXQG-UHFFFAOYSA-N	6.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C6OTRIKET	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	2.4×10^{4}		Wang et al. (2017)	Q	81, 240
XAHWCAXZWOTSBC-UHFFFAOYSA-N	5.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CO356OCOOH	6.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_6$	4.5×10^{6}		Wang et al. (2017)	Q	81, 240
MVKXXKVCXUKLOS-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:SBUACCOOH	8.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_5$	5.3×10^{2}		Wang et al. (2017)	Q	81, 240
DTGNYNGASXJUMP-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:SBUACEONE	1.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_3$	3.3×10^{1}		Wang et al. (2017)	Q	81, 240
ZKPTYCJWRHHBOW-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:BOX2COMOOH	9.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	2.1×10^{4}		Wang et al. (2017)	Q	81, 240
YCDXONIQHOVSSF-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:BOXCOCOME	1.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_3$	6.3		Wang et al. (2017)	Q	81, 240
ZAZUOXBHFXAWMD-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	81, 241
MCM:C23O3ECO3H	1.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_6$	5.1×10^{4}		Wang et al. (2017)	Q	81, 240
FWVKIPPVGIEQRB-UHFFFAOYSA-N	8.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MC6OTKTOOH	4.5×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_6$	9.3×10^{4}		Wang et al. (2017)	Q	81, 240
DJTBKMNUYULRIV-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:MC6OTRIKET	9.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	5.9×10^{3}		Wang et al. (2017)	Q	81, 240
FJYCWZCSXDGURV-UHFFFAOYSA-N	2.6×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PRCOOPRONE	1.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_3$	5.0×10^{1}		Wang et al. (2017)	Q	81, 240
AIJLJYUDTAJRDN-UHFFFAOYSA-N	3.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PRNOCOPOOH	9.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{12}O_5$	6.8×10^{5}		Wang et al. (2017)	Q	81, 240
RGEURRORAZXRIV-UHFFFAOYSA-N	1.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C1013CO	1.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_3$	8.3×10^{1}		Wang et al. (2017)	Q	81, 240
DPRGOCIPALHGLN-UHFFFAOYSA-N	6.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:BZFUCO	1.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_4$	4.2×10^{6}		Wang et al. (2017)	Q	81, 240
MFFNSLKCUZEAFI-UHFFFAOYSA-N	1.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:MALNHYOHCO	2.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_4H_2O_5$	1.0×10^{9}		Wang et al. (2017)	Q	81, 240
DBWAPECJPVXLJZ-UHFFFAOYSA-N	1.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:ACPRONEOH	2.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	1.3×10^{4}		Wang et al. (2017)	Q	81, 240
LBOLMEABDOYQGX-UHFFFAOYSA-N	7.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C23O3MOH	4.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	2.0×10^{4}		Wang et al. (2017)	Q	81, 240
WHFDSTOTVFOUIH-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:ACBUONAOH	4.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	5.1×10^{4}		Wang et al. (2017)	Q	81, 240
UGJVDYQVVBKWGL-UHFFFAOYSA-N	2.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:ACBUONBOH	2.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	6.8×10^{3}		Wang et al. (2017)	Q	81, 240
GYQPXJWBTJDNGC-UHFFFAOYSA-N	7.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C23O3EOH	4.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
BVDDSYZMRAYYIJ-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C6OTKETOH	4.4×10^{4}	16000	Wieser et al. (2023)	Q	439
$C_6H_8O_5$	1.5×10^{6}		Wang et al. (2017)	Q	81, 239
NOUUUBJIFPBZMZ-UHFFFAOYSA-N	2.0×10^{6}		Wang et al. (2017)	Q	81, 240
	6.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:EBFUCO	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	5.0×10^{6}		Wang et al. (2017)	Q	81, 240
QFGGPABGKQEYQI-UHFFFAOYSA-N	7.3×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:SBUACCOH	1.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}O_4$	4.5×10^{3}		Wang et al. (2017)	Q	81, 240
SUDJMSTXSVVFNQ-UHFFFAOYSA-N	5.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:IPBFUCO	9.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	4.6×10^{6}		Wang et al. (2017)	Q	81, 240
NHSFIZKDULUUEP-UHFFFAOYSA-N	6.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:MC6OTKETOH	8.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	7.1×10^{5}		Wang et al. (2017)	Q	81, 240
GQVIXHCRVNFYGI-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:PBFUCO	8.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	3.6×10^{6}		Wang et al. (2017)	Q	81, 240
PKKIVTPUHZVJRM-UHFFFAOYSA-N	7.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C23O3CCHO	1.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_4$	2.1×10^{4}		Wang et al. (2017)	Q	81, 240
JQZIMULKJBYVEJ-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C23O3MCHO	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	6.0×10^{3}		Wang et al. (2017)	Q	81, 240
KNKMVXKCHLTCEX-UHFFFAOYSA-N	8.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C5OCO3M	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	5.6×10^{3}		Wang et al. (2017)	Q	81, 240
MFFVRQLCBYBQSQ-UHFFFAOYSA-N	4.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C23O3ECHO	1.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	3.2×10^{3}		Wang et al. (2017)	Q	81, 240
RCPFVGJRKWBYKE-UHFFFAOYSA-N	4.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C1014CO	4.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_4$	2.0×10^{4}		Wang et al. (2017)	Q	81, 240
MPJVRMHYAPYGFM-UHFFFAOYSA-N	4.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:BCLKBOC	7.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_4$	3.6×10^{4}		Wang et al. (2017)	Q	81, 240
YETGIZICMMLUOK-UHFFFAOYSA-N	5.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C148CO	5.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{20}O_5$	3.5×10^{5}		Wang et al. (2017)	Q	81, 240
WKRISEJACIFSSJ-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C148OOH	6.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_6$	3.0×10^{6}		Wang et al. (2017)	Q	81, 240
QNGFZXSUHFZFIE-UHFFFAOYSA-N	4.4×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C148OH	1.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_5$	7.6×10^{6}		Wang et al. (2017)	Q	81, 240
LXDPLKVHKWYPKP-UHFFFAOYSA-N	9.8×10^{4}		Wang et al. (2017)	Q	81, 241

Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:ACETC2CO2H	2.9×10^3		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	4.8×10^4		Wang et al. (2017)	Q	81, 240
RFEXARYJXBYPLD-UHFFFAOYSA-N	6.5×10^4		Wang et al. (2017)	Q	81, 241
MCM:C24O3CCO2H	1.6×10^5		Wang et al. (2017)	Q	81, 239
$C_5H_6O_5$	3.5×10^6		Wang et al. (2017)	Q	81, 240
HSSKPURIBYAXCO-UHFFFAOYSA-N	7.3×10^4		Wang et al. (2017)	Q	81, 241
MCM:IPRACBCO2H	3.5×10^3		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	6.9×10^3		Wang et al. (2017)	Q	81, 240
WTLNOANVTIKPEE-UHFFFAOYSA-N	5.0×10^3		Wang et al. (2017)	Q	81, 241
MCM:MTBEALCO2H	2.8×10^3		Wang et al. (2017)	Q	81, 239
$C_5H_8O_4$	2.1×10^3		Wang et al. (2017)	Q	81, 240
BXXOFUQIACXFIW-UHFFFAOYSA-N	2.0×10^3		Wang et al. (2017)	Q	81, 241
MCM:C1013CO2H	3.0×10^3		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_4$	3.1×10^4		Wang et al. (2017)	Q	81, 240
QWGCLZMSSSTRLX-UHFFFAOYSA-N	5.0×10^4		Wang et al. (2017)	Q	81, 241
MCM:CO14O3CO2H	3.3×10^6		Wang et al. (2017)	Q	81, 239
$C_4H_4O_5$	5.4×10^4		Wang et al. (2017)	Q	81, 240
OPFWUCMVKDVVTF-UHFFFAOYSA-N	1.7×10^5		Wang et al. (2017)	Q	81, 241
MCM:C23O3CCO2H	2.3×10^6		Wang et al. (2017)	Q	81, 239
$C_5H_6O_5$	9.1×10^6		Wang et al. (2017)	Q	81, 240
WRKCXTWVOWDGBE-UHFFFAOYSA-N	1.7×10^5		Wang et al. (2017)	Q	81, 241
MCM:C23O3MCO2H	2.0×10^6		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	1.6×10^6		Wang et al. (2017)	Q	81, 240
OGSBZWITKXVLIV-UHFFFAOYSA-N	9.3×10^4		Wang et al. (2017)	Q	81, 241
MCM:C23O3ECO2H	1.7×10^6		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	6.0×10^5		Wang et al. (2017)	Q	81, 240
OEONINCNUUTEPU-UHFFFAOYSA-N	2.5×10^4		Wang et al. (2017)	Q	81, 241

A3.9 Ethers (ROR)

Table A3.9: Ethers (ROR)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dimethyl ether	9.9×10^{-3}		Duchowicz et al. (2020)	V	187
CH_3OCH_3	1.7×10^{-3}		HSDB (2015)	V	
[115-10-6]	7.6×10^{-2}		Mackay et al. (2006c)	V	
LCGLNKUTAGEVQW-UHFFFAOYSA-N	1.3×10^{-1}		Mackay et al. (1993)	V	
	9.9×10^{-3}		Hine and Mookerjee (1975)	V	
	9.8×10^{-3}		Hine and Weimar (1965)	R	
	1.0×10^{-2}	4900	Bagno et al. (1991)	T	475
	1.5×10^{-2}		Yaws (2003)	X	238, 28
	6.5×10^{-3}		Hayer et al. (2022)	Q	20
	5.1×10^{-2}		Duchowicz et al. (2020)	Q	
	3.0×10^{-3}		Wang et al. (2017)	Q	81, 239
	3.0×10^{-2}		Wang et al. (2017)	Q	81, 240
	1.1×10^{-2}		Wang et al. (2017)	Q	81, 241
	7.1×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
	1.8×10^{-2}		Hilal et al. (2008)	Q	
	1.4×10^{-2}		Modarresi et al. (2007)	Q	68
	7.5×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	8.4×10^{-3}		Katritzky et al. (1998)	Q	
	2.2×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	5.3×10^{-2}		Russell et al. (1992)	Q	360
	1.2×10^{-2}		Suzuki et al. (1992)	Q	233
	1.5×10^{-2}		Yaws (1999)	?	21, 28
	6.2×10^{-3}		Abraham and Weathersby (1994)	?	21
	9.9×10^{-3}		Abraham et al. (1990)	?	
ethyl methyl ether	8.2×10^{-3}		Duchowicz et al. (2020)	V	187
$C_2H_5OCH_3$	1.4×10^{-2}		Bagno et al. (1991)	T	475
[540-67-0]	1.9×10^{-2}		Duchowicz et al. (2020)	Q	
XOBKSJJDNFUZPF-UHFFFAOYSA-N	1.5×10^{-2}		HSDB (2015)	Q	100
	1.5×10^{-2}		Hilal et al. (2008)	Q	
	3.0×10^{-2}		English and Carroll (2001)	Q	231, 232
	9.7×10^{-3}		Katritzky et al. (1998)	Q	
	1.9×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	8.9×10^{-3}		Saxena and Hildemann (1996)	E	403
	1.8×10^{-2}		Yaws (1999)	?	21
diethyl ether	9.9×10^{-3}	5800	Burkholder et al. (2019)	L	1
$C_2H_5OC_2H_5$	2.0×10^{-2}	5800	Burkholder et al. (2015)	L	
[60-29-7]	9.9×10^{-3}	5800	Brockbank (2013)	L	1
RTZKZFJDLAIYFH-UHFFFAOYSA-N	5.0×10^{-3}		Steward et al. (1973)	L	14
	9.6×10^{-3}	5000	Allott et al. (1973)	L	
	1.1×10^{-2}	6600	Hiatt (2013)	M	
	9.5×10^{-2}		Helburn et al. (2008)	M	

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.0×10^{-2}	5700	Ondo and Dohnal (2007)	M	1
	1.1×10^{-2}		Nielsen et al. (1994)	M	
	3.3×10^{-3}		Yu (1992)	M	12
	7.0×10^{-3}	3900	Lamarche and Droste (1989)	M	347
	6.3×10^{-3}		Guitart et al. (1989)	M	14
	1.3×10^{-2}	7400	Bachofen and Farhi (1971)	M	
	6.3×10^{-3}		Brody et al. (1971)	M	14
	7.8×10^{-3}		Signer et al. (1969)	M	
	5.1×10^{-3}		Eger et al. (1963)	M	14
	1.1×10^{-2}		Mackay et al. (2006c)	V	
	1.0×10^{-2}	5800	Fukuchi et al. (2002)	V	
	1.1×10^{-2}		Mackay et al. (1993)	V	
	8.7×10^{-3}		Hwang et al. (1992)	V	
	1.1×10^{-2}		Hine and Weimar (1965)	V	
	1.1×10^{-2}		Butler and Ramchandani (1935)	V	
	6.0×10^{-3}	5700	Bagno et al. (1991)	T	475
	1.2×10^{-2}		Yaws (2003)	X	238
	4.3×10^{-3}		Keshavarz et al. (2022)	Q	
	6.8×10^{-3}		Duchowicz et al. (2020)	Q	185
	2.1×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.6×10^{-2}		Wang et al. (2017)	Q	81, 240
	2.2×10^{-3}		Wang et al. (2017)	Q	81, 241
	7.7×10^{-3}		Li et al. (2014)	Q	242
	1.3×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
	7.0×10^{-3}		Hilal et al. (2008)	Q	
	1.3×10^{-2}		Modarresi et al. (2007)	Q	68
		5300	Kühne et al. (2005)	Q	
	8.6×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	2.4×10^{-2}		English and Carroll (2001)	Q	231, 232
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
	1.7×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	4.6×10^{-2}		Russell et al. (1992)	Q	280
	7.3×10^{-3}		Suzuki et al. (1992)	Q	233
	8.0×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		5700	Kühne et al. (2005)	?	
	1.2×10^{-2}		Yaws (1999)	?	21
	5.8×10^{-3}		Abraham and Weathersby (1994)	?	21
	7.7×10^{-3}		Hoff et al. (1993)	?	21
	6.0×10^{-3}		Abraham et al. (1990)	?	

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
diethyl ether-d10 $C_2D_5OC_2D_5$ [2679-89-2] RTZKZFJDLAIYFH-MWUKXHIBSA-N	1.3×10^{-2}	6500	Hiatt (2013)	M	
methyl propyl ether $CH_3OC_3H_7$ [557-17-5] VNKYTQGIUYNRMY-UHFFFAOYSA-N	6.6×10^{-3}		Duchowicz et al. (2020)	V	187
	6.7×10^{-3}		Meylan and Howard (1991)	V	
	6.7×10^{-3}		Hine and Mookerjee (1975)	V	
	6.9×10^{-3}		Yaws (2003)	X	238
	2.0×10^{-2}		Duchowicz et al. (2020)	Q	
	5.2×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	8.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.1×10^{-2}		Hilal et al. (2008)	Q	
	6.9×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.1×10^{-2}		Katritzky et al. (1998)	Q	
	1.5×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	7.3×10^{-3}		Suzuki et al. (1992)	Q	233
	6.5×10^{-3}		Meylan and Howard (1991)	Q	
	6.9×10^{-3}		Yaws (1999)	?	21
methyl 2-propyl ether $CH_3OC_3H_7$ (methyl isopropyl ether) [598-53-8] RMGHERXMTMUMMV-UHFFFAOYSA-N	1.1×10^{-2}		Duchowicz et al. (2020)	V	187
	1.2×10^{-2}		Hine and Mookerjee (1975)	V	
	1.2×10^{-2}		Yaws (2003)	X	259
	1.1×10^{-2}		Yaws (2003)	X	238
	7.1×10^{-3}		Dupeux et al. (2022)	Q	260
	7.8×10^{-3}		Duchowicz et al. (2020)	Q	
	1.4×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
	8.2×10^{-3}		Hilal et al. (2008)	Q	
	1.2×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.1×10^{-2}		Katritzky et al. (1998)	Q	
	6.5×10^{-3}		Suzuki et al. (1992)	Q	233
	1.1×10^{-2}		Yaws (1999)	?	21
divinyl ether C_4H_6O [109-93-3] QYKIQEUNHZKYBP-UHFFFAOYSA-N	5.4×10^{-4}		Steward et al. (1973)	L	14
	5.4×10^{-4}		Allott et al. (1973)	L	14
	1.2×10^{-3}		Duchowicz et al. (2020)	V	187
	5.6×10^{-4}		Yaws (2003)	X	238, 14
	7.3×10^{-2}		Duchowicz et al. (2020)	Q	
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	6.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
	3.8×10^{-4}		Hilal et al. (2008)	Q	
	2.0×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	5.8×10^{-4}		Abraham and Weathersby (1994)	?	21
methyl butyl ether	6.6×10^{-3}	6100	Brockbank (2013)	L	1, 520
$C_5H_{12}O$	5.5×10^{-3}		Duchowicz et al. (2020)	V	187
[628-28-4]	4.4×10^{-3}		Amoore and Buttery (1978)	V	
CXBDYQVECUFKRK-UHFFFAOYSA-N	7.1×10^{-3}		Yaws (2003)	X	238
	2.1×10^{-2}		Duchowicz et al. (2020)	Q	
	4.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	5.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
	9.6×10^{-3}		Modarresi et al. (2007)	Q	68
	5.6×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.1×10^{-2}		Katritzky et al. (1998)	Q	
2-methoxybutane	6.7×10^{-3}		Duchowicz et al. (2020)	V	187
$C_5H_{12}O$	7.1×10^{-3}		Yaws (2003)	X	238
(methyl *sec*-butyl ether)	8.1×10^{-3}		Duchowicz et al. (2020)	Q	
[6795-87-5]	7.3×10^{-3}		Gharagheizi et al. (2012)	Q	
FVNIMHIOIXPIQT-UHFFFAOYSA-N	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	7.2×10^{-3}		Gharagheizi et al. (2010)	Q	247
	6.2×10^{-3}		Hilal et al. (2008)	Q	
	1.6×10^{-2}		Modarresi et al. (2007)	Q	68
	8.6×10^{-3}		Yaws (1999)	?	21
methyl isobutyl ether	4.3×10^{-3}	6700	Brockbank (2013)	L	
$C_5H_{12}O$	4.5×10^{-3}		Duchowicz et al. (2020)	V	187
[625-44-5]	7.2×10^{-3}		Yaws (2003)	X	238
ZYVYEJXMYBUCMN-UHFFFAOYSA-N	8.1×10^{-3}		Duchowicz et al. (2020)	Q	
	2.3×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
	7.1×10^{-3}		Modarresi et al. (2007)	Q	68
	5.6×10^{-3}		Yaffe et al. (2003)	Q	249, 273
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
	8.6×10^{-3}		Yaws (1999)	?	21

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl *tert*-butyl ether	1.2×10^{-2}	5100	Schwardt et al. (2021)	L	1
$CH_3OC(CH_3)_3$	1.3×10^{-2}	5900	Brockbank (2013)	L	1
(MTBE)	1.7×10^{-2}	9100	Hiatt (2013)	M	
[1634-04-4]	2.4×10^{-2}	18000	Zhang et al. (2013)	M	326
BZLVMXJERCGZMT-UHFFFAOYSA-N	3.2×10^{-2}		Zhang et al. (2013)	M	327
	1.9×10^{-2}	5300	Hwang et al. (2010)	M	33, 521, 11
	1.1×10^{-2}	4800	Sieg et al. (2009)	M	328
	1.1×10^{-2}	4400	Falabella and Teja (2008)	M	11, 340
	1.5×10^{-2}	5900	Böhme et al. (2008)	M	
	1.2×10^{-2}	5100	Haimi et al. (2006)	M	522
	1.2×10^{-2}	5000	Arp and Schmidt (2004)	M	523
	1.4×10^{-2}	4500	Fischer et al. (2004)	M	
	7.2×10^{-3}	3200	Bierwagen and Keller (2001)	M	
	1.7×10^{-2}		Miller and Stuart (2000)	M	73
	2.3×10^{-2}		Park et al. (1997)	M	
	1.9×10^{-2}	15000	Robbins et al. (1993)	M	524
	1.4×10^{-2}		Mackay et al. (2006c)	V	
	1.0×10^{-1}	3700	Fukuchi et al. (2002)	V	
	1.6×10^{-2}		Park et al. (1997)	V	
	1.4×10^{-2}		Mackay et al. (1993)	V	
	2.0×10^{-2}		Hwang et al. (1992)	V	
	1.7×10^{-2}		Guthrie (1973)	V	
	1.7×10^{-2}		Bagno et al. (1991)	T	475
	1.8×10^{-2}		Yaws (2003)	X	259
	1.0×10^{-2}		Dupeux et al. (2022)	Q	260
	5.7×10^{-3}		Keshavarz et al. (2022)	Q	
	3.5×10^{-3}		Duchowicz et al. (2020)	Q	185
	1.3×10^{-3}		Wang et al. (2017)	Q	81, 239
	6.0×10^{-3}		Wang et al. (2017)	Q	81, 240
	1.5×10^{-2}		Wang et al. (2017)	Q	81, 241
	2.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	3.9×10^{-3}		Hilal et al. (2008)	Q	
	1.3×10^{-2}		Modarresi et al. (2007)	Q	68
		6300	Kühne et al. (2005)	Q	
	1.8×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.4×10^{-2}		English and Carroll (2001)	Q	231, 232
	1.1×10^{-2}		Katritzky et al. (1998)	Q	
	8.6×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	4.3×10^{-3}		Suzuki et al. (1992)	Q	233
	1.7×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		6000	Kühne et al. (2005)	?	
	1.8×10^{-2}		Yaws (1999)	?	21

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethyl propyl ether	8.7×10^{-3}		Duchowicz et al. (2020)	V	187
$C_2H_5OC_3H_7$	8.6×10^{-3}		Hine and Mookerjee (1975)	V	
[628-32-0]	8.6×10^{-3}		Butler and Ramchandani (1935)	V	
NVJUHMXYKCUMQA-UHFFFAOYSA-N	6.4×10^{-3}		Yaws (2003)	X	238
	7.7×10^{-3}		Howard and Meylan (1997)	X	448
	7.0×10^{-3}		Duchowicz et al. (2020)	Q	
	8.2×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	7.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
	7.9×10^{-3}		Hilal et al. (2008)	Q	
	1.4×10^{-2}		Modarresi et al. (2007)	Q	68
	8.6×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
	5.7×10^{-3}		Suzuki et al. (1992)	Q	233
	7.9×10^{-3}		Yaws (1999)	?	21
ethyl isopropyl ether	8.1×10^{-3}		Yaws (2003)	X	238
$C_5H_{12}O$	2.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[625-54-7]	9.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
XSJVWZAETSBXKU-UHFFFAOYSA-N					
2,2-dimethoxypropane	1.4×10^{-1}		Ebert et al. (2023)	?	317
$C_5H_{12}O_2$					
[77-76-9]					
HEWZVZIVELJPQZ-UHFFFAOYSA-N					
methyl 1,2-dimethylpropyl ether	4.6×10^{-3}		Yaws (2003)	X	238
$C_6H_{14}O$	3.8×10^{-3}		Gharagheizi et al. (2012)	Q	
[62016-49-3]	5.7×10^{-3}		Gharagheizi et al. (2010)	Q	247
JPUDLQKLSRSRGN-UHFFFAOYSA-N					
methyl 1-ethylpropyl ether	4.4×10^{-3}		Yaws (2003)	X	238
$C_6H_{14}O$	4.3×10^{-3}		Gharagheizi et al. (2012)	Q	
[36839-67-5]	4.2×10^{-3}		Gharagheizi et al. (2010)	Q	247
CQRFEDVNTJTKFU-UHFFFAOYSA-N					
methyl 1-methylbutyl ether	4.2×10^{-3}		Yaws (2003)	X	238
$C_6H_{14}O$	6.9×10^{-3}		Gharagheizi et al. (2012)	Q	
[6795-88-6]	4.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
XSAJCGUYMQTAHL-UHFFFAOYSA-N					
methyl 2,2-dimethylpropyl ether	4.5×10^{-3}		Yaws (2003)	X	238
$C_6H_{14}O$	1.2×10^{-3}		Gharagheizi et al. (2012)	Q	
[1118-00-9]	4.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
JILHZKWLEAKYRC-UHFFFAOYSA-N					

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl 2-methylbutyl ether	4.3×10^{-3}		Yaws (2003)	X	238
$C_6H_{14}O$	2.1×10^{-3}		Gharagheizi et al. (2012)	Q	
[62016-48-2]	3.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
XGLHRCWEOMNVKS-UHFFFAOYSA-N					
methyl 3-methylbutyl ether	4.3×10^{-3}		Yaws (2003)	X	238
$C_6H_{14}O$	3.1×10^{-3}		Gharagheizi et al. (2012)	Q	
[626-91-5]	3.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
ZQAYBCWERYRAMF-UHFFFAOYSA-N					
methyl pentyl ether	3.8×10^{-3}		Yaws (2003)	X	238
$C_6H_{14}O$	3.9×10^{-3}		Gharagheizi et al. (2012)	Q	
[628-80-8]	3.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
DBUJFULDVAZULB-UHFFFAOYSA-N					
2-methoxy-2-methylbutane	9.7×10^{-3}	6600	Brockbank (2013)	L	1
$C_6H_{14}O$	5.3×10^{-2}	9400	Hwang et al. (2010)	M	521, 11
(*tert*-amyl methyl ether)	1.0×10^{-2}	7000	Haimi et al. (2006)	M	525
[994-05-8]	8.6×10^{-3}	6500	Arp and Schmidt (2004)	M	
HVZJRWJGKQPSFL-UHFFFAOYSA-N	5.2×10^{-3}		Miller and Stuart (2000)	M	73
	1.0×10^{-2}		Dohnal and Hovorka (1999)	M	
	7.0×10^{-3}		Park et al. (1997)	M	
	8.1×10^{-3}		Park et al. (1997)	V	
	4.2×10^{-3}		Yaws (2003)	X	238
	3.9×10^{-3}		Yaws (2003)	X	238
	4.7×10^{-2}		Keshavarz et al. (2022)	Q	
	3.6×10^{-3}		Duchowicz et al. (2020)	Q	300
	1.3×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.8×10^{-3}		Gharagheizi et al. (2010)	Q	247
	3.8×10^{-3}		Gharagheizi et al. (2010)	Q	247
		6600	Kühne et al. (2005)	Q	
	7.5×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		6900	Kühne et al. (2005)	?	
	5.4×10^{-3}		Yaws (1999)	?	21
	5.0×10^{-3}	7600	Pankow et al. (1996)	?	
1-ethoxy-butane	7.6×10^{-3}	5700	Brockbank (2013)	L	1
$C_6H_{14}O$	6.4×10^{-3}		Miller and Stuart (2000)	M	73
(ethyl butyl ether)	7.8×10^{-3}		Mackay et al. (2006c)	V	
[628-81-9]	7.8×10^{-3}		Mackay et al. (1993)	V	
PZHIWRCQKBBTOW-UHFFFAOYSA-N	4.0×10^{-3}		Yaws (2003)	X	238
	6.7×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
		5900	Kühne et al. (2005)	Q	
		5000	Kühne et al. (2005)	?	

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethyl isobutyl ether	4.9×10^{-3}		Yaws (2003)	X	238
$C_6H_{14}O$	3.5×10^{-3}		Gharagheizi et al. (2012)	Q	
[627-02-1]	4.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
RQUBQBFVDOLUKC-UHFFFAOYSA-N					
ethyl *sec*-butyl ether	4.9×10^{-3}		Yaws (2003)	X	238
$C_6H_{14}O$	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[2679-87-0]	5.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
VSCUCHUDCLERMY-UHFFFAOYSA-N					
ethyl *tert*-butyl ether	7.2×10^{-3}	6900	Brockbank (2013)	L	
$C_2H_5OC(CH_3)_3$	1.2×10^{-1}	13000	Hwang et al. (2010)	M	521, 11
(ETBE)	6.3×10^{-3}	6600	Sieg et al. (2009)	M	328
[637-92-3]	4.4×10^{-3}	4300	Falabella and Teja (2008)	M	11, 340
NUMQCACRALPSHD-UHFFFAOYSA-N	6.4×10^{-3}	7300	Haimi et al. (2006)	M	526
	6.1×10^{-3}	6500	Arp and Schmidt (2004)	M	
	4.2×10^{-3}		Miller and Stuart (2000)	M	73
	5.2×10^{-3}		Yaws (2003)	X	238
	7.8×10^{-3}		Keshavarz et al. (2022)	Q	
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	300
	1.1×10^{-3}		Wang et al. (2017)	Q	81, 239
	4.1×10^{-3}		Wang et al. (2017)	Q	81, 240
	1.5×10^{-2}		Wang et al. (2017)	Q	81, 241
	2.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	5.2×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
	6.0×10^{-3}		Duchowicz et al. (2020)	?	186, 21
	3.7×10^{-3}	7600	Pankow et al. (1996)	?	
dipropyl ether	2.9×10^{-3}	6400	Brockbank (2013)	L	1
$C_3H_7OC_3H_7$	3.0×10^{-3}		Li and Carr (1993)	M	
[111-43-3]	2.9×10^{-3}		Li et al. (1993)	M	
POLCUAVZOMRGSN-UHFFFAOYSA-N	2.2×10^{-3}	9100	Hartkopf and Karger (1973)	M	
	3.9×10^{-3}		Mackay et al. (2006c)	V	
	3.9×10^{-3}		Mackay et al. (1993)	V	
	5.7×10^{-3}		Hwang et al. (1992)	V	
	2.9×10^{-3}		Hine and Mookerjee (1975)	V	
	2.8×10^{-3}		Butler and Ramchandani (1935)	V	
	4.5×10^{-3}		Yaws (2003)	X	259
	4.5×10^{-3}		Yaws (2003)	X	238
	1.2×10^{-3}		Dupeux et al. (2022)	Q	260
	7.8×10^{-3}		Keshavarz et al. (2022)	Q	
	7.2×10^{-3}		Duchowicz et al. (2020)	Q	185
	4.4×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
	6.0×10^{-3}		Hilal et al. (2008)	Q	
	7.5×10^{-3}		Modarresi et al. (2007)	Q	68
		5900	Kühne et al. (2005)	Q	
	4.5×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.1×10^{-2}		Katritzky et al. (1998)	Q	
	1.0×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	4.3×10^{-3}		Suzuki et al. (1992)	Q	233
	4.5×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		7300	Kühne et al. (2005)	?	
	4.5×10^{-3}		Yaws (1999)	?	21
	1.9×10^{-3}		Hoff et al. (1993)	?	21
	4.5×10^{-3}		Yaws and Yang (1992)	?	21
	2.9×10^{-3}		Abraham et al. (1990)	?	
diisopropyl ether	4.5×10^{-3}	6600	Brockbank (2013)	L	1
$C_3H_7OC_3H_7$	1.5×10^{-2}	8400	Hwang et al. (2010)	M	521, 11
[108-20-3]	3.9×10^{-3}	6400	Arp and Schmidt (2004)	M	
ZAFNJMIOTHYJRJ-UHFFFAOYSA-N	4.3×10^{-3}		Miller and Stuart (2000)	M	73
	4.7×10^{-3}		Dohnal and Hovorka (1999)	M	
	4.8×10^{-3}		Nielsen et al. (1994)	M	
	4.2×10^{-3}		Li and Carr (1993)	M	
	4.4×10^{-3}		Li et al. (1993)	M	
	2.8×10^{-3}		Guitart et al. (1989)	M	14
	4.3×10^{-3}		HSDB (2015)	V	
	3.9×10^{-3}		Mackay et al. (2006c)	V	
	4.8×10^{-3}	6200	Fukuchi et al. (2002)	V	
	3.1×10^{-3}	6400	Pankow et al. (1996)	V	
	3.9×10^{-3}		Mackay et al. (1993)	V	
	9.9×10^{-4}		Hine and Mookerjee (1975)	V	
	9.8×10^{-4}		Hine and Weimar (1965)	V	
	5.7×10^{-3}		Yaws (2003)	X	259
	5.6×10^{-3}		Yaws (2003)	X	238
	5.7×10^{-3}		Dupeux et al. (2022)	Q	260
	7.8×10^{-3}		Keshavarz et al. (2022)	Q	
	1.1×10^{-3}		Duchowicz et al. (2020)	Q	
	1.8×10^{-3}		Wang et al. (2017)	Q	81, 239
	6.2×10^{-3}		Wang et al. (2017)	Q	81, 240
	1.2×10^{-2}		Wang et al. (2017)	Q	81, 241
	2.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	5.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
	3.7×10^{-3}		Hilal et al. (2008)	Q	
	9.6×10^{-3}		Modarresi et al. (2007)	Q	68

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		6600	Kühne et al. (2005)	Q	
	4.5×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
	8.0×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	3.5×10^{-3}		Suzuki et al. (1992)	Q	233
	3.9×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		7200	Kühne et al. (2005)	?	
	5.6×10^{-3}		Yaws (1999)	?	21
	5.7×10^{-3}		Yaws and Yang (1992)	?	21
	9.9×10^{-4}		Abraham et al. (1990)	?	
propyl isopropyl ether $C_6H_{14}O$ [627-08-7] JIEJJGMNDWIGBJ-UHFFFAOYSA-N	5.0×10^{-3}		Yaws (2003)	X	238
	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	5.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
	6.3×10^{-3}		Modarresi et al. (2007)	Q	68
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
2-ethoxy-2-methylbutane $C_7H_{16}O$ (*tert*-amyl ethyl ether) [919-94-8] KFRVYYGHSPLXSZ-UHFFFAOYSA-N	5.0×10^{-3}	7400	Brockbank (2013)	L	
	4.8×10^{-3}	7600	Haimi et al. (2006)	M	527
	5.2×10^{-4}		Duchowicz et al. (2020)	V	187
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	2.4×10^{-3}		Hilal et al. (2008)	Q	
	1.1×10^{-2}		Modarresi et al. (2007)	Q	68
tert-butyl isopropyl ether $C_7H_{16}O$ [17348-59-3] HNFSPSWQNZVCTB-UHFFFAOYSA-N	6.6×10^{-4}		Yaws (1999)	?	21
dipropylene glycol monomethyl ether $C_7H_{16}O_3$ [34590-94-8] WGYZMNBUZFHYRX-UHFFFAOYSA-N	8.6×10^{3}		Bartelt-Hunt et al. (2008)	?	21
dibutyl ether $C_4H_9OC_4H_9$ [142-96-1] DURPTKYDGMDSBL-UHFFFAOYSA-N	2.1×10^{-3}	6700	Brockbank (2013)	L	
	7.2×10^{-3}	10000	Hwang et al. (2010)	M	521, 11
	2.2×10^{-3}		Li and Carr (1993)	M	
	1.3×10^{-3}		Li et al. (1993)	M	
	2.1×10^{-3}		Ioffe et al. (1984)	M	
	2.1×10^{-3}		Mackay et al. (2006c)	V	
	2.1×10^{-3}		Mackay et al. (1993)	V	
	1.6×10^{-3}		Pierotti et al. (1959)	X	416

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.4×10^{-2}		Keshavarz et al. (2022)	Q	
	7.4×10^{-3}		Duchowicz et al. (2020)	Q	
	1.6×10^{-3}		Li et al. (2014)	Q	242
	2.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	3.1×10^{-3}		Hilal et al. (2008)	Q	
	6.1×10^{-3}		Modarresi et al. (2007)	Q	68
		6600	Kühne et al. (2005)	Q	
	1.8×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	9.9×10^{-3}		Katritzky et al. (1998)	Q	
	6.4×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	2.2×10^{-3}		Russell et al. (1992)	Q	280
	2.5×10^{-3}		Suzuki et al. (1992)	Q	233
	1.6×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		7000	Kühne et al. (2005)	?	
	1.8×10^{-2}		Yaws (1999)	?	21
	1.6×10^{-3}		Abraham et al. (1990)	?	
diisobutyl ether $C_8H_{18}O$ [628-55-7] SZNYYWIUQFZLLT-UHFFFAOYSA-N	3.7×10^{-3}		Hilal et al. (2008)	Q	
di-*sec*-butyl ether $C_8H_{18}O$ [6863-58-7] HHBZZTKMMLDNDN-UHFFFAOYSA-N	1.8×10^{-3}		Yaws (2003)	X	259
	1.8×10^{-3}		Yaws (2003)	X	238
	1.0×10^{-3}		Dupeux et al. (2022)	Q	260
	8.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.7×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.8×10^{-3}		Yaws (1999)	?	21
di-*tert*-butyl ether $C_8H_{18}O$ [6163-66-2] AQEFLFZSWDEAIP-UHFFFAOYSA-N	2.1×10^{-3}		Yaws (2003)	X	238
	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
	3.0×10^{-3}		Yaws (1999)	?	21
2-methoxy-2,4,4-trimethylpentane $C_9H_{20}O$ (methyl *tert*-octyl ether) [62108-41-2] IKZVAPMTXDXWMX-UHFFFAOYSA-N	1.9×10^{-3}		Ebert et al. (2023)	?	528
2-methoxy-2-methylheptane $C_9H_{20}O$ [76589-16-7] KJRACWZCOVHBQU-UHFFFAOYSA-N	1.9×10^{-3}	8100	Haimi et al. (2006)	M	529

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-ethoxy-2,4,4-trimethylpentane $C_{10}H_{22}O$ (ethyl tert-octyl ether) [187103-12-4] JGPJRBWLBUGAQN-UHFFFAOYSA-N	7.7×10^{-4}	6900	Haimi et al. (2006)	M	530
1,1'-oxybispentane	3.5×10^{-4}		Yaws (2003)	X	259
$C_{10}H_{22}O$	3.5×10^{-4}		Yaws (2003)	X	238
(dipentyl ether)	4.5×10^{-4}		Dupeux et al. (2022)	Q	260
[693-65-2]	4.3×10^{-3}		Gharagheizi et al. (2012)	Q	
AOPDRZXCEAKHHW-UHFFFAOYSA-N	4.3×10^{-4}		Gharagheizi et al. (2010)	Q	247
	2.7×10^{-3}		Hilal et al. (2008)	Q	
	1.0×10^{-3}		Yaws (1999)	?	21
			Brockbank (2013)	W	531
1,1'-oxybis(3-methylbutane)	6.8×10^{-3}		Duchowicz et al. (2020)	V	187
$C_{10}H_{22}O$	6.6×10^{-3}		HSDB (2015)	V	
(diisopentyl ether)	1.1×10^{-3}		Duchowicz et al. (2020)	Q	
[544-01-4]	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
AQZGPSLYZOOYQP-UHFFFAOYSA-N	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	3.3×10^{-3}		Hilal et al. (2008)	Q	
	4.8×10^{-3}		Modarresi et al. (2007)	Q	68
1,1'-oxybishexane	2.9×10^{-4}		Yaws (2003)	X	238
$C_{12}H_{26}O$	5.6×10^{-3}		Gharagheizi et al. (2012)	Q	
(dihexyl ether)	1.7×10^{-4}		Gharagheizi et al. (2010)	Q	247
[112-58-3]	1.8×10^{-3}		Hilal et al. (2008)	Q	
BPIUIOXAFBGMNB-UHFFFAOYSA-N	3.0×10^{-3}		Yaws (1999)	?	21
			Brockbank (2013)	W	532
1-ethoxy-3,7-dimethyloctane	6.7×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_{26}O$	5.3×10^{-3}		Zhang et al. (2010)	Q	288, 290
[22810-10-2]	1.3×10^{-3}		Zhang et al. (2010)	Q	288, 291
HCHHIPCZJSRFRT-UHFFFAOYSA-N	2.5×10^{-4}		Zhang et al. (2010)	Q	288, 292
diheptyl ether	2.8×10^{-5}		Yaws (2003)	X	238
$C_{14}H_{30}O$	8.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
[629-64-1]					
UJEGHEMJVNQWOJ-UHFFFAOYSA-N					
dioctyl ether	1.3×10^{-4}		Yaws (2003)	X	238
$C_{16}H_{34}O$	6.7×10^{-5}		Gharagheizi et al. (2010)	Q	247
[629-82-3]	8.2×10^{-2}		Yaws (1999)	?	21
NKJOXAZJBOMXID-UHFFFAOYSA-N					

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methoxycyclohexane $C_7H_{14}O$ [931-56-6] GHDIHPNJQVDFBL-UHFFFAOYSA-N	3.1×10^{-2}		Hilal et al. (2008)	Q	
methyl cedryl ether $C_{16}H_{28}O$ [19870-74-7] HRGPYCVTDOECMG-WALBABNVSA-N	2.5×10^{-3}		Zhang et al. (2010)	Q	288, 289
	2.4×10^{-3}		Zhang et al. (2010)	Q	288, 290
	7.7×10^{-3}		Zhang et al. (2010)	Q	288, 291
	1.2×10^{-3}		Zhang et al. (2010)	Q	288, 292
dimethoxymethane $CH_3OCH_2OCH_3$ (methylal) [109-87-5] NKDDWNXOKDWJAK-UHFFFAOYSA-N	6.1×10^{-2}	4700	Brockbank (2013)	L	
	6.3×10^{-2}	4800	Ondo and Dohnal (2007)	M	1
	6.1×10^{-2}		HSDB (2015)	V	
	5.7×10^{-2}		Pierotti et al. (1959)	X	416
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	4.6×10^{-1}		Duchowicz et al. (2020)	Q	185
	7.1×10^{-2}		Wang et al. (2017)	Q	81, 239
	3.6×10^{-1}		Wang et al. (2017)	Q	81, 240
	6.5×10^{-2}		Wang et al. (2017)	Q	81, 241
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	2.3×10^{-1}		Hilal et al. (2008)	Q	
	6.9×10^{-2}		Modarresi et al. (2007)	Q	68
	5.7×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	6.9×10^{-2}		Yaws (1999)	?	21, 12
trimethoxymethane $HC(OCH_3)_3$ [149-73-5] PYOKUURKVVELLB-UHFFFAOYSA-N	6.9×10^{-1}		Guthrie (1973)	V	
diethoxymethane $C_5H_{12}O_2$ [462-95-3] KLKFAASOGCDTDT-UHFFFAOYSA-N	1.5×10^{-1}		Duchowicz et al. (2020)	V	187
	7.5×10^{-2}		Duchowicz et al. (2020)	Q	
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	7.2×10^{-2}		Modarresi et al. (2007)	Q	68
1,1-diethoxyethane $(C_2H_5O)_2CHCH_3$ (acetal) [105-57-7] DHKHKXVYLBGOIT-UHFFFAOYSA-N	1.0×10^{-1}		Duchowicz et al. (2020)	V	187
	1.0×10^{-1}		HSDB (2015)	V	
	1.0×10^{-1}		Hine and Mookerjee (1975)	V	
	1.2×10^{-1}		Abney (2021)	Q	401
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	5.7×10^{-2}		Hilal et al. (2008)	Q	
	6.9×10^{-2}		Modarresi et al. (2007)	Q	68
	1.1×10^{-1}		Yaws (1999)	?	21

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-diethoxyethane	1.6×10^{-1}		Duchowicz et al. (2020)	V	187
$C_2H_5OC_2H_4OC_2H_5$	1.6×10^{-1}		HSDB (2015)	V	
[629-14-1]	1.6×10^{-1}		Hine and Mookerjee (1975)	V	
LZDKZFUFMNSQCJ-UHFFFAOYSA-N	1.2×10^{-1}		Howard and Meylan (1997)	X	448
	8.3×10^{-2}		Duchowicz et al. (2020)	Q	
	3.9×10^{-1}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	68
1,1,1-trimethoxyethane	6.4×10^{-1}		Guthrie (1973)	V	
$CH_3C(OCH_3)_3$					
[1445-45-0]					
HDPNBNXLBDFELL-UHFFFAOYSA-N					
1,2-dimethoxyethane	1.3	7300	Brockbank (2013)	L	1, 533
$C_4H_{10}O_2$	2.1		O'Farrell and Waghorne (2010)	M	
[110-71-4]	1.4	7200	Ondo and Dohnal (2007)	M	1
XTHFKEDIFFGKHM-UHFFFAOYSA-N	1.4	7100	Cabani et al. (1978)	T	
	9.0		HSDB (2015)	Q	100
	5.3×10^{-1}		Hilal et al. (2008)	Q	
3-oxa-1-hexanol	2.0×10^{1}	8400	Cabani et al. (1978)	T	
$C_5H_{12}O_2$	6.6×10^{2}		HSDB (2015)	Q	100
(2-propoxyethanol)	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
[2807-30-9]	9.9		Raventos-Duran et al. (2010)	Q	245
YEYKMVJDLWJFOA-UHFFFAOYSA-N	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	246
	1.0×10^{1}		Hilal et al. (2008)	Q	
	5.8		Nirmalakhandan et al. (1997)	Q	
3-oxa-1-heptanol	1.3×10^{1}	8300	Brockbank (2013)	L	
$C_6H_{14}O_2$	3.5	7700	Hiatt (2013)	M	
(2-butoxyethanol; butyl cellosolve)	1.3×10^{1}	8300	Kim et al. (2000)	M	33
[111-76-2]	2.7		Johanson and Dynésius (1988)	M	14
POAOYUHQDCAZBD-UHFFFAOYSA-N	1.6×10^{1}	8900	Cabani et al. (1978)	T	
	1.7×10^{1}		Keshavarz et al. (2022)	Q	
	7.4		Duchowicz et al. (2020)	Q	185
	5.4		Wang et al. (2017)	Q	81, 239
	1.9×10^{1}		Wang et al. (2017)	Q	81, 240
	3.2		Wang et al. (2017)	Q	81, 241
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	272, 244
	7.8		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	246
	7.7		Hilal et al. (2008)	Q	
	1.9×10^{1}		Modarresi et al. (2007)	Q	68
	4.5		Nirmalakhandan et al. (1997)	Q	
	6.2		Duchowicz et al. (2020)	?	186, 21
	2.8×10^{1}		Yaws (1999)	?	21, 12

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methoxy-2-propanol	4.8		Johanson and Dynésius (1988)	M	14
$C_4H_{10}O_2$	1.1×10^{1}		Hilal et al. (2008)	C	
[107-98-2]	9.2		Keshavarz et al. (2022)	Q	
ARXJGSRGQADJSQ-UHFFFAOYSA-N	6.7		Duchowicz et al. (2020)	Q	300
	8.3		Wang et al. (2017)	Q	81, 239
	4.7×10^{1}		Wang et al. (2017)	Q	81, 240
	4.9		Wang et al. (2017)	Q	81, 241
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{1}		Hilal et al. (2008)	Q	
	2.8×10^{1}		Modarresi et al. (2007)	Q	68
	1.1×10^{1}		Yaffe et al. (2003)	Q	249, 250
	3.5		Katritzky et al. (1998)	Q	
	1.1×10^{1}		Duchowicz et al. (2020)	?	186, 21
4-methyl-3-oxa-1-pentanol	4.8		Johanson and Dynésius (1988)	M	14
$C_5H_{12}O_2$	1.2×10^{1}		Keshavarz et al. (2022)	Q	
(2-isopropoxyethanol)	2.6		Duchowicz et al. (2020)	Q	185
[109-59-1]	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	272, 244
HCGFUIQPSOCUHI-UHFFFAOYSA-N	7.8		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	246
	7.9		Hilal et al. (2008)	Q	
	2.7×10^{1}		Modarresi et al. (2007)	Q	68
	1.1×10^{1}		Duchowicz et al. (2020)	?	186, 21
1,2-dibutoxyethane	9.9×10^{-1}		HSDB (2015)	V	
$C_{10}H_{22}O_2$	1.4×10^{-1}		Hilal et al. (2008)	Q	
[112-48-1]	1.1×10^{-1}		Modarresi et al. (2007)	Q	68
GDXHBFHOEYVPED-UHFFFAOYSA-N					
3,6-dioxa-1-decanol	1.4×10^{3}		Kim et al. (2000)	M	
$C_8H_{18}O_3$					
(butyl carbitol)					
[112-34-5]					
OAYXUHPQHDHDDZ-UHFFFAOYSA-N					
diethylene glycol dibutyl ether	2.5	13000	Brockbank (2013)	L	
$C_{12}H_{26}O_3$	3.9		Duchowicz et al. (2020)	V	187
[112-73-2]	6.1		Yaws (2003)	X	238, 12
KZVBBTZJMSWGTK-UHFFFAOYSA-N	1.3		Duchowicz et al. (2020)	Q	
	6.0		Gharagheizi et al. (2010)	Q	247
	3.5		Hilal et al. (2008)	Q	
	1.5		Modarresi et al. (2007)	Q	68
	4.0		Yaws (1999)	?	21, 12

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl vinyl ether	1.5×10^{-3}		HSDB (2015)	V	
C_3H_6O	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
[107-25-5]	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
XJRBAMWJDBPFIM-UHFFFAOYSA-N	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	246
ethyl vinyl ether	1.8×10^{-3}		Duchowicz et al. (2020)	V	187
C_4H_8O	2.3×10^{-2}		Duchowicz et al. (2020)	Q	
[109-92-2]	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
FJKIXWOMBXYWOQ-UHFFFAOYSA-N	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
propyl vinyl ether $C_5H_{10}O$ [764-47-6] OVGRCEFMXPHEBL-UHFFFAOYSA-N	3.1×10^{-3}	4800	Hwang et al. (2010)	M	521, 11
allyl glycidyl ether $C_6H_{10}O_2$ [106-92-3] LSWYGACWGAICNM-UHFFFAOYSA-N	2.1		Ebert et al. (2023)	?	317
butyl vinyl ether	4.6×10^{-3}		Duchowicz et al. (2020)	V	187
$C_6H_{12}O$	4.5×10^{-3}		HSDB (2015)	V	
[111-34-2]	7.3×10^{-4}		Dupeux et al. (2022)	Q	260
UZKWTJUDCOPSNM-UHFFFAOYSA-N	2.5×10^{-2}		Duchowicz et al. (2020)	Q	
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	2.5×10^{-3}		Modarresi et al. (2007)	Q	68
isobutyl vinyl ether	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
$C_6H_{12}O$	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	245
[109-53-5]	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	246
OZCMOJQQLBXBKI-UHFFFAOYSA-N	1.9×10^{-4}		Hilal et al. (2008)	Q	
	2.5×10^{-3}		Modarresi et al. (2007)	Q	68
benzyl methyl ether	1.1×10^{-1}		Duchowicz et al. (2020)	V	187
$C_8H_{10}O$	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
[538-86-3]					
GQKZBCPTCWJTAS-UHFFFAOYSA-N					
benzyl ethyl ether	6.7×10^{-2}		Dupeux et al. (2022)	Q	260
$C_9H_{12}O$					
[539-30-0]					
AXPZDYVDTMMLNB-UHFFFAOYSA-N					

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methoxybenzene	2.9×10^{-2}	4200	Brockbank (2013)	L	
$C_6H_5OCH_3$	2.9×10^{-2}	4200	Brockbank et al. (2013)	M	
(anisole)	2.6×10^{-2}	4800	Dewulf et al. (1999)	M	
[100-66-3]	3.2×10^{-2}		Li and Carr (1993)	M	
RDOXTESZEPMUJZ-UHFFFAOYSA-N	2.0×10^{-2}		Duchowicz et al. (2020)	V	187
	3.1×10^{-2}		Mackay et al. (2006c)	V	
	4.0×10^{-2}		Mackay et al. (1993)	V	
	2.3×10^{-3}		Hine and Mookerjee (1975)	V	
	2.3×10^{-3}		Hine and Weimar (1965)	R	
	2.7×10^{-3}		Yaws (2003)	X	259
	2.7×10^{-3}		Yaws (2003)	X	238
	6.9×10^{-2}		Schüürmann (2000)	C	21
	1.9×10^{-2}		Dupeux et al. (2022)	Q	260
	1.2×10^{-1}		Duchowicz et al. (2020)	Q	
	2.3×10^{-3}		HSDB (2015)	Q	100
	1.9×10^{-2}		Li et al. (2014)	Q	242
	1.3×10^{-1}		Gharagheizi et al. (2010)	Q	247
	9.0×10^{-3}		Hilal et al. (2008)	Q	
	3.3×10^{-2}		Modarresi et al. (2007)	Q	68
		4500	Kühne et al. (2005)	Q	
	8.6×10^{-3}		Yao et al. (2002)	Q	230
	1.2×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	2.3×10^{-3}		Suzuki et al. (1992)	Q	233
		4300	Kühne et al. (2005)	?	
	2.7×10^{-3}		Yaws (1999)	?	21
	2.5×10^{-2}		Abraham et al. (1990)	?	
ethoxybenzene	1.7×10^{-2}		Li and Carr (1993)	M	
$C_8H_{10}O$	2.2×10^{-2}		Duchowicz et al. (2020)	V	187
(phenetole)	2.2×10^{-2}		HSDB (2015)	V	
[103-73-1]	2.3×10^{-2}		Mackay et al. (2006c)	V	
DLRJIFUOBPOJNS-UHFFFAOYSA-N	4.4×10^{-2}		Duchowicz et al. (2020)	Q	
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	6.5×10^{-3}		Hilal et al. (2008)	Q	
	2.9×10^{-2}		Modarresi et al. (2007)	Q	68
	2.6×10^{-1}		Katritzky et al. (1998)	Q	
	1.0×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	1.7×10^{-2}		Abraham et al. (1990)	?	
1,2-dimethoxybenzene		5100	Kühne et al. (2005)	Q	
$C_8H_{10}O_2$		2400	Kühne et al. (2005)	?	
[91-16-7]					
ABDKAPXRBAPSQN-UHFFFAOYSA-N					

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-phenoxyethanol	2.1×10^{2}		Duchowicz et al. (2020)	V	187
$C_8H_{10}O_2$	2.0×10^{2}		HSDB (2015)	V	
[122-99-6]	4.0×10^{1}		Duchowicz et al. (2020)	Q	
QCDWFXQBSFUVSP-UHFFFAOYSA-N	3.4×10^{1}		Hilal et al. (2008)	Q	
	1.4×10^{2}		Modarresi et al. (2007)	Q	68
2-(phenylmethoxy)-ethanol	8.2×10^{1}		Duchowicz et al. (2020)	V	187
$C_9H_{12}O_2$	4.4×10^{1}		Duchowicz et al. (2020)	Q	
[622-08-2]	1.6×10^{3}		Raventos-Duran et al. (2010)	Q	243, 244
CUZKCNWZBXLAJX-UHFFFAOYSA-N	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{3}		Raventos-Duran et al. (2010)	Q	246
	1.5×10^{2}		Hilal et al. (2008)	Q	
	7.0×10^{2}		Modarresi et al. (2007)	Q	68
1,2,3-trimethoxybenzene $C_9H_{12}O_3$ [634-36-6] CRUILBNAQILVHZ-UHFFFAOYSA-N	3.6		Schüürmann (2000)	V	
1-methoxy-4-(1-propenyl)-benzene	9.9×10^{-2}	6200	van Roon et al. (2005)	V	
$C_{10}H_{12}O$	1.0×10^{-1}		Yaws (2003)	X	259
(anethole)	3.7×10^{-2}		Dupeux et al. (2022)	Q	260
[104-46-1]	1.4×10^{-1}		HSDB (2015)	Q	100
RUVINXPYWBROJD-UHFFFAOYSA-N	2.0×10^{-2}		Hilal et al. (2008)	Q	
	1.0×10^{-1}		Yaws (1999)	?	21
2-methoxy-4-(2-propenyl)-phenol	9.2		McFall et al. (2020)	M	
$C_{10}H_{12}O_2$	5.0		Duchowicz et al. (2020)	V	187
(eugenol)	6.9		Martins et al. (2017)	V	316
[97-53-0]	5.1		HSDB (2015)	V	
RRAFCDWBNXTKKO-UHFFFAOYSA-N	7.2	9700	van Roon et al. (2005)	V	
	3.9		Dupeux et al. (2022)	Q	260
	3.5×10^{-1}		Abney (2021)	Q	401
	2.0×10^{1}		Duchowicz et al. (2020)	Q	
	5.7		McFall et al. (2020)	Q	476
1,2-dimethoxy-4-(2-propenyl)-benzene	1.8		Duchowicz et al. (2020)	V	187
$C_{11}H_{14}O_2$	1.8		HSDB (2015)	V	
[93-15-2]	1.0		Duchowicz et al. (2020)	Q	
ZYEMGPIYFIJGTP-UHFFFAOYSA-N	3.6		Hilal et al. (2008)	Q	
	1.9×10^{-1}		Modarresi et al. (2007)	Q	68

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
diphenyl ether	1.9×10^{-2}		Brockbank (2013)	L	
$C_{12}H_{10}O$	3.5×10^{-2}		Duchowicz et al. (2020)	V	187
[101-84-8]	3.5×10^{-2}		HSDB (2015)	V	
USIUVYZYUHIAEV-UHFFFAOYSA-N	3.7×10^{-2}		Mackay et al. (2006c)	V	
	1.1×10^{-1}		Kurz and Ballschmiter (1999)	V	
	3.7×10^{-2}		Mackay et al. (1993)	V	
	1.8×10^{-2}		Yaws (2003)	X	238
	2.9×10^{-1}		Duchowicz et al. (2020)	Q	
	1.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
	1.7×10^{-2}		Hilal et al. (2008)	Q	
	1.7×10^{-1}		Modarresi et al. (2007)	Q	68
	1.9×10^{-2}		Yaws (1999)	?	21
(phenoxymethyl)-oxirane	1.2×10^{1}		Duchowicz et al. (2020)	V	187
$C_9H_{10}O_2$	1.2×10^{1}		HSDB (2015)	V	
[122-60-1]	4.8		Duchowicz et al. (2020)	Q	
FQYUMYWMJTYZTK-UHFFFAOYSA-N	6.1×10^{-1}		Hilal et al. (2008)	Q	
	1.9		Modarresi et al. (2007)	Q	68
1-dodecyl-4-phenoxybenzene	3.4×10^{-3}		Zhang et al. (2010)	Q	288, 289
$C_{24}H_{34}O$	1.4×10^{-3}		Zhang et al. (2010)	Q	288, 290
[119345-02-7]	1.7×10^{-2}		Zhang et al. (2010)	Q	288, 291
XSAHYEQPUFJGKW-UHFFFAOYSA-N	7.7×10^{-2}		Zhang et al. (2010)	Q	288, 292
2,2,4-trimethyl-4-(4-(4-(2,4,4-trimethylpentan-2-yl)phenoxy)phenyl)pentane	1.3×10^{-3}		Zhang et al. (2010)	Q	288, 289
$C_{28}H_{42}O$	1.2×10^{-3}		Zhang et al. (2010)	Q	288, 290
[61702-88-3]	5.4×10^{-2}		Zhang et al. (2010)	Q	288, 291
AJDONJVWDSZZQF-UHFFFAOYSA-N	6.9×10^{-3}		Zhang et al. (2010)	Q	288, 292
etofenprox $C_{25}H_{28}O_3$ [80844-07-1] YREQHYQNNWYQCJ-UHFFFAOYSA-N	7.4×10^{1}		Maniere et al. (2011)	?	166
di-*tert*-butyl *sec*-butylidene diperoxide	1.2×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_{26}O_4$	6.1×10^{-5}		Zhang et al. (2010)	Q	288, 290
[2167-23-9]	1.6×10^{-2}		Zhang et al. (2010)	Q	288, 291
HQOVXPHOJANJBR-UHFFFAOYSA-N	1.1		Zhang et al. (2010)	Q	288, 292
peroxide, 1,1-dimethylethyl 1-methyl-1-phenylethyl	1.4×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{13}H_{20}O_2$	4.8×10^{-3}		Zhang et al. (2010)	Q	288, 290
[3457-61-2]	1.6×10^{-2}		Zhang et al. (2010)	Q	288, 291
BIISIZOQPWZPPS-UHFFFAOYSA-N	1.9×10^{-1}		Zhang et al. (2010)	Q	288, 292

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
di-*tert*-butyl 1,1,4,4-tetramethyltetramethylene diperoxide	3.9×10^{-3}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_{34}O_4$	7.9×10^{-4}		Zhang et al. (2010)	Q	288, 290
[78-63-7]	1.3×10^{-1}		Zhang et al. (2010)	Q	288, 291
DMWVYCCGCQPJEA-UHFFFAOYSA-N	3.4×10^{-1}		Zhang et al. (2010)	Q	288, 292
1,4-bis(1-*tert*-butylperoxy-1-methyl-ethyl)benzene	1.0×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{20}H_{34}O_4$	1.8×10^{-2}		Zhang et al. (2010)	Q	288, 290
[2781-00-2]	2.9×10^{-1}		Zhang et al. (2010)	Q	288, 291
GWQOYRSARAWVTC-UHFFFAOYSA-N	8.6		Zhang et al. (2010)	Q	288, 292
MCM:CH3OCH2OOH	2.2×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_6O_3$	6.9×10^{1}		Wang et al. (2017)	Q	81, 240
CDXAGPPPWKCPRI-UHFFFAOYSA-N	7.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ETHOXOOH	7.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_4O_3$	1.7×10^{2}		Wang et al. (2017)	Q	81, 240
NOEKFNMWGHEGBN-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DMMAOOH	5.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_8O_4$	3.0×10^{2}		Wang et al. (2017)	Q	81, 240
SHLFZQKLTPTTSZ-UHFFFAOYSA-N	1.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DMMBOOH	5.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_8O_4$	5.6×10^{1}		Wang et al. (2017)	Q	81, 240
HODDSHZVZWXLHR-UHFFFAOYSA-N	2.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:ETOMEOOH	1.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_3H_8O_3$	3.9×10^{1}		Wang et al. (2017)	Q	81, 240
NZBMKAZNWPZJND-UHFFFAOYSA-N	6.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MEMOXYCO3H	2.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_4$	7.1×10^{1}		Wang et al. (2017)	Q	81, 240
PWWCDEMRYRBWOJ-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DIETETOOH	1.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	1.3×10^{1}		Wang et al. (2017)	Q	81, 240
CXWWPQGYBJCHJL-UHFFFAOYSA-N	4.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ETOC2OOH	1.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	8.1×10^{1}		Wang et al. (2017)	Q	81, 240
NYVGIYPKZJSYSP-UHFFFAOYSA-N	6.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ETOMECO3H	2.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	3.4×10^{1}		Wang et al. (2017)	Q	81, 240
ULYBJOMJQUHMOL-UHFFFAOYSA-N	4.8		Wang et al. (2017)	Q	81, 241

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:IPRMETOOH	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	4.5		Wang et al. (2017)	Q	81, 240
PSBSELFEZHDPTA-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:BOXMOOH	1.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	2.0×10^{1}		Wang et al. (2017)	Q	81, 240
DCHWALHTYQHXTG-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:EIPEOOH	8.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	3.0		Wang et al. (2017)	Q	81, 240
ZZXLAMSYBUVKJS-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:IPROC21OOH	1.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	6.6		Wang et al. (2017)	Q	81, 240
VGMUBGNCFVOQDX-UHFFFAOYSA-N	2.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MTBEAOOH	8.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	8.5		Wang et al. (2017)	Q	81, 240
BGZKVDIFKPQYHL-UHFFFAOYSA-N	6.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MTBEBCO3H	1.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	4.7		Wang et al. (2017)	Q	81, 240
NGYXBYFCPPVOQA-UHFFFAOYSA-N	3.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:MTBEBOOH	8.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_3$	2.5×10^{1}		Wang et al. (2017)	Q	81, 240
FPTBRWWJTBOWHN-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:BOXMCO3H	1.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	1.7×10^{1}		Wang et al. (2017)	Q	81, 240
BMXLBBYCODRNIJ-UHFFFAOYSA-N	8.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:DIIPRETOOH	8.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	1.6		Wang et al. (2017)	Q	81, 240
PFVPTWUDXVSVAC-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ETBEACO3H	1.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	3.4		Wang et al. (2017)	Q	81, 240
UAVAAIVEDVDYSQ-UHFFFAOYSA-N	3.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:ETBEAOOH	8.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	1.7×10^{1}		Wang et al. (2017)	Q	81, 240
ITRUGVUCIYLYDK-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ETBEBOOH	8.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	2.5		Wang et al. (2017)	Q	81, 240
VOZHKKMLSSYDIG-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ETBECCO3H	1.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	8.9		Wang et al. (2017)	Q	81, 240
AELSWALKLVZVPO-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:ETBECOOH	8.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	2.0×10^{1}		Wang et al. (2017)	Q	81, 240
WJMPPRSRRBMJID-UHFFFAOYSA-N	5.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:IPROMC2OOH	1.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	2.2×10^{1}		Wang et al. (2017)	Q	81, 240
JCIUPJDJCBRYHD-UHFFFAOYSA-N	2.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:IPROMCCO3H	1.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_4$	7.8		Wang et al. (2017)	Q	81, 240
SFJQIQZNOBLTBZ-UHFFFAOYSA-N	7.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:BCSOZ	9.1		Wang et al. (2017)	Q	81, 239
$C_{15}H_{24}O_3$	2.0×10^{-1}		Wang et al. (2017)	Q	81, 240
DXZCAIRIBLPJLG-UHFFFAOYSA-N	7.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CH3OCH2OH	8.1		Wang et al. (2017)	Q	81, 239
$C_2H_6O_2$	5.4×10^{1}		Wang et al. (2017)	Q	81, 240
VHWYCFISAQVCCP-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DMMAOH	1.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_3H_8O_3$	4.1×10^{2}		Wang et al. (2017)	Q	81, 240
YANOHILBFNXRFM-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DMMBOH	2.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_3H_8O_3$	4.6×10^{1}		Wang et al. (2017)	Q	81, 240
IIGJYLXJNYBXEO-UHFFFAOYSA-N	9.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ETOMEOH	6.8		Wang et al. (2017)	Q	81, 239
$C_3H_8O_2$	3.0×10^{1}		Wang et al. (2017)	Q	81, 240
RRLWYLINGKISHN-UHFFFAOYSA-N	3.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MO2EOLA2OH	9.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_8O_3$	9.6×10^{3}		Wang et al. (2017)	Q	81, 240
CSCSROFYRUZJJH-UHFFFAOYSA-N	4.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MO2EOLAOOH	8.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_3H_8O_4$	2.8×10^{4}		Wang et al. (2017)	Q	81, 240
PFSIOEPXGRVTPO-UHFFFAOYSA-N	6.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:MO2EOLB2OH	2.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_3H_8O_3$	2.0×10^{4}		Wang et al. (2017)	Q	81, 240
ONSWVOSXVUHESJ-UHFFFAOYSA-N	4.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:MO2EOLBOOH	6.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_3H_8O_4$	1.4×10^{5}		Wang et al. (2017)	Q	81, 240
VULCDXDIAONDTM-UHFFFAOYSA-N	2.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:DIETETOH	6.0		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_2$	1.7×10^{1}		Wang et al. (2017)	Q	81, 240
CAFAOQIVXSSFSY-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:EOX2ETA2OH	8.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	6.6×10^{3}		Wang et al. (2017)	Q	81, 240
WWVBRUMYFUDEJQ-UHFFFAOYSA-N	4.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:EOX2ETB2OH	2.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	8.9×10^{3}		Wang et al. (2017)	Q	81, 240
RZYMXMZJVMXDRP-UHFFFAOYSA-N	2.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:EOX2OLAOOH	6.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_4$	1.7×10^{4}		Wang et al. (2017)	Q	81, 240
OSAXOMWTXDBXFG-UHFFFAOYSA-N	4.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:EOX2OLBOOH	6.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_4$	6.2×10^{4}		Wang et al. (2017)	Q	81, 240
IWDPPKCJRWMAAT-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:H2C3OCOH	2.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	1.0×10^{4}		Wang et al. (2017)	Q	81, 240
OAPWFUZUONIVKV-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:H2C3OCOOH	6.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_4$	1.3×10^{5}		Wang et al. (2017)	Q	81, 240
ZZOFHQOVQLUGOX-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:IPRMEETOH	4.2		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_2$	9.3		Wang et al. (2017)	Q	81, 240
BFSUQRCCKXZXEX-UHFFFAOYSA-N	7.4		Wang et al. (2017)	Q	81, 241
MCM:PR2OHMOOOH	7.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_4$	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
BIISZUJLPYTCKS-UHFFFAOYSA-N	2.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:PROH2MOX	8.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_{10}O_3$	7.6×10^{3}		Wang et al. (2017)	Q	81, 240
OEYNWAWWSZUGDU-UHFFFAOYSA-N	9.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:BOXMOH	4.7		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	1.5×10^{1}		Wang et al. (2017)	Q	81, 240
CRHLZRRTZDFDAJ-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:EIPEOH	3.4		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	6.3		Wang et al. (2017)	Q	81, 240
MGMXTRZFWPWZFH-UHFFFAOYSA-N	7.4		Wang et al. (2017)	Q	81, 241
MCM:HIEPOXB	1.5×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_4$	1.8×10^{8}		Wang et al. (2017)	Q	81, 240
YTIKZIBPNMOYQX-UHFFFAOYSA-N	5.6×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:IEACO3H	7.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	3.6×10^{3}		Wang et al. (2017)	Q	81, 240
WBOLSVSGSKMCPN-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:IECCO3H	7.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_5$	2.7×10^{3}		Wang et al. (2017)	Q	81, 240
CEWHGLGNUIHIJU-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:IEPOXA	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	9.3×10^{4}		Wang et al. (2017)	Q	81, 240
CIDUHKBATDRWPE-UHFFFAOYSA-N	4.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:IEPOXC	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	4.7×10^{4}		Wang et al. (2017)	Q	81, 240
REKLCZSNEUFIBP-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:IPROC21OH	5.6		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	1.0×10^{1}		Wang et al. (2017)	Q	81, 240
PWLPTLCMMFJZIU-UHFFFAOYSA-N	9.8		Wang et al. (2017)	Q	81, 241
MCM:MTBEAOH	3.4		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	7.4		Wang et al. (2017)	Q	81, 240
NHNNIMVRQJIZFW-UHFFFAOYSA-N	2.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MTBEBOH	4.8		Wang et al. (2017)	Q	81, 239
$C_5H_{12}O_2$	1.5×10^{1}		Wang et al. (2017)	Q	81, 240
VMPUAIZSESMILD-UHFFFAOYSA-N	3.6		Wang et al. (2017)	Q	81, 241
MCM:BOX2E2OH	5.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	3.6×10^{3}		Wang et al. (2017)	Q	81, 240
WQHNZXURJISVCT-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:BOX2OHAOOH	4.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_4$	3.6×10^{4}		Wang et al. (2017)	Q	81, 240
XRZMTAXNHOGTME-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:BOX2OHBOOH	4.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_4$	8.1×10^{3}		Wang et al. (2017)	Q	81, 240
LCMMTUJPIXBSDS-UHFFFAOYSA-N	2.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:BOXOHETOH	1.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_3$	6.0×10^{3}		Wang et al. (2017)	Q	81, 240
QLKNFVRAYYHHDF-UHFFFAOYSA-N	7.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:DIIPRETOH	3.2		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	3.5		Wang et al. (2017)	Q	81, 240
FRKCZFUUIQCQPC-UHFFFAOYSA-N	4.8		Wang et al. (2017)	Q	81, 241
MCM:ETBEAOH	3.7		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	1.0×10^{1}		Wang et al. (2017)	Q	81, 240
WOSZILCYMCIWFB-UHFFFAOYSA-N	3.0		Wang et al. (2017)	Q	81, 241
MCM:ETBEBOH	3.2		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	4.1		Wang et al. (2017)	Q	81, 240
DUNYNUFVLYAWTI-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	81, 241

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:ETBECOH	3.7		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	8.5		Wang et al. (2017)	Q	81, 240
BDLXTDLGTWNUFM-UHFFFAOYSA-N	2.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:IPROMC2OH	6.5		Wang et al. (2017)	Q	81, 239
$C_6H_{14}O_2$	1.3×10^{1}		Wang et al. (2017)	Q	81, 240
ZFEKANLLFQEKED-UHFFFAOYSA-N	4.2		Wang et al. (2017)	Q	81, 241
1-butoxy-2-propanol	5.0		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O_2$	1.7×10^{1}		Wang et al. (2017)	Q	81, 240
(MCM:BOX2PROL)	8.7×10^{-1}		Wang et al. (2017)	Q	81, 241
[5131-66-8]					
RWNUSVWFHDHRCJ-UHFFFAOYSA-N					
MCM:BOXOHPROL	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O_3$	7.8×10^{3}		Wang et al. (2017)	Q	81, 240
ITIQJVOJGXCBQB-UHFFFAOYSA-N	6.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:BOXPOLAOOH	3.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O_4$	2.6×10^{4}		Wang et al. (2017)	Q	81, 240
JGCUFCZSCOGTSN-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:BOXPOLBOOH	4.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O_4$	6.0×10^{3}		Wang et al. (2017)	Q	81, 240
AJCGQJRNRRPZGZ-UHFFFAOYSA-N	9.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:BOXPR2OH	5.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{16}O_3$	2.9×10^{3}		Wang et al. (2017)	Q	81, 240
XKPKIGSYCLTAJO-UHFFFAOYSA-N	4.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:BCSOZOH	1.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{26}O_5$	1.1×10^{5}		Wang et al. (2017)	Q	81, 240
JQRHKAPCWHNLMS-UHFFFAOYSA-N	3.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:BCSOZOOH	8.5×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{26}O_6$	1.4×10^{5}		Wang et al. (2017)	Q	81, 240
VCKYKGHDZKOMMJ-UHFFFAOYSA-N	5.0×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:MEMOXYCHO	2.1		Wang et al. (2017)	Q	81, 239
$C_3H_6O_2$	2.0×10^{1}		Wang et al. (2017)	Q	81, 240
YSEFYOVWKJXNCH-UHFFFAOYSA-N	3.0		Wang et al. (2017)	Q	81, 241
MCM:EOX2ETCHO	2.0		Wang et al. (2017)	Q	81, 239
$C_4H_8O_2$	6.9		Wang et al. (2017)	Q	81, 240
IAHZBRPNDIVNNR-UHFFFAOYSA-N	2.3		Wang et al. (2017)	Q	81, 241
MCM:EPXC4DIAL	6.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_3$	7.1×10^{3}		Wang et al. (2017)	Q	81, 240
IRJHVNZVWOCVLV-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	81, 241

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:EPXDLCO3H	7.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_5$	9.6×10^{4}		Wang et al. (2017)	Q	81, 240
OKYIQGCZHSMTGV-UHFFFAOYSA-N	7.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:EPXMC4DIAL	3.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_3$	1.2×10^{3}		Wang et al. (2017)	Q	81, 240
SYCYSIWUSJFZTN-UHFFFAOYSA-N	7.4		Wang et al. (2017)	Q	81, 241
MCM:EPXMDLCO3H	3.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_5$	3.1×10^{4}		Wang et al. (2017)	Q	81, 240
LLYFBEXLHOFXFI-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MTBEBCHO	1.1		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_2$	1.5		Wang et al. (2017)	Q	81, 240
HSCUZOQCNBPBST-UHFFFAOYSA-N	5.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:BOX2ECHO	1.2		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	6.5		Wang et al. (2017)	Q	81, 240
RPLPGIHCAYAYKX-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
MCM:BZEMUCCO3H	2.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_5$	1.1×10^{5}		Wang et al. (2017)	Q	81, 240
LTCNUSVDDXPSIF-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:BZEPOXMUC	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_3$	5.4×10^{3}		Wang et al. (2017)	Q	81, 240
NQHJMOLWTXQPLS-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:EPXM2C4DAL	2.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	3.0×10^{2}		Wang et al. (2017)	Q	81, 240
QTKFOEFUZGORGI-UHFFFAOYSA-N	4.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:EPXM2DCO3H	2.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	6.8×10^{3}		Wang et al. (2017)	Q	81, 240
CFBRPHMFNHCZFV-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ETBEACHO	9.8×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	1.2		Wang et al. (2017)	Q	81, 240
HHIYJPQUMUPZIZ-UHFFFAOYSA-N	4.5×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:ETBECCHO	9.8×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	3.5		Wang et al. (2017)	Q	81, 240
SMUYZOMGNHBYHU-UHFFFAOYSA-N	6.8		Wang et al. (2017)	Q	81, 241
MCM:IPROMCCHO	1.6		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_2$	3.3		Wang et al. (2017)	Q	81, 240
AAPDVSFWBQNMLJ-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	81, 241
MCM:EPXMEC4DAL	1.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	2.8×10^{2}		Wang et al. (2017)	Q	81, 240
MOJUYSNCEBTQMW-UHFFFAOYSA-N	2.5		Wang et al. (2017)	Q	81, 241

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:EPXMEDCO3H	1.7×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	3.7×10^{3}		Wang et al. (2017)	Q	81, 240
IBELTJZUJIPVRI-UHFFFAOYSA-N	5.6		Wang et al. (2017)	Q	81, 241
MCM:OXYEPOXMUC	5.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_3$	6.8×10^{2}		Wang et al. (2017)	Q	81, 240
QLTFECLMPRWGQQ-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:OXYMUCCO3H	6.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_5$	6.6×10^{3}		Wang et al. (2017)	Q	81, 240
PBSKNYKKTPMDFL-UHFFFAOYSA-N	8.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:OETLMUCO3H	5.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	4.0×10^{3}		Wang et al. (2017)	Q	81, 240
UVJSWMTUJCHEOZ-UHFFFAOYSA-N	5.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:OETLPOXMUC	4.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	4.6×10^{2}		Wang et al. (2017)	Q	81, 240
NORSPZZKBNMHEY-UHFFFAOYSA-N	5.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:IEACHO	7.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	4.2×10^{3}		Wang et al. (2017)	Q	81, 240
SXTKPSXTIDLSQV-UHFFFAOYSA-N	3.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:IECCHO	7.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_8O_3$	1.9×10^{3}		Wang et al. (2017)	Q	81, 240
FUNIHXJAXNKVQS-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:BZEMUCOH	1.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	1.7×10^{9}		Wang et al. (2017)	Q	81, 240
HYRDKGAOZPVDDL-UHFFFAOYSA-N	1.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:BZEMUCOOH	7.6×10^{10}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_6$	1.2×10^{9}		Wang et al. (2017)	Q	81, 240
YPGXWAYLBNMEJL-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:OXYMUCOH	3.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	1.3×10^{8}		Wang et al. (2017)	Q	81, 240
SKTLSFGOHJFJLD-UHFFFAOYSA-N	9.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:OXYMUCOOH	4.6×10^{11}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_6$	2.9×10^{8}		Wang et al. (2017)	Q	81, 240
ZBCSCRLAPOVYAB-UHFFFAOYSA-N	1.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:OETLMUCOH	2.6×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	7.4×10^{7}		Wang et al. (2017)	Q	81, 240
BKCWOZADWPGCRT-UHFFFAOYSA-N	4.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:OETLMUCOOH	4.2×10^{11}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_6$	1.7×10^{8}		Wang et al. (2017)	Q	81, 240
OMPONQJDZISYFQ-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PRONEMOOOH	1.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_4$	8.1×10^{2}		Wang et al. (2017)	Q	81, 240
WKDIYCKWLNCFHJ-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PRONEMOX	1.4		Wang et al. (2017)	Q	81, 239
$C_4H_8O_2$	1.4×10^{1}		Wang et al. (2017)	Q	81, 240
CUZLJOLBIRPEFB-UHFFFAOYSA-N	8.1		Wang et al. (2017)	Q	81, 241
MCM:EPXKTMCO3H	2.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	3.2×10^{4}		Wang et al. (2017)	Q	81, 240
ABDSVLWFPNKKBV-UHFFFAOYSA-N	4.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:EPXMKTCO3H	2.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_5$	3.2×10^{4}		Wang et al. (2017)	Q	81, 240
CAGQARJHZCESJI-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:BOXPROBOOH	7.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_4$	2.0×10^{2}		Wang et al. (2017)	Q	81, 240
YHFJWWLEGMYFFZ-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:BOXPRONE	8.1×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_2$	8.0		Wang et al. (2017)	Q	81, 240
UYNCDYOFUJEUQN-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	81, 241
MCM:BOXPROOOH	7.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_4$	6.3×10^{3}		Wang et al. (2017)	Q	81, 240
YUTHBWBUPOPMPG-UHFFFAOYSA-N	2.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:EPXEKTCO3H	2.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	2.4×10^{4}		Wang et al. (2017)	Q	81, 240
PGCJNBUAAIEYIA-UHFFFAOYSA-N	2.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:TLEMUCCO3H	1.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_5$	2.0×10^{5}		Wang et al. (2017)	Q	81, 240
RISGILSSNRWCFR-UHFFFAOYSA-N	5.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:EBZMUCCO3H	1.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_5$	9.6×10^{4}		Wang et al. (2017)	Q	81, 240
GTEVSPXWKYUSQE-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:MXYMUCCO3H	7.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_5$	3.6×10^{4}		Wang et al. (2017)	Q	81, 240
ROKAXOITEMHIEK-UHFFFAOYSA-N	3.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:PXYMUCCO3H	7.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_5$	5.5×10^{4}		Wang et al. (2017)	Q	81, 240
AYUPQGRQZSTAMO-UHFFFAOYSA-N	1.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:IPBZMUCO3H	1.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	5.6×10^{4}		Wang et al. (2017)	Q	81, 240
SKJBPGYNTSYQCQ-UHFFFAOYSA-N	9.3×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:METLMUCO3H	6.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	1.7×10^{4}		Wang et al. (2017)	Q	81, 240
CXRRYJPLLOUVIM-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:PBZMUCCO3H	9.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	5.4×10^{4}		Wang et al. (2017)	Q	81, 240
ZGGPGQBINYKWGU-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:PETLMUCO3H	6.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	2.6×10^{4}		Wang et al. (2017)	Q	81, 240
KWWJCAVGGMMMRV-UHFFFAOYSA-N	7.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:TM123OXMUC	4.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	3.9×10^{3}		Wang et al. (2017)	Q	81, 240
XYHNNFZVTWOCNN-UHFFFAOYSA-N	1.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:TM124MUO3H	4.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	1.2×10^{4}		Wang et al. (2017)	Q	81, 240
FTWAFKXUKWKGAJ-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:TM135MUO3H	5.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	3.4×10^{4}		Wang et al. (2017)	Q	81, 240
JNFPQQOSCDIIIK-UHFFFAOYSA-N	6.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DMEBMUO3H	4.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{14}O_5$	1.7×10^{4}		Wang et al. (2017)	Q	81, 240
JWBQDZWURHDWCA-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DETLMUO3H	3.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{16}O_5$	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
QEEAHFHJZRPBGG-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:BCKSOZ	3.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{22}O_4$	1.4×10^{2}		Wang et al. (2017)	Q	81, 240
JTZKRSQXPBULRM-UHFFFAOYSA-N	1.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:PRONEMOXOH	2.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
RETWRLMOZHRKHX-UHFFFAOYSA-N	6.6		Wang et al. (2017)	Q	81, 241
MCM:BOXPRONBOH	1.2×10^{2}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_3$	3.2×10^{2}		Wang et al. (2017)	Q	81, 240
ANPLAICHKIQBPV-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	81, 241
MCM:BOXPRONOH	2.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{14}O_3$	1.0×10^{4}		Wang et al. (2017)	Q	81, 240
NQJNHGUTJISDHM-UHFFFAOYSA-N	9.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:TM123MUCCO	2.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	4.1×10^{7}		Wang et al. (2017)	Q	81, 240
ZVWGUKJQFRZUIG-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:TM123MUCOH	2.6×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	3.7×10^{8}		Wang et al. (2017)	Q	81, 240
JUUFKUYJQYFRGA-UHFFFAOYSA-N	1.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:TM123MUOOH	1.7×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_6$	2.7×10^{8}		Wang et al. (2017)	Q	81, 240
LLVDHGQYZCXGKH-UHFFFAOYSA-N	1.9×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:EPXALMKT	2.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	9.8×10^{2}		Wang et al. (2017)	Q	81, 240
QIJMAVIYYVSLPO-UHFFFAOYSA-N	4.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:EPXMALKT	2.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_3$	9.8×10^{2}		Wang et al. (2017)	Q	81, 240
MWBGBWUOLRJCDU-UHFFFAOYSA-N	3.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:EPXEALKT	2.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_3$	1.0×10^{3}		Wang et al. (2017)	Q	81, 240
HQSBJPSKMKUTIT-UHFFFAOYSA-N	9.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:EBZPOXMUC	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_3$	9.1×10^{3}		Wang et al. (2017)	Q	81, 240
UTCVUMOGNJSPDS-UHFFFAOYSA-N	6.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MXYEPOXMUC	6.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_3$	3.5×10^{3}		Wang et al. (2017)	Q	81, 240
VLMKIGFKBHEGBU-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:PXYEPOXMUC	6.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_3$	5.4×10^{3}		Wang et al. (2017)	Q	81, 240
LGKLIBFTBUCZPW-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:IPBZPOXMUC	9.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	6.6×10^{3}		Wang et al. (2017)	Q	81, 240
NUCYHGVQTCVYLO-UHFFFAOYSA-N	4.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:METLPOXMUC	5.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	1.9×10^{3}		Wang et al. (2017)	Q	81, 240
SWHMTTAIKVELRE-UHFFFAOYSA-N	4.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PBZPOXMUC	8.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	6.0×10^{3}		Wang et al. (2017)	Q	81, 240
AHKQGNMGHQLOPP-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PETLPOXMUC	5.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	3.0×10^{3}		Wang et al. (2017)	Q	81, 240
UTBNMXYREJYVNQ-UHFFFAOYSA-N	6.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:TM124OXMUC	3.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
HFTMUUPKJAPOHL-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:TM135OXMUC	4.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_3$	3.7×10^{3}		Wang et al. (2017)	Q	81, 240
JFCWARPMSNNZLY-UHFFFAOYSA-N	3.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DMEBPOXMUC	3.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{14}O_3$	2.0×10^{3}		Wang et al. (2017)	Q	81, 240
VGOICOHBXPGRQT-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DETLPOXMUC	3.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{16}O_3$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
VPGNNECRJBEQEI-UHFFFAOYSA-N	6.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:BZEMUCCO	1.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_5$	1.1×10^{8}		Wang et al. (2017)	Q	81, 240
KQXCODNTIAPVKL-UHFFFAOYSA-N	3.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:TLEMUCCO	3.7×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_5$	1.7×10^{7}		Wang et al. (2017)	Q	81, 240
AJWOUZMMNQLKHW-UHFFFAOYSA-N	3.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:TLEMUCOH	6.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_5$	1.5×10^{9}		Wang et al. (2017)	Q	81, 240
WPTVRQIFDQMAMS-UHFFFAOYSA-N	5.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:TLEMUCOOH	1.0×10^{12}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_6$	4.8×10^{9}		Wang et al. (2017)	Q	81, 240
DVPKQTIPCHKXBD-UHFFFAOYSA-N	4.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:EBZMUCCO	3.5×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_5$	7.6×10^{6}		Wang et al. (2017)	Q	81, 240
MYHWFJZUBUHIGJ-UHFFFAOYSA-N	2.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:EBZMUCOH	5.6×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	1.0×10^{9}		Wang et al. (2017)	Q	81, 240
VKTUBYIQTACODT-UHFFFAOYSA-N	3.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:EBZMUCOOH	9.1×10^{11}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_6$	3.3×10^{9}		Wang et al. (2017)	Q	81, 240
KWCWGZCSJYJCAS-UHFFFAOYSA-N	8.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:MXYMUCCO	2.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_5$	3.3×10^{6}		Wang et al. (2017)	Q	81, 240
KJOIECUJZBFUMR-UHFFFAOYSA-N	9.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MXYMUCOH	3.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	3.9×10^{8}		Wang et al. (2017)	Q	81, 240
UZLLCOIUEBQPHF-UHFFFAOYSA-N	4.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:MXYMUCOOH	5.6×10^{11}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_6$	1.2×10^{9}		Wang et al. (2017)	Q	81, 240
ZYWDOJNDZBPDDO-UHFFFAOYSA-N	8.3×10^{3}		Wang et al. (2017)	Q	81, 241

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:OXYMUCCO	1.7×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_5$	1.9×10^{6}		Wang et al. (2017)	Q	81, 240
RJHLIQPRSGXWHC-UHFFFAOYSA-N	2.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PXYMUCCO	2.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_5$	4.9×10^{6}		Wang et al. (2017)	Q	81, 240
UICQALDYFNTPHO-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:PXYMUCOH	3.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_5$	5.1×10^{8}		Wang et al. (2017)	Q	81, 240
MIBKDAKBVPRIGB-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:PXYMUCOOH	5.6×10^{11}		Wang et al. (2017)	Q	81, 239
$C_8H_{12}O_6$	1.6×10^{9}		Wang et al. (2017)	Q	81, 240
GSJPWDRXFYTPMH-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:IPBZMUCCO	3.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	1.3×10^{7}		Wang et al. (2017)	Q	81, 240
XOMPDNKHXMMXOK-UHFFFAOYSA-N	5.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:IPBZMUCOH	5.3×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	6.5×10^{8}		Wang et al. (2017)	Q	81, 240
AKVRVUIGBHJRNQ-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:IPBZMUCOOH	8.5×10^{11}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_6$	2.1×10^{9}		Wang et al. (2017)	Q	81, 240
LSOCHQKLDSXALN-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:METLMUCCO	1.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	3.7×10^{6}		Wang et al. (2017)	Q	81, 240
ZRMCSOCJQIXUEX-UHFFFAOYSA-N	5.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:METLMUCOH	3.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	1.8×10^{8}		Wang et al. (2017)	Q	81, 240
ARJLZFCPXRPKBS-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:METLMUCOOH	5.0×10^{11}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_6$	6.0×10^{8}		Wang et al. (2017)	Q	81, 240
UXABECSPQFCGIJ-UHFFFAOYSA-N	2.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:OETLMUCCO	1.6×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	2.0×10^{6}		Wang et al. (2017)	Q	81, 240
JSKKVRLLVVSVCZ-UHFFFAOYSA-N	9.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PBZMUCCO	2.7×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	1.1×10^{7}		Wang et al. (2017)	Q	81, 240
FCRYPGHUONBQCX-UHFFFAOYSA-N	9.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PBZMUCOH	4.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	5.8×10^{8}		Wang et al. (2017)	Q	81, 240
VYXNVIKZUYYSSA-UHFFFAOYSA-N	1.9×10^{4}		Wang et al. (2017)	Q	81, 241

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PBZMUCOOH	7.3×10^{11}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_6$	2.0×10^{9}		Wang et al. (2017)	Q	81, 240
FCKGMMNUJIAHAV-UHFFFAOYSA-N	5.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:PETLMUCCO	1.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	5.9×10^{6}		Wang et al. (2017)	Q	81, 240
RORTYMWKJCCJQU-UHFFFAOYSA-N	6.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PETLMUCOH	3.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	2.5×10^{8}		Wang et al. (2017)	Q	81, 240
ZLOWXLKYIJYQIH-UHFFFAOYSA-N	8.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:PETLMUCOOH	5.0×10^{11}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_6$	8.1×10^{8}		Wang et al. (2017)	Q	81, 240
RSNULGXAYPPPGL-UHFFFAOYSA-N	3.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:TM124MUCCO	2.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_5$	9.8×10^{6}		Wang et al. (2017)	Q	81, 240
DQECTOJLTKBSTJ-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:TM124MUCOH	2.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	1.0×10^{8}		Wang et al. (2017)	Q	81, 240
KPYCPCVRGFCQPX-UHFFFAOYSA-N	7.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:TM124MUOOH	1.4×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_6$	6.8×10^{7}		Wang et al. (2017)	Q	81, 240
DQFPDDPNMNSRMG-UHFFFAOYSA-N	3.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:TM135MUOH	2.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_5$	2.4×10^{8}		Wang et al. (2017)	Q	81, 240
CZQCDAJVGDGQTR-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:TM135MUOOH	1.4×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{14}O_6$	1.2×10^{8}		Wang et al. (2017)	Q	81, 240
FIFCCDBMOKNVLN-UHFFFAOYSA-N	2.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:DMEBMUOH	1.7×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_5$	1.3×10^{8}		Wang et al. (2017)	Q	81, 240
MURMIEBRJYKLPQ-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:DMEBMUOOH	1.2×10^{10}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{16}O_6$	6.2×10^{7}		Wang et al. (2017)	Q	81, 240
QHUZCFCKANZAOE-UHFFFAOYSA-N	3.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DETLMUOH	1.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_5$	8.5×10^{7}		Wang et al. (2017)	Q	81, 240
BLCXZNPOSIAMRZ-UHFFFAOYSA-N	5.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:DETLMUOOH	9.8×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{18}O_6$	4.2×10^{7}		Wang et al. (2017)	Q	81, 240
ZGRWZBBDFVAIEE-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:ETOMECO2H	2.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_8O_3$	3.6×10^{2}		Wang et al. (2017)	Q	81, 240
YZGQDNOIGFBYKF-UHFFFAOYSA-N	7.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MTBEBCO2H	1.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}O_3$	3.9×10^{1}		Wang et al. (2017)	Q	81, 240
BKBZFJRHYSCZQA-UHFFFAOYSA-N	8.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:BOXMCO2H	1.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{12}O_3$	1.2×10^{2}		Wang et al. (2017)	Q	81, 240
AJQOASGWDCBKCJ-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:EPXDLCO2H	9.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_4O_4$	1.5×10^{5}		Wang et al. (2017)	Q	81, 240
BIFCJMYQXQSHFE-UHFFFAOYSA-N	5.4×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:EPXMDLCO2H	5.4×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_6O_4$	5.9×10^{4}		Wang et al. (2017)	Q	81, 240
HNJRQDPCPFMZIJ-UHFFFAOYSA-N	2.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:BZEMUCCO2H	2.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_6O_4$	4.8×10^{5}		Wang et al. (2017)	Q	81, 240
YYDFWEKDUXDLMC-UHFFFAOYSA-N	3.7×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:EPXM2DCO2H	2.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	2.6×10^{4}		Wang et al. (2017)	Q	81, 240
TVFMSHFDVSCCSQ-UHFFFAOYSA-N	6.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:EPXMEDCO2H	2.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	1.5×10^{4}		Wang et al. (2017)	Q	81, 240
CTYOPZSWGBYACX-UHFFFAOYSA-N	5.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:OXYMUCCO2H	7.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_4$	8.1×10^{4}		Wang et al. (2017)	Q	81, 240
CDVXJWVOWNWWPU-UHFFFAOYSA-N	7.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:OETLMUCO2H	6.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	5.1×10^{4}		Wang et al. (2017)	Q	81, 240
UVQOKFRFLASUOJ-UHFFFAOYSA-N	3.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:EPXKTMCO2H	3.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	5.3×10^{4}		Wang et al. (2017)	Q	81, 240
BXVGKWFSHJVVPB-UHFFFAOYSA-N	6.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:EPXMKTCO2H	3.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_8O_4$	1.1×10^{5}		Wang et al. (2017)	Q	81, 240
FTLSPZDBESPPRR-UHFFFAOYSA-N	3.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:EPXEKTCO2H	2.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{10}O_4$	1.8×10^{5}		Wang et al. (2017)	Q	81, 240
XBMXXNQRKRSRRJ-UHFFFAOYSA-N	5.0×10^{5}		Wang et al. (2017)	Q	81, 241

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:TLEMUCCO2H	1.7×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_8O_4$	8.3×10^{5}		Wang et al. (2017)	Q	81, 240
YZQFSRDEODCLRC-UHFFFAOYSA-N	1.3×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:EBZMUCCO2H	1.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_4$	5.0×10^{5}		Wang et al. (2017)	Q	81, 240
BSMJHSATRRVHTI-UHFFFAOYSA-N	6.8×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:MXYMUCCO2H	9.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_4$	4.2×10^{5}		Wang et al. (2017)	Q	81, 240
BMJHPUYAWBLOER-UHFFFAOYSA-N	3.2×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:PXYMUCCO2H	9.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}O_4$	2.9×10^{5}		Wang et al. (2017)	Q	81, 240
FMBYVAMRNZYNGO-UHFFFAOYSA-N	8.3×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:IPBZMUCO2H	1.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	3.2×10^{5}		Wang et al. (2017)	Q	81, 240
LXYULRJMRUJREP-UHFFFAOYSA-N	2.2×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:METLMUCO2H	8.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	2.1×10^{5}		Wang et al. (2017)	Q	81, 240
TZAADSLPRMCSBM-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:PBZMUCCO2H	1.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	3.0×10^{5}		Wang et al. (2017)	Q	81, 240
MSVJIRWCUUEXSY-UHFFFAOYSA-N	2.9×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:PETLMUCO2H	8.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	1.4×10^{5}		Wang et al. (2017)	Q	81, 240
YZGPSCFZKHZHEQ-UHFFFAOYSA-N	2.6×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:TM124MUO2H	4.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	1.4×10^{5}		Wang et al. (2017)	Q	81, 240
VDBMALGYQLXWML-UHFFFAOYSA-N	4.3×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:TM135MUO2H	6.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}O_4$	3.8×10^{5}		Wang et al. (2017)	Q	81, 240
RLMHTEATULORAU-UHFFFAOYSA-N	2.1×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:DMEBMUO2H	5.4×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{14}O_4$	2.0×10^{5}		Wang et al. (2017)	Q	81, 240
GTDCDBIZJZUTJP-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:DETLMUO2H	4.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{16}O_4$	1.4×10^{5}		Wang et al. (2017)	Q	81, 240
FTAMRHAZJZCWNK-UHFFFAOYSA-N	5.5×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:DMCOOH	2.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_5$	3.7×10^{3}		Wang et al. (2017)	Q	81, 240
ISFGCMQHKVEPTP-UHFFFAOYSA-N	1.9×10^{2}		Wang et al. (2017)	Q	81, 241

Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MMF	1.2		Wang et al. (2017)	Q	81, 239
$C_3H_6O_3$	2.1		Wang et al. (2017)	Q	81, 240
VKWJMTLAAJULGF-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	81, 241
MCM:MMFOOH	9.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_5$	5.6×10^{2}		Wang et al. (2017)	Q	81, 240
AAAZTRZXKHTMLL-UHFFFAOYSA-N	9.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DMCOH	7.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_4$	7.4×10^{2}		Wang et al. (2017)	Q	81, 240
YGODNDLTUXBUQH-UHFFFAOYSA-N	6.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MMFOH	3.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_4$	1.5×10^{2}		Wang et al. (2017)	Q	81, 240
GDDJZBRTXIGGHV-UHFFFAOYSA-N	4.5×10^{1}		Wang et al. (2017)	Q	81, 241
GOLIG1 $C_4H_6O_5$ LEKXYOUPWKVTGM-UHFFFAOYSA-N	1.5×10^{12}	19000	Wieser et al. (2023)	Q	439
GOLIG2 $C_4H_8O_6$ GWSRJJGBNXJVPO-UHFFFAOYSA-N	1.5×10^{15}	24000	Wieser et al. (2023)	Q	439
GOLIG3 $C_4H_{10}O_7$ ADECTKUVLJSMDK-UHFFFAOYSA-N	3.8×10^{18}	29000	Wieser et al. (2023)	Q	439
MGLYFB $C_6H_{10}O_6$ UCPBJDKPOQEXSQ-UHFFFAOYSA-N	7.1×10^{8}	23000	Wieser et al. (2023)	Q	439
MGLYOXDA $C_6H_{10}O_5$ QMSLRDMQAWWKIZ-UHFFFAOYSA-N	2.0×10^{8}	16000	Wieser et al. (2023)	Q	439
MGLYOXDB $C_6H_{12}O_6$ IUHMFBWAUOLAFM-UHFFFAOYSA-N	1.5×10^{13}	22000	Wieser et al. (2023)	Q	439

A3.10 Heterocycles with oxygen

Table A3.10: Heterocycles with oxygen

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
β-propiolactone $C_3H_4O_2$ [57-57-8] VEZXCJBBBCKRPI-UHFFFAOYSA-N	1.3×10^{1}		Ebert et al. (2023)	?	317
2-methyl-1,3-dioxolane $C_4H_8O_2$ [497-26-7] HTWIZMNMTWYQRN-UHFFFAOYSA-N	7.9×10^{-1}		Ebert et al. (2023)	?	317
DIEPOXO3 $C_5H_8O_3$ QGQUFAZKBSHWQB-UHFFFAOYSA-N	1.3×10^{3}	14000	Wieser et al. (2023)	Q	439
IEPOXO4 $C_5H_8O_3$ DNQIATHBSKHPLN-UHFFFAOYSA-N	2.1×10^{4}	14000	Wieser et al. (2023)	Q	439
2,2-dimethyl-1,3-dioxolane $C_5H_{10}O_2$ [2916-31-6] SIJBDWPVNAYVGY-UHFFFAOYSA-N	4.8×10^{-1}		Ebert et al. (2023)	?	317
METHFDIOL $C_5H_{10}O_3$ UNAIOYXCADSMDR-UHFFFAOYSA-N	9.0×10^{5}	11000	Wieser et al. (2023)	Q	439
3,4-dihydro-2-methoxy-2H-pyran $C_6H_{10}O_2$ [4454-05-1] XCYWUZHUTJDTGS-UHFFFAOYSA-N	9.7×10^{-2}		Ebert et al. (2023)	?	317
maltol $C_6H_6O_3$ [118-71-8] XPCTZQVDEJYUGT-UHFFFAOYSA-N	7.3×10^{2}		Abraham et al. (2019)	Q	
2-methylfuran C_5H_6O [534-22-5] VQKFNUFAXTZWDK-UHFFFAOYSA-N	1.5×10^{-3}	4100	Wieland et al. (2015)	M	534
3-methylfuran C_5H_6O [930-27-8] KJRRQXYWFQKJIP-UHFFFAOYSA-N	3.2×10^{-3}		Wu et al. (2022a)	Q	415

Table A3.10: Heterocycles with oxygen (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-furanmethanol	1.3×10^{2}		Duchowicz et al. (2020)	V	187
$C_5H_6O_2$	1.2×10^{2}		HSDB (2015)	V	
(furfuryl alcohol)	2.5×10^{1}		Yaws (2003)	X	259
[98-00-0]	2.2×10^{1}		Dupeux et al. (2022)	Q	260
XPFVYQJUAUNWIW-UHFFFAOYSA-N	2.4×10^{1}		Duchowicz et al. (2020)	Q	
	5.3×10^{1}		Gharagheizi et al. (2012)	Q	
	6.2×10^{1}		Raventos-Duran et al. (2010)	Q	272, 244
	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	246
	3.4×10^{1}		Hilal et al. (2008)	Q	
	4.8×10^{1}		Modarresi et al. (2007)	Q	68
	4.8×10^{2}		Katritzky et al. (1998)	Q	
	1.1×10^{2}		Yaws (1999)	?	21, 12
tetrahydropyran-2-methanol	6.5×10^{2}		Duchowicz et al. (2020)	V	187
$C_6H_{12}O_2$	5.2×10^{1}		Duchowicz et al. (2020)	Q	
[100-72-1]	6.2×10^{1}		Raventos-Duran et al. (2010)	Q	272, 244
ROTONRWJLXYJBD-UHFFFAOYSA-N	3.1×10^{2}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{3}		Raventos-Duran et al. (2010)	Q	246
	9.0×10^{1}		Hilal et al. (2008)	Q	
	8.5×10^{1}		Modarresi et al. (2007)	Q	68
oxirane	5.8×10^{-2}	3200	Conway et al. (1983)	M	
C_2H_4O	8.3×10^{-2}		Lide and Frederikse (1995)	V	
(ethylene oxide)	8.6×10^{-2}		Mackay et al. (1993)	V	
[75-21-8]	5.0×10^{-2}		Hwang et al. (1992)	V	
IAYPIBMASNFSPL-UHFFFAOYSA-N	6.0×10^{-2}		Keshavarz et al. (2022)	Q	
	1.4×10^{-1}		Duchowicz et al. (2020)	Q	
	9.3×10^{-3}		Wang et al. (2017)	Q	81, 239
	5.9×10^{-2}		Wang et al. (2017)	Q	81, 240
	6.0×10^{-2}		Wang et al. (2017)	Q	81, 241
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	2.9×10^{-2}		Modarresi et al. (2007)	Q	68
	6.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.0×10^{-2}		Katritzky et al. (1998)	Q	
	6.7×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	4.1×10^{-2}		Yaws (1999)	?	21
1,2-epoxypropane	1.4×10^{-1}		Duchowicz et al. (2020)	V	187
C_3H_6O	1.4×10^{-1}		HSDB (2015)	V	
(1,2-propylene oxide)	1.2×10^{-1}		Mackay et al. (2006c)	V	
[75-56-9]	1.2×10^{-1}		Lide and Frederikse (1995)	V	
GOOHAUXETOMSMM-UHFFFAOYSA-N	1.2×10^{-1}		Mackay et al. (1993)	V	
	1.7×10^{-1}		Yaws (2003)	X	238, 12
	5.2×10^{-2}		Goldstein (1982)	X	448
	5.1×10^{-2}	3500	Goldstein (1982)	X	299
	6.3×10^{-2}		Duchowicz et al. (2020)	Q	

Table A3.10: Heterocycles with oxygen (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-1}		Gharagheizi et al. (2010)	Q	247
	1.7×10^{-2}		Hilal et al. (2008)	Q	
	1.5×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	1.3×10^{-2}		Katritzky et al. (1998)	Q	
	1.4×10^{-1}		Yaws (1999)	?	21, 12
phenyloxirane	6.2×10^{-1}		HSDB (2015)	V	
C_8H_8O	5.8×10^{-1}		Mackay et al. (2006c)	V	
(styrene oxide)	5.8×10^{-1}		Mackay et al. (1993)	V	
[96-09-3]	6.2×10^{-1}		Meylan and Howard (1991)	V	
AWMVMTVKBNGEAK-UHFFFAOYSA-N	2.5×10^{-1}		Hilal et al. (2008)	Q	
	5.5×10^{-1}		Modarresi et al. (2007)	Q	68
	1.0		Meylan and Howard (1991)	Q	
oxacyclopentadiene	1.8×10^{-3}		HSDB (2015)	V	
C_4H_4O	1.8×10^{-3}		Mackay et al. (2006c)	V	
(furan; furfuran)	1.8×10^{-3}		Mackay et al. (1993)	V	
[110-00-9]	1.8×10^{-3}		Yaws (2003)	X	259
YLQBMQCUIZJEEH-UHFFFAOYSA-N	1.8×10^{-3}		Yaws (2003)	X	238
	2.2×10^{-3}		Dupeux et al. (2022)	Q	260
	4.6×10^{-3}		Hayer et al. (2022)	Q	20
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.3×10^{-3}		Hilal et al. (2008)	Q	
	1.9×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	4.3×10^{-3}		Yao et al. (2002)	Q	230
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
	1.8×10^{-3}		Yaws (1999)	?	21
	1.8×10^{-3}		Yaws and Yang (1992)	?	21
dibenzofuran	7.4×10^{-2}	5800	Brockbank (2013)	L	
$C_{12}H_8O$	4.6×10^{-2}		Duchowicz et al. (2020)	V	187
(2,2'-biphenylene oxide)	4.7×10^{-2}		HSDB (2015)	V	
[132-64-9]	7.1×10^{-2}		Mackay et al. (2006b)	V	
TXCDCPKCNAJMEE-UHFFFAOYSA-N	7.2×10^{-2}		Govers and Krop (1998)	V	
	9.1×10^{-2}		Mackay et al. (1992b)	X	366
	8.9×10^{-3}		Yaws (2003)	X	238
	2.8×10^{-1}		Duchowicz et al. (2020)	Q	
	9.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
	8.2×10^{-2}		Saçan et al. (2005)	Q	
	4.7×10^{-2}		Govers and Krop (1998)	Q	

Table A3.10: Heterocycles with oxygen (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-furancarboxaldehyde	2.6		Duchowicz et al. (2020)	V	187
$C_5H_4O_2$	2.6		HSDB (2015)	V	
(furfural; 2-furanaldehyde)	2.7		Mackay et al. (2006c)	V	
[98-01-1]	2.7		Mackay et al. (1995)	V	
HYBBIBNJHNGZAN-UHFFFAOYSA-N	3.0		Yaws (2003)	X	259
	3.0		Yaws (2003)	X	238
	9.6		Dupeux et al. (2022)	Q	260
	8.4×10^{-1}		Duchowicz et al. (2020)	Q	
	1.7		Gharagheizi et al. (2012)	Q	
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	6.2		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	3.0		Gharagheizi et al. (2010)	Q	247
	6.0		Hilal et al. (2008)	Q	
	8.1×10^{-1}		Modarresi et al. (2007)	Q	68
	7.2×10^{-2}		Emel'yanenko et al. (2007)	Q	417
	7.2×10^{-2}		Hertel and Sommer (2006)	Q	417
		6100	Kühne et al. (2005)	Q	
		5900	Kühne et al. (2005)	?	
	3.0		Yaws (1999)	?	21
5-methylfurfural	4.7		Ebert et al. (2023)	?	317
$C_6H_6O_2$					
[620-02-0]					
OUDFNZMQXZILJD-UHFFFAOYSA-N					
2,2-dimethyloxirane	2.9×10^{-2}		Ebert et al. (2023)	?	317
C_4H_8O					
(isobutylene oxide)					
[558-30-5]					
GELKGHVAFRCJNA-UHFFFAOYSA-N					
tetrahydrofuran	1.5×10^{-1}	5700	Brockbank (2013)	L	
C_4H_8O	1.5×10^{-1}	5700	Ondo and Dohnal (2007)	M	1
(THF)	6.4×10^{-1}		Welke et al. (1998)	M	
[109-99-9]	6.0×10^{-1}	4200	Pividal et al. (1992)	M	
WYURNTSHIVDZCO-UHFFFAOYSA-N	2.2×10^{-1}		Signer et al. (1969)	M	
	1.4×10^{-1}	5700	Cabani et al. (1971b)	T	
	6.0×10^{-2}		Yaws (2003)	X	238, 12
	1.1×10^{-1}		Keshavarz et al. (2022)	Q	
	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
	8.5×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	6.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
	1.1×10^{-1}		Hilal et al. (2008)	Q	
	3.5×10^{-2}		Modarresi et al. (2007)	Q	68

Table A3.10: Heterocycles with oxygen (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		4000	Kühne et al. (2005)	Q	
	1.5×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	1.3×10^{-1}		English and Carroll (2001)	Q	231, 232
	2.4×10^{-2}		Katritzky et al. (1998)	Q	
	1.3×10^{-1}		Suzuki et al. (1992)	Q	233
	1.4×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		3200	Kühne et al. (2005)	?	
	1.9×10^{-1}		Yaws (1999)	?	21, 12
	1.4×10^{-1}		Abraham et al. (1990)	?	
tetrahydrofuran-d8 C_4D_8O (THF-d8) [1693-74-9] WYURNTSHIVDZCO-SVYQBANQSA-N	2.3×10^{-1}	8000	Hiatt (2013)	M	
2-methyltetrahydrofuran	1.5×10^{-3}		Mackay et al. (1993)	V	
$CH_3C_4H_7O$	1.1×10^{-1}	6200	Cabani et al. (1971b)	T	
[96-47-9]	1.5×10^{-1}		Keshavarz et al. (2022)	Q	
JWUJQDFVADABEY-UHFFFAOYSA-N	5.3×10^{-2}		Duchowicz et al. (2020)	Q	
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	6.1×10^{-2}		Hilal et al. (2008)	Q	
	1.7×10^{-2}		Modarresi et al. (2007)	Q	68
		4400	Kühne et al. (2005)	Q	
	1.0×10^{-1}		English and Carroll (2001)	Q	231, 261
	2.4×10^{-2}		Katritzky et al. (1998)	Q	
	9.0×10^{-2}		Suzuki et al. (1992)	Q	233
	1.1×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		5400	Kühne et al. (2005)	?	
2,5-dimethyltetrahydrofuran	5.5×10^{-2}	6800	Cabani et al. (1971b)	T	
$(CH_3)_2C_4H_6O$	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
[1003-38-9]	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
OXMIDRBAFOEOQT-UHFFFAOYSA-N	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	3.1×10^{-2}		Hilal et al. (2008)	Q	
	2.5×10^{-2}		Modarresi et al. (2007)	Q	68
	7.9×10^{-2}		English and Carroll (2001)	Q	231, 232
tetrahydropyran	8.1×10^{-2}	5800	Brockbank (2013)	L	1
$C_5H_{10}O$	8.3×10^{-2}	5900	Ondo and Dohnal (2007)	M	1
(THP)	1.0×10^{-1}		Mackay et al. (2006c)	V	
[142-68-7]	1.0×10^{-1}		Mackay et al. (1993)	V	
DHXVGJBLRPWPCS-UHFFFAOYSA-N	7.8×10^{-2}	5900	Cabani et al. (1971b)	T	
	1.5×10^{-1}		Keshavarz et al. (2022)	Q	
	1.4×10^{-1}		Duchowicz et al. (2020)	Q	
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244

Table A3.10: Heterocycles with oxygen (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.1×10^{-1}		Hilal et al. (2008)	Q	
	6.9×10^{-2}		Modarresi et al. (2007)	Q	68
	7.9×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.0×10^{-1}		English and Carroll (2001)	Q	231, 275
	2.6×10^{-2}		Katritzky et al. (1998)	Q	
	9.9×10^{-2}		Suzuki et al. (1992)	Q	233
	7.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	7.9×10^{-2}		Abraham et al. (1990)	?	
3-methyltetrahydropyran $C_6H_{12}O$ [26093-63-0] UJQZTMFRMLEYQN-UHFFFAOYSA-N		4700	Kühne et al. (2005)	Q	
		5300	Kühne et al. (2005)	?	
3,4-dihydro-2H-pyran C_5H_8O [110-87-2] BUDQDWGNQVEFAC-UHFFFAOYSA-N		3500	Kühne et al. (2005)	Q	
		3600	Kühne et al. (2005)	?	
1,3-dioxolane $C_3H_6O_2$ [646-06-0] WNXJIVFYUVYPPR-UHFFFAOYSA-N	4.3×10^{-1}	4800	Ondo and Dohnal (2007)	M	1
	4.0×10^{-1}	4800	Cabani et al. (1971b)	T	
	8.1×10^{-2}		Keshavarz et al. (2022)	Q	
	2.1		Duchowicz et al. (2020)	Q	185
	1.5		Hilal et al. (2008)	Q	
	2.2×10^{-1}		Modarresi et al. (2007)	Q	68
	4.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
1,3-dioxane $C_4H_8O_2$ [505-22-6] VDFVNEFVBPFDSB-UHFFFAOYSA-N	1.8		O'Farrell and Waghorne (2010)	M	
	2.1		Hilal et al. (2008)	Q	
1,4-dioxane $C_4H_8O_2$ (dioxane) [123-91-1] RYHBNJHYFVUHQT-UHFFFAOYSA-N	1.8	5800	Brockbank (2013)	L	1
	2.3	6600	Hiatt (2013)	M	
	2.0	5800	Ondo and Dohnal (2007)	M	1
	2.0		Welke et al. (1998)	M	
	1.4	5100	Kolb et al. (1992)	M	278
	2.1		Park et al. (1987)	M	
	4.4		Ioffe et al. (1984)	M	81
	1.4		Friant and Suffet (1979)	M	38
	2.2		Rohrschneider (1973)	M	
	1.9		Hwang et al. (1992)	V	
	1.1		Amoore and Buttery (1978)	V	
	2.0	5800	Cabani et al. (1971b)	T	
	1.1		Hayer et al. (2022)	Q	20
	1.1×10^{-1}		Keshavarz et al. (2022)	Q	
	2.8		Duchowicz et al. (2020)	Q	185

Table A3.10: Heterocycles with oxygen (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	245
	1.6		Raventos-Duran et al. (2010)	Q	246
	3.3		Hilal et al. (2008)	Q	
	1.3		Modarresi et al. (2007)	Q	68
		5200	Kühne et al. (2005)	Q	
	1.5		English and Carroll (2001)	Q	231, 232
	8.2×10^{-1}		Russell et al. (1992)	Q	280
	2.1		Duchowicz et al. (2020)	?	186, 21
		6100	Kühne et al. (2005)	?	
	1.8		Yaws (1999)	?	21
	2.0		Betterton (1992)	?	535
	2.2		Betterton (1992)	?	536
	1.4		Yaws and Yang (1992)	?	21
1,4-dioxane-d8 $C_4D_8O_2$ (dioxane-d8) [17647-74-4] RYHBNJHYFVUHQT-SVYQBANQSA-N	2.8	6800	Hiatt (2013)	M	
trioxane $C_3H_6O_3$ [110-88-3] BGJSXRVXTHVRSN-UHFFFAOYSA-N	9.6×10^{-1}		Yaws (2003)	X	259
	2.7		Dupeux et al. (2022)	Q	260
4-methyl-1,3-dioxolan-2-one $C_4H_6O_3$ (propylene carbonate) [108-32-7] RUOJZAUFBMNUDX-UHFFFAOYSA-N	2.9×10^{2}		Duchowicz et al. (2020)	V	187
	2.9×10^{2}		HSDB (2015)	V	
	1.6×10^{-1}		Duchowicz et al. (2020)	Q	
	1.4×10^{2}		Abraham et al. (1990)	?	
1,3,3-trimethyl-2-oxabicyclo[2.2.2]octane	5.9×10^{-2}		Kish et al. (2013)	M	
$C_{10}H_{18}O$ (eucalyptol; 1,8-cineole) [470-82-6] WEEGYLXZBRQIMU-UHFFFAOYSA-N	1.2×10^{-1}		Amoore and Buttery (1978)	M	
	9.0×10^{-2}		Duchowicz et al. (2020)	V	187
	7.5×10^{-2}		Copolovici and Niinemets (2005)	V	
	7.4×10^{-2}		Niinemets and Reichstein (2002)	V	
	7.8×10^{-2}		Amoore and Buttery (1978)	V	
	5.3×10^{-3}		Duchowicz et al. (2020)	Q	
	2.2×10^{-2}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	68
limonene oxide $C_{10}H_{16}O$ [1195-92-2] CCEFMUBVSUDRLG-UHFFFAOYSA-N	5.6×10^{-2}		Fichan et al. (1999)	M	
	5.5×10^{-2}		Duchowicz et al. (2020)	V	187
	2.7×10^{-2}	4600	van Roon et al. (2005)	V	
	4.8×10^{-2}		Duchowicz et al. (2020)	Q	

Table A3.10: Heterocycles with oxygen (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dibenzo[b, e][1,4]dioxin	8.9×10^{-2}		Duchowicz et al. (2020)	V	187
$C_{12}H_8O_2$	9.0×10^{-2}		HSDB (2015)	V	
(dibenzo-p-dioxin)	8.5×10^{-2}		Mackay et al. (2006b)	V	
[262-12-4]	9.5×10^{-3}		Saçan et al. (2005)	V	
NFBOHOGPQUYFRF-UHFFFAOYSA-N	8.5×10^{-2}		Govers and Krop (1998)	V	
	8.1×10^{-2}		Shiu et al. (1988)	V	
	2.0		Duchowicz et al. (2020)	Q	
	2.7×10^{-2}		Saçan et al. (2005)	Q	
	6.3×10^{-2}		Wang and Wong (2002)	Q	537
	9.1×10^{-2}		Govers and Krop (1998)	Q	
piperonal	1.8×10^{1}		Duchowicz et al. (2020)	V	187
$C_8H_6O_3$	1.8×10^{1}		HSDB (2015)	V	
[120-57-0]	1.6×10^{2}		Duchowicz et al. (2020)	Q	
SATCULPHIDQDRE-UHFFFAOYSA-N	4.1×10^{2}		Hilal et al. (2008)	Q	
	1.1×10^{1}		Modarresi et al. (2007)	Q	68
paraldehyde	5.8×10^{-1}		Duchowicz et al. (2020)	V	187
$C_6H_{12}O_3$	2.5×10^{-1}		HSDB (2015)	V	
[123-63-7]	4.7		Duchowicz et al. (2020)	Q	
SQYNKIJPMDEDEG-UHFFFAOYSA-N	3.6×10^{-1}		Hilal et al. (2008)	Q	
	2.1		Modarresi et al. (2007)	Q	68
	6.4×10^{-1}		Yaws (1999)	?	21, 38
benzofuran	1.9×10^{-2}		HSDB (2015)	Q	100
C_8H_6O	1.9×10^{-2}		Hilal et al. (2008)	Q	
[271-89-6]					
IANQTJSKSUMEQM-UHFFFAOYSA-N					
γ-nonalactone	1.8×10^{-1}		Hertel and Sommer (2006)	Q	417
$C_9H_{16}O_2$					
[104-61-0]					
OALYTRUKMRCXNH-UHFFFAOYSA-N					
xanthene	1.3×10^{-1}		Abraham et al. (2019)	Q	
$C_{13}H_{10}O$					
[92-83-1]					
GJCOSYZMQJWQCA-UHFFFAOYSA-N					
1,5,5,9-tetramethyl-13-oxatricyclo(8.3.0.0(4,9))tridecane	2.0×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_{28}O$	2.9×10^{-1}		Zhang et al. (2010)	Q	288, 290
(ambroxan)	6.5×10^{-2}		Zhang et al. (2010)	Q	288, 291
[3738-00-9]	1.1×10^{-3}		Zhang et al. (2010)	Q	288, 292
YPZUZOLGGMJZJO-UHFFFAOYSA-N					

Table A3.10: Heterocycles with oxygen (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylcyclopenta[g]-2-benzopyran	7.6×10^{-2}		HSDB (2015)	V	
$C_{18}H_{26}O$	7.5×10^{-2}		Zhang et al. (2010)	Q	288, 289
[1222-05-5]	8.2		Zhang et al. (2010)	Q	288, 290
ONKNPOPIGWHAQC-UHFFFAOYSA-N	8.4×10^{-2}		Zhang et al. (2010)	Q	288, 291
	9.9×10^{-3}		Zhang et al. (2010)	Q	288, 292
cinmethylin $C_{18}H_{26}O_2$ [87818-31-3] QMTNOLKHSWIQBE-FGTMMUONSA-N	1.3×10^{1}		Ebert et al. (2023)	?	319
milbemycin A4 $C_{32}H_{46}O_7$ (milbemectin A4) [51596-11-3] VOZIAWLUULBIPN-LRBNAKOISA-N	7.7×10^{6}		Ebert et al. (2023)	?	319

A3.11 Oxidized terpenoids

Table A3.11: Oxidized terpenoids

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(1S-endo)-1,7,7-trimethyl-bicyclo[2.2.1]heptan-2-ol	4.5×10^{-1}		Fichan et al. (1999)	M	
$C_{10}H_{18}O$	7.2×10^{-1}		Duchowicz et al. (2020)	V	187
(1S-endo-(-)-borneol)	4.0×10^{-1}		Duchowicz et al. (2020)	Q	
[464-45-9]					
DTGKSKDOIYIVQL-QXFUBDJGSA-N					
(1R)-1,3,3-trimethylbicyclo[2.2.1]heptan-2-ol	3.6×10^{-1}		Fichan et al. (1999)	M	
$C_{10}H_{18}O$	3.6×10^{-1}		Duchowicz et al. (2020)	V	187
(endo-(+)-fenchyl alcohol)	4.0×10^{-1}		Duchowicz et al. (2020)	Q	
[2217-02-9]					
IAIHUHQCLTYTSF-OYNCUSHFSA-N					
2-(4-methyl-3-cyclohexen-1-yl)-2-propanol	4.4	2200	Copolovici and Niinemets (2005)	M	
$C_{10}H_{18}O$	4.1		Copolovici and Niinemets (2005)	V	
(α-terpineol)	6.0×10^{-1}	4800	van Roon et al. (2005)	V	
[98-55-5]	4.2		Niinemets and Reichstein (2002)	V	
WUOACPNHFRMFPN-UHFFFAOYSA-N	7.4×10^{-1}	5400	Li et al. (1998)	V	
	6.5		Dupeux et al. (2022)	Q	260
	3.6		Hilal et al. (2008)	Q	
	8.2×10^{-1}		Modarresi et al. (2007)	Q	68
1,2-dimethyl-3-(1-methylethenyl)-cyclopentanol	5.3×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{10}H_{18}O$	4.0×10^{-1}	17000	Li et al. (1998)	V	
(plinol)	3.4×10^{-1}		Duchowicz et al. (2020)	Q	
[72402-00-7]	1.2		Hilal et al. (2008)	Q	
ZRVPDCMGGOSDKG-UHFFFAOYSA-N	1.6		Modarresi et al. (2007)	Q	68
1-methyl-4-(1-methylethyl)-7-oxabicyclo[2.2.1]heptane	3.9×10^{-2}		Helburn et al. (2008)	M	
$C_{10}H_{18}O$	7.4×10^{-2}		Copolovici and Niinemets (2005)	V	
(1,4-cineole)	1.4×10^{-1}	4000	van Roon et al. (2005)	V	
[470-67-7]					
RFFOTVCVTJUTAD-UHFFFAOYSA-N					
1,7,7-trimethyl-bicyclo[2.2.1]heptan-2-one	1.2×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{10}H_{16}O$	1.2×10^{-1}		HSDB (2015)	V	
(camphor)	1.1		Copolovici and Niinemets (2005)	V	
[76-22-2]	5.4×10^{-1}	4800	van Roon et al. (2005)	V	
DSSYKIVIOFKYAU-UHFFFAOYSA-N	8.2×10^{-1}		Niinemets and Reichstein (2002)	V	
	2.3×10^{-2}		Duchowicz et al. (2020)	Q	
	3.5×10^{-1}		Modarresi et al. (2007)	Q	68

Table A3.11: Oxidized terpenoids (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,7,7-trimethyl-3-oxatricyclo[4.1.1.0(2,4)]octane	2.3×10^{-2}		Fichan et al. (1999)	M	
$C_{10}H_{16}O$	2.3×10^{-2}		Duchowicz et al. (2020)	V	187
((-)-α-pinene oxide)	2.4×10^{-2}		Copolovici and Niinemets (2005)	V	
[1686-14-2]	5.4×10^{-2}	4400	van Roon et al. (2005)	V	
NQFUSWIGRKFAHK-UHFFFAOYSA-N	2.2×10^{-2}		Duchowicz et al. (2020)	Q	
5-methyl-2-(1-methylethylidene)-cyclohexanone	2.8×10^{-1}	5300	van Roon et al. (2005)	V	
$C_{10}H_{16}O$	1.7×10^{-1}		HSDB (2015)	Q	100
(pulegone)					
[89-82-7]					
NZGWDASTMWDZIW-UHFFFAOYSA-N					
exo-2-[(1,7,7-trimethylbicyclo[2.2.1]hept-2-yl)-oxy]ethanol	1.0	4100	Li et al. (1998)	V	
$C_{12}H_{22}O_2$					
(arbanol)					
[7070-15-7]					
IWWCSDGEIDYEJV-JBLDHEPKSA-N					
bornyl acetate	3.8×10^{-4}	1700	Copolovici and Niinemets (2015)	M	
$C_{12}H_{20}O_2$					
[5655-61-8]					
KGEKLUUHTZCSIP-SCVCMEIPSA-N					
β-ionone	1.2		Fichan et al. (1999)	M	
$C_{13}H_{20}O$	1.2×10^{-1}		Duchowicz et al. (2020)	V	187
[79-77-6]	1.5×10^{-2}		Abney (2021)	Q	401
PSQYTAPXSHCGMF-BQYQJAHWSA-N	6.6×10^{-3}		Duchowicz et al. (2020)	Q	
nerolidol	3.2×10^{-4}	4300	Copolovici and Niinemets (2015)	M	
$C_{15}H_{26}O$					
[7212-44-4]					
FQTLCLSUCSAZDY-UHFFFAOYSA-N					

A3.12 Miscellaneous

Table A3.12: Miscellaneous

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
oxoethanoic acid	1.1×10^{2}	4800	Burkholder et al. (2019)	L	462
OHCCOOH	1.1×10^{2}	4800	Burkholder et al. (2015)	L	462
(glyoxylic acid)	1.1×10^{2}	4800	Sander et al. (2011)	L	
[298-12-4]	1.1×10^{2}	4800	Ip et al. (2009)	M	
HHLFWLYXYJOTON-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	81, 239
	1.5×10^{1}		Wang et al. (2017)	Q	81, 240
	6.9×10^{1}		Wang et al. (2017)	Q	81, 241
	3.3×10^{3}		HSDB (2015)	Q	100
	7.8×10^{4}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{8}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{3}		Raventos-Duran et al. (2010)	Q	246
	8.9×10^{1}		Saxena and Hildemann (1996)	E	403
			Warneck (2005)	?	538
hydroxyethanoic acid	2.8×10^{2}	4000	Burkholder et al. (2019)	L	462, 539
$HOCH_2COOH$	2.8×10^{2}	4000	Burkholder et al. (2015)	L	462, 540
(glycolic acid)	2.8×10^{2}	4000	Sander et al. (2011)	L	
[79-14-1]	2.8×10^{2}	4000	Ip et al. (2009)	M	
AEMRFAOFKBGASW-UHFFFAOYSA-N	1.9×10^{3}		Wang et al. (2017)	Q	81, 239
	1.4×10^{5}		Wang et al. (2017)	Q	81, 240
	5.3×10^{4}		Wang et al. (2017)	Q	81, 241
	1.2×10^{3}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{4}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	246
2-hydroxyethanal	3.9×10^{2}	4600	Burkholder et al. (2019)	L	462
$HOCH_2CHO$	3.9×10^{2}	4600	Burkholder et al. (2015)	L	462
(hydroxyacetaldehyde; glycolaldehyde)	4.1×10^{2}	4600	Betterton and Hoffmann (1988)	M	462
[141-46-8]	9.9×10^{2}		Lee and Zhou (1993)	C	88
WGCNASOHLSPBMP-UHFFFAOYSA-N	2.9×10^{2}		Keshavarz et al. (2022)	Q	
	1.8×10^{1}		Duchowicz et al. (2020)	Q	300
	1.3×10^{1}		Wang et al. (2017)	Q	81, 239
	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
	4.2		Wang et al. (2017)	Q	81, 241
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	272, 244
	7.8×10^{3}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	6.5×10^{2}		Hilal et al. (2008)	Q	
	2.4×10^{2}		Modarresi et al. (2007)	Q	68
		7600	Kühne et al. (2005)	Q	
	4.1×10^{2}		Duchowicz et al. (2020)	?	186, 21
		4600	Kühne et al. (2005)	?	

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
propanonal	3.5×10^{1}	7500	Burkholder et al. (2019)	L	462
CH_3COCHO	3.5×10^{1}	7500	Burkholder et al. (2015)	L	462
(methylglyoxal; pyruvaldehyde)	3.2×10^{2}		Zhou and Mopper (1990)	M	71
[78-98-8]	3.4×10^{1}	7500	Betterton and Hoffmann (1988)	M	462
AIJULSRZWUXGPQ-UHFFFAOYSA-N	3.7×10^{2}		Lee and Zhou (1993)	C	88
	5.4×10^{1}		Wang et al. (2017)	Q	81, 239
	1.3×10^{1}		Wang et al. (2017)	Q	81, 240
	2.9×10^{-2}		Wang et al. (2017)	Q	81, 241
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	272, 244
	4.9×10^{2}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	246
	1.4×10^{1}		Modarresi et al. (2007)	Q	68
		6200	Kühne et al. (2005)	Q	
	8.2		Katritzky et al. (1998)	Q	
		7600	Kühne et al. (2005)	?	
2-oxopropanoic acid	3.1×10^{3}	5100	Burkholder et al. (2019)	L	
$CH_3COCOOH$	3.1×10^{3}	5100	Burkholder et al. (2015)	L	
(pyruvic acid)	3.1×10^{3}	5100	Sander et al. (2011)	L	
[127-17-3]	3.1×10^{3}	5100	Sander et al. (2006)	L	
LCTONWCANYUPML-UHFFFAOYSA-N	3.0×10^{3}	5300	Staudinger and Roberts (2001)	L	
	3.1×10^{3}	5100	Khan et al. (1995)	M	
	3.1×10^{3}		Khan et al. (1992)	M	
	3.1×10^{3}	5200	Khan and Brimblecombe (1992)	M	
	2.2×10^{4}		Keshavarz et al. (2022)	Q	
	2.3×10^{2}		Duchowicz et al. (2020)	Q	185
	7.8×10^{3}		Wang et al. (2017)	Q	81, 239
	5.0×10^{1}		Wang et al. (2017)	Q	81, 240
	1.9×10^{1}		Wang et al. (2017)	Q	81, 241
	1.6×10^{3}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{6}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{3}		Raventos-Duran et al. (2010)	Q	246
	2.6×10^{3}		Hilal et al. (2008)	Q	
	2.6×10^{3}		Modarresi et al. (2007)	Q	68
		5600	Kühne et al. (2005)	Q	
	3.1×10^{3}		Duchowicz et al. (2020)	?	186, 21
		5300	Kühne et al. (2005)	?	
3-oxopropanoic acid	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$OHCCH_2COOH$	1.2×10^{4}		Wang et al. (2017)	Q	81, 240
[926-61-4]	1.7×10^{4}		Wang et al. (2017)	Q	81, 241
OAKURXIZZOAYBC-UHFFFAOYSA-N	6.9×10^{1}		Saxena and Hildemann (1996)	E	403

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-hydroxypropanoic acid	1.2×10^{2}		Duchowicz et al. (2020)	V	187
$CH_3CHOHCOOH$	1.2×10^{2}		HSDB (2015)	V	
(lactic acid)	1.1×10^{3}		Duchowicz et al. (2020)	Q	
[50-21-5]	9.9×10^{2}		Raventos-Duran et al. (2010)	Q	243, 244
JVTAAEKCZFNVCJ-UHFFFAOYSA-N	9.9×10^{3}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	246
	6.9×10^{5}		Saxena and Hildemann (1996)	E	403
glycidaldehyde	1.9×10^{1}		HSDB (2015)	Q	100
$C_3H_4O_2$					
[765-34-4]					
IWYRWIUNAVNFPE-UHFFFAOYSA-N					
trimethylene oxide	4.0×10^{-1}		Duchowicz et al. (2020)	V	187
C_3H_6O	3.9×10^{-1}		HSDB (2015)	V	
(1,3-epoxypropane; 1,3-propylene oxide; oxetane)	1.2×10^{-1}		Duchowicz et al. (2020)	Q	
[503-30-0]					
AHHWIHXENZJRFG-UHFFFAOYSA-N					
2,3-dihydroxypropanal	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_3$	2.6×10^{4}		Wang et al. (2017)	Q	81, 240
(glyceraldehyde)	8.1×10^{2}		Wang et al. (2017)	Q	81, 241
[367-47-5]	2.0×10^{8}		Saxena and Hildemann (1996)	E	403
MNQZXJOMYWMBOU-UHFFFAOYSA-N					
dihydroxyacetone	1.8×10^{6}		HSDB (2015)	V	
$C_3H_6O_3$	5.5×10^{3}		Wang et al. (2017)	Q	81, 239
[96-26-4]	3.8×10^{3}		Wang et al. (2017)	Q	81, 240
RXKJFZQQPQGTFL-UHFFFAOYSA-N	5.0×10^{3}		Wang et al. (2017)	Q	81, 241
2-methoxyethanol	4.4	7500	Hiatt (2013)	M	
$C_3H_8O_2$	2.2×10^{-4}	-730	Ashworth et al. (1988)	M	541, 42, 279
(methyl cellosolve)	1.4×10^{1}		Johanson and Dynésius (1988)	M	14
[109-86-4]	3.7×10^{1}	7300	Cabani et al. (1978)	T	
XNWFRZJHXBZDAG-UHFFFAOYSA-N	6.8		Keshavarz et al. (2022)	Q	
	1.4×10^{1}		Duchowicz et al. (2020)	Q	185
	8.9		Wang et al. (2017)	Q	81, 239
	5.4×10^{1}		Wang et al. (2017)	Q	81, 240
	1.3×10^{1}		Wang et al. (2017)	Q	81, 241
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{2}		Raventos-Duran et al. (2010)	Q	246
	2.1×10^{1}		Hilal et al. (2008)	Q	
	4.0×10^{1}		Modarresi et al. (2007)	Q	68
	1.5×10^{1}		Nirmalakhandan et al. (1997)	Q	
	3.0×10^{1}		Duchowicz et al. (2020)	?	186, 21

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-oxobutanoic acid	8.3×10^{3}		Wang et al. (2017)	Q	81, 239
$OHC(CH_2)_2COOH$	3.2×10^{5}		Wang et al. (2017)	Q	81, 240
[692-29-5]	2.1×10^{4}		Wang et al. (2017)	Q	81, 241
UIUJIQZEACWQSV-UHFFFAOYSA-N	4.9×10^{1}		Saxena and Hildemann (1996)	E	403
2,3-dihydroxybutanedioic acid	4.9×10^{15}		Burkholder et al. (2019)	L	
HOOCCHOHCHOHCOOH	4.9×10^{15}		Burkholder et al. (2015)	L	
(tartaric acid)			Compernolle and Müller (2014a)	V	542
[87-69-4]	1.3×10^{13}		Yaws (2003)	X	238, 12
FEWJPZIEWOKRBE-JCYAYHJZSA-N	5.1×10^{10}		Gharagheizi et al. (2012)	Q	
	1.3×10^{13}		Gharagheizi et al. (2010)	Q	247
	9.9×10^{15}		Saxena and Hildemann (1996)	E	403
3-oxapentane-1,5-diol	3.3×10^{4}		Yaws (2003)	X	259
$HO(CH_2)_2O(CH_2)_2OH$	3.3×10^{4}		Yaws (2003)	X	238
(diethylene glycol)	9.0×10^{3}		Dupeux et al. (2022)	Q	260
[111-46-6]	2.5×10^{3}		Olsen et al. (2016)	Q	427
MTHSVFCYNBDYFN-UHFFFAOYSA-N	1.6×10^{3}		Olsen et al. (2016)	Q	428
	1.7×10^{3}		Olsen et al. (2016)	Q	429
	4.9×10^{3}		HSDB (2015)	Q	100
	7.7×10^{3}		Gharagheizi et al. (2012)	Q	
	3.8×10^{4}		Gharagheizi et al. (2010)	Q	247
	2.4×10^{4}		Hilal et al. (2008)	Q	
	2.2×10^{4}		Yao et al. (2002)	Q	230
	2.0×10^{7}		Saxena and Hildemann (1996)	E	403
	3.3×10^{4}		Yaws (1999)	?	21
hydroxybutanedioic acid	2.7×10^{8}		Compernolle and Müller (2014a)	V	
$HOOCCH_2CHOHCOOH$	1.7×10^{9}		Yaws (2003)	X	238, 374
(malic acid)	1.2×10^{7}		HSDB (2015)	Q	100
[6915-15-7]	5.3×10^{8}		Gharagheizi et al. (2012)	Q	
BJEPYKJPYRNKOW-UHFFFAOYSA-N	1.4×10^{9}		Gharagheizi et al. (2010)	Q	247
	2.0×10^{11}		Saxena and Hildemann (1996)	E	403
2-ethoxyethanol	8.9		Johanson and Dynésius (1988)	M	14
$C_4H_{10}O_2$	3.3×10^{1}		Abraham et al. (1994a)	R	
[110-80-5]	2.8×10^{1}	8000	Cabani et al. (1978)	T	
ZNQVEEAIQZEUHB-UHFFFAOYSA-N	9.2		Keshavarz et al. (2022)	Q	
	5.8		Duchowicz et al. (2020)	Q	300
	7.4		Wang et al. (2017)	Q	81, 239
	3.4×10^{1}		Wang et al. (2017)	Q	81, 240
	9.8		Wang et al. (2017)	Q	81, 241
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	246
	1.6×10^{1}		Hilal et al. (2008)	Q	
	3.2×10^{1}		Modarresi et al. (2007)	Q	68
	7.5		Nirmalakhandan et al. (1997)	Q	

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.1×10^{1}		Duchowicz et al. (2020)	?	186, 21
	1.9×10^{1}		Yaws (1999)	?	21, 12
2-methoxy-1-propanol $C_4H_{10}O_2$ [1589-47-5] YTTFFPATQICAQN-UHFFFAOYSA-N	5.5×10^{2}		HSDB (2015)	Q	100
1,1-dimethoxyethane $C_4H_{10}O_2$ [534-15-6] SPEUIVXLLWOEMJ-UHFFFAOYSA-N	1.5×10^{-1}		HSDB (2015)	Q	100
4-methylene-2-oxetanone $C_4H_4O_2$ (acetyl ketene) [674-82-8] WASQWSOJHCZDFK-UHFFFAOYSA-N	1.6×10^{-2}		HSDB (2015)	Q	100
2(5H)-furanone $C_4H_4O_2$ [497-23-4] VIHAEDVKXSOUAT-UHFFFAOYSA-N	3.5×10^{-1}		Wang et al. (2017)	Q	81, 239
	3.6×10^{2}		Wang et al. (2017)	Q	81, 240
	1.4×10^{3}		Wang et al. (2017)	Q	81, 241
	1.0		HSDB (2015)	Q	100
2,2'-bioxirane $C_4H_6O_2$ [1464-53-5] ZFIVKAOQEXOYFY-UHFFFAOYSA-N	2.8×10^{2}		HSDB (2015)	Q	100
γ-butyrolactone $C_4H_6O_2$ [96-48-0] YEJRWHAVMIAJKC-UHFFFAOYSA-N	1.9×10^{2}		Duchowicz et al. (2020)	V	187
	1.9×10^{2}		HSDB (2015)	V	
	6.5×10^{1}		Dupeux et al. (2022)	Q	260
	1.2		Duchowicz et al. (2020)	Q	
ethyloxirane C_4H_8O (1,2-epoxybutane) [106-88-7] RBACIKXCRWGCBB-UHFFFAOYSA-N	5.5×10^{-2}		Duchowicz et al. (2020)	V	187
	5.5×10^{-2}		HSDB (2015)	V	
	6.9×10^{-2}		Duchowicz et al. (2020)	Q	
2,3-epoxy-2-methyl-1,4-butanediol $C_5H_{10}O_3$ (IEPOX) FLVAIUDBQNOKHB-UHFFFAOYSA-N	5.0×10^{4}		Wang et al. (2017)	Q	81, 239
	1.3×10^{5}		Wang et al. (2017)	Q	81, 240
	3.2×10^{4}		Wang et al. (2017)	Q	81, 241
	2.7×10^{4}		Pye et al. (2013)	Q	494
			Chan et al. (2010)	Q	543
	1.3×10^{6}		Eddingsaas et al. (2010)	Q	544
	1.9×10^{5}		Vasilakos et al. (2021)	E	545
	3.0×10^{5}		Woo and McNeill (2015)	?	468

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MEDICO1CO $C_5H_8O_4$ RRXXDUUNVWXRFN-UHFFFAOYSA-N	2.5×10^{7}	12000	Wieser et al. (2023)	Q	439
MEDICO4CO $C_5H_8O_4$ GXKSWJOBVXKANI-UHFFFAOYSA-N	3.1×10^{6}	12000	Wieser et al. (2023)	Q	439
METRICO $C_5H_{10}O_4$ LCGBCDAYKOJPSO-UHFFFAOYSA-N	7.3×10^{6}	12000	Wieser et al. (2023)	Q	439
2,3-epoxy-6-oxo-heptenal $C_7H_8O_3$ (MCM:TLEPOXMUC) YHZQHUOBDYTWMQ-UHFFFAOYSA-N	1.1×10^{4} 1.4×10^{4} 2.8×10^{3} 2.5×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) McNeill et al. (2012)	Q Q Q Q	81, 239 81, 240 81, 241
3-hydroxy-2-butanone $C_4H_8O_2$ (acetoin) [513-86-0] ROWKJAVDOGWPAT-UHFFFAOYSA-N	3.1 5.7×10^{-1} 7.8 1.1×10^{2} 1.2×10^{1} 9.9×10^{-1}		Wu et al. (2022b) Straver and de Loos (2005) Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) HSDB (2015)	M M Q Q Q Q	546 81, 239 81, 240 81, 241 100
2-(vinyloxy)ethanol $C_4H_8O_2$ (ethylene glycol monovinyl ether) [764-48-7] VUIWJRYTWUGOOF-UHFFFAOYSA-N	3.9×10^{1}		HSDB (2015)	Q	100
2-methyloxetane C_4H_8O [2167-39-7] FZIIBDOXPQOKBP-UHFFFAOYSA-N	1.2×10^{-1}		HSDB (2015)	Q	100
5-oxopentanoic acid $OHC(CH_2)_3COOH$ [5746-02-1] VBKPPDYGFUZOAJ-UHFFFAOYSA-N	3.9×10^{1}		Saxena and Hildemann (1996)	E	403
2-oxopentanedioic acid $HOOC(CH_2)_2COCOOH$ (α-keto glutaric acid) [328-50-7] KPGXRSRHYNQIFN-UHFFFAOYSA-N	9.9×10^{6}		Saxena and Hildemann (1996)	E	403

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tetrahydro-2-furanmethanol	4.4×10^{1}		Yaws (2003)	X	259
$C_5H_{10}O_2$	1.7×10^{2}		Dupeux et al. (2022)	Q	260
(tetrahydrofurfuryl alcohol)	2.4×10^{3}		HSDB (2015)	Q	100
[97-99-4]					
BSYVTEYKTMYBMK-UHFFFAOYSA-N					
xylose	8.2×10^{3}		HSDB (2015)	Q	100
$C_5H_{10}O_5$					
[58-86-6]					
PYMYPHUHKUWMLA-VPENINKCSA-N					
2-(2-methoxyethoxy)ethanol	6.2×10^{5}		HSDB (2015)	Q	100
$C_5H_{12}O_3$					
(diethylene glycol monomethyl ether)					
[111-77-3]					
SBASXUCJHJRPEV-UHFFFAOYSA-N					
3,6-dioxaoctane-1,8-diol	1.1×10^{4}		Olsen et al. (2016)	Q	427
$HO(CH_2CH_2O)_3H$	5.9×10^{3}		Olsen et al. (2016)	Q	428
(triethylene glycol)	6.7×10^{3}		Olsen et al. (2016)	Q	429
[112-27-6]	3.1×10^{5}		HSDB (2015)	Q	100
ZIBGPFATKBEMQZ-UHFFFAOYSA-N	8.9×10^{9}		Saxena and Hildemann (1996)	E	403
2-oxepanone	5.5×10^{-2}		HSDB (2015)	Q	100
$C_6H_{10}O_2$					
(caprolactone)					
[502-44-3]					
PAPBSGBWRJIAAV-UHFFFAOYSA-N					
glycidyl ether	7.6×10^{2}		HSDB (2015)	Q	100
$C_6H_{10}O_3$					
(diglycidyl ether)					
[2238-07-5]					
GYZLOYUZLJXAJU-UHFFFAOYSA-N					
4-hydroxy-4-methyl-2-pentanone	3.8×10^{1}		Duchowicz et al. (2020)	V	187
$C_6H_{12}O_2$	1.3×10^{1}		Yaws (2003)	X	259
(diacetone alcohol)	3.1×10^{2}		Dupeux et al. (2022)	Q	260
[123-42-2]	7.4×10^{-2}		Duchowicz et al. (2020)	Q	
SWXVUIWOUIDPGS-UHFFFAOYSA-N	7.6×10^{1}		Wang et al. (2017)	Q	81, 239
	8.0×10^{2}		Wang et al. (2017)	Q	81, 240
	6.8×10^{1}		Wang et al. (2017)	Q	81, 241
	2.3×10^{3}		HSDB (2015)	Q	547
1-propoxy-2-propanol	2.9×10^{2}		HSDB (2015)	Q	547
$C_6H_{14}O_2$					
[1569-01-3]					
FENFUOGYJVOCRY-UHFFFAOYSA-N					

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-(2-ethoxyethoxy)ethanol	4.4×10^{2}		Duchowicz et al. (2020)	V	187
$C_6H_{14}O_3$	4.5×10^{2}		HSDB (2015)	V	
(diethylene glycol monoethyl ether)	9.0×10^{2}		Dupeux et al. (2022)	Q	260
[111-90-0]	6.4×10^{1}		Duchowicz et al. (2020)	Q	
XXJWXESWEXIICW-UHFFFAOYSA-N					
2,5,8-trioxanonane	1.9×10^{1}		Duchowicz et al. (2020)	V	187
$C_6H_{14}O_3$	1.9×10^{1}		HSDB (2015)	V	
(diglyme)	6.2		Duchowicz et al. (2020)	Q	
[111-96-6]					
SBZXBUIDTXKZTM-UHFFFAOYSA-N					
oxydipropanol	1.8×10^{3}		HSDB (2015)	V	
$C_6H_{14}O_3$					
(dipropylene glycol)					
[25265-71-8]					
SZXQTJUDPRGNJN-UHFFFAOYSA-N					
p-benzoquinone	2.1×10^{-2}		HSDB (2015)	V	
$C_6H_4O_2$	5.1		Wang et al. (2017)	Q	81, 239
(1,4-benzoquinone)	1.7×10^{4}		Wang et al. (2017)	Q	81, 240
[106-51-4]	2.3×10^{1}		Wang et al. (2017)	Q	81, 241
AZQWKYJCGOJGHM-UHFFFAOYSA-N	2.1×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	7.7		Katritzky et al. (1998)	Q	
5-hydroxymethylfurfural	1.8×10^{4}		HSDB (2015)	Q	100
$C_6H_6O_3$					
(5-hydroxymethyl-2-furfuraldehyde)					
[67-47-0]					
NOEGNKMFWQHSLB-UHFFFAOYSA-N					
5-hydroxy-2-(hydroxymethyl)-4H-pyran-4-one	4.1×10^{1}		HSDB (2015)	Q	100
$C_6H_6O_4$					
(kojic acid)					
[501-30-4]					
BEJNERDRQOWKJM-UHFFFAOYSA-N					
2-hydroxy-1,2,3-propanetricarboxylic acid	3.1×10^{15}		Burkholder et al. (2019)	L	
$C_6H_8O_7$	3.1×10^{15}		Burkholder et al. (2015)	L	
(citric acid)			Compernolle and Müller (2014a)	V	548
[77-92-9]	7.6×10^{12}		Yaws (2003)	X	238, 12
KRKNYBCHXYNGOX-UHFFFAOYSA-N	4.8×10^{11}		Gharagheizi et al. (2012)	Q	
	7.9×10^{12}		Gharagheizi et al. (2010)	Q	247
	3.0×10^{16}		Saxena and Hildemann (1996)	E	403

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(butoxymethyl)oxirane	4.0×10^{-1}		Duchowicz et al. (2020)	V	187
$C_7H_{14}O_2$	3.9×10^{-1}		HSDB (2015)	V	
(n-butyl glycidyl ether)	8.9×10^{-1}		Duchowicz et al. (2020)	Q	
[2426-08-6]					
YSUQLAYJZDEMOT-UHFFFAOYSA-N					
1-(1,1-dimethylethoxy)-2-propanol	2.1		HSDB (2015)	V	
$C_7H_{16}O_2$					
(propylene glycol mono-t-butyl ether)					
[57018-52-7]					
GQCZPFJGIXHZMB-UHFFFAOYSA-N					
2-[2-(2-methoxyethoxy)ethoxy]ethanol	2.8×10^{8}		HSDB (2015)	Q	100
$C_7H_{16}O_4$					
(triethylene glycol monomethyl ether)					
[112-35-6]					
JLGLQAWTXXGVEM-UHFFFAOYSA-N					
2-methyl-*p*-benzoquinone	3.1		Wang et al. (2017)	Q	81, 239
$C_7H_6O_2$	6.9×10^{3}		Wang et al. (2017)	Q	81, 240
[553-97-9]	2.1×10^{1}		Wang et al. (2017)	Q	81, 241
VTWDKFNVVLAELH-UHFFFAOYSA-N	5.2×10^{3}		HSDB (2015)	Q	100
patulin	9.0×10^{4}		HSDB (2015)	Q	100
$C_7H_6O_4$					
[149-29-1]					
ZRWPUFFVAOMMNM-UHFFFAOYSA-N					
1-hydroxy-3-methoxybenzene	1.7×10^{2}		Abraham et al. (1994a)	R	
$C_7H_8O_2$	1.7×10^{2}		Keshavarz et al. (2022)	Q	
(3-methoxyphenol)	4.7×10^{2}		Duchowicz et al. (2020)	Q	300
[150-19-6]	2.0×10^{2}		Raventos-Duran et al. (2010)	Q	243, 244
ASHGTJPOSUFTGB-UHFFFAOYSA-N	2.5×10^{2}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{2}		Raventos-Duran et al. (2010)	Q	246
	1.3×10^{2}		Hilal et al. (2008)	Q	
	6.4×10^{1}		Modarresi et al. (2007)	Q	68
	5.0×10^{2}		Nirmalakhandan et al. (1997)	Q	
	1.7×10^{2}		Duchowicz et al. (2020)	?	186, 21
mequinol	6.9×10^{-1}		Yaws (2003)	X	238, 14
$C_7H_8O_2$	1.9×10^{1}		HSDB (2015)	Q	100
(4-methoxyphenol)	6.9×10^{-1}		Gharagheizi et al. (2010)	Q	247
[150-76-5]	2.0		Yaws (1999)	?	21, 14
NWVVVBRKAWDGAB-UHFFFAOYSA-N					

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-hydroxy-2-methoxybenzene	8.6		McFall et al. (2020)	M	
$C_7H_8O_2$	9.0	7900	Wieland et al. (2015)	M	549
(guaiacol; 2-methoxyphenol)	7.7		Sagebiel et al. (1992)	M	
[90-05-1]	9.1	7600	Sagebiel et al. (1992)	M	
LHGVFZTZFXWLCP-UHFFFAOYSA-N	9.6		Mackay et al. (2006c)	V	
	7.7		Sagebiel et al. (1992)	V	
	4.1×10^{1}		Leuenberger et al. (1985)	V	418
	5.0		Abraham et al. (1994a)	R	
	1.1×10^{1}		Keshavarz et al. (2022)	Q	
	5.6×10^{-1}		Abney (2021)	Q	401
	8.7		Duchowicz et al. (2020)	Q	300
	8.2		McFall et al. (2020)	Q	476
	5.2		Hilal et al. (2008)	Q	
	7.7		Modarresi et al. (2007)	Q	68
		6700	Kühne et al. (2005)	Q	
	1.2×10^{1}		English and Carroll (2001)	Q	231, 275
	6.4×10^{1}		Katritzky et al. (1998)	Q	
	5.1×10^{2}		Nirmalakhandan et al. (1997)	Q	
	8.2		Duchowicz et al. (2020)	?	186, 21
		7800	Kühne et al. (2005)	?	
	3.3×10^{-1}		Yaws (1999)	?	21, 14
1,4-dimethoxybenzene	2.8×10^{-3}		HSDB (2015)	Q	100
$C_8H_{10}O_2$					
(hydroquinone dimethyl ether)					
[150-78-7]					
OHBQPCCCRFSCAX-UHFFFAOYSA-N					
4-methyl-2-methoxyphenol	7.7		Sagebiel et al. (1992)	M	
$C_8H_{10}O_2$	7.1	7400	Sagebiel et al. (1992)	M	
[93-51-6]	1.0×10^{1}		Sagebiel et al. (1992)	V	
PETRWTHZSKVLRE-UHFFFAOYSA-N	1.6×10^{1}		Keshavarz et al. (2022)	Q	
	5.2		Duchowicz et al. (2020)	Q	
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	272, 244
	3.1		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{2}		Raventos-Duran et al. (2010)	Q	246
	5.2		Hilal et al. (2008)	Q	
	2.5		Modarresi et al. (2007)	Q	68
		7100	Kühne et al. (2005)	Q	
	7.3		Yaffe et al. (2003)	Q	249, 250
	6.2×10^{1}		Katritzky et al. (1998)	Q	
	7.4		Duchowicz et al. (2020)	?	186, 21
		7900	Kühne et al. (2005)	?	

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tyrosol $C_8H_{10}O_2$ (4-hydroxybenzeneethanol) [501-94-0] YCCILVSKPBXVIP-UHFFFAOYSA-N	3.5×10^{5}		McFall et al. (2020)	Q	476
1,3-dimethoxy-2-hydroxybenzene $C_8H_{10}O_3$ (2,6-dimethoxyphenol) [91-10-1] KLIDCXVFHGNTTM-UHFFFAOYSA-N	3.7×10^{1}		Sagebiel et al. (1992)	M	
	5.0×10^{1}	6700	Sagebiel et al. (1992)	M	
	1.2×10^{2}		Sagebiel et al. (1992)	V	
	1.6×10^{1}		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	
	7.8×10^{2}		Raventos-Duran et al. (2010)	Q	272, 244
	4.9×10^{2}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{3}		Raventos-Duran et al. (2010)	Q	246
	3.5×10^{2}		Hilal et al. (2008)	Q	
	1.1×10^{2}		Modarresi et al. (2007)	Q	68
		7300	Kühne et al. (2005)	Q	
	4.3×10^{1}		Duchowicz et al. (2020)	?	186, 21
		7600	Kühne et al. (2005)	?	
hexahydro-1,3-isobenzofurandione $C_8H_{10}O_3$ (hexahydrophthalic anhydride) [85-42-7] MUTGBJKUEZFXGO-UHFFFAOYSA-N	4.7×10^{-1}		HSDB (2015)	Q	100
vanillyl alcohol $C_8H_{10}O_3$ [498-00-0] ZENOXNGFMSCLLL-UHFFFAOYSA-N	9.6×10^{4}		McFall et al. (2020)	M	
	2.0×10^{5}		McFall et al. (2020)	Q	476
1-methoxy-4-methylbenzene $C_8H_{10}O$ [104-93-8] CHLICZRVGGXEOD-UHFFFAOYSA-N	2.1×10^{-3}		HSDB (2015)	Q	100
dimethoxane $C_8H_{14}O_4$ [828-00-2] PHMNXPYGVPEQSJ-UHFFFAOYSA-N	8.0×10^{1}		HSDB (2015)	Q	100
RO5R5 $C_8H_{14}O_4$ MESHXYGXEHAFFE-UHFFFAOYSA-N	1.3×10^{5}	17000	Wieser et al. (2023)	Q	439
5-hydroxy-2-octanone $C_8H_{16}O_2$ (C82CO5OH) KZPPEBIAPHLFQD-UHFFFAOYSA-N	1.6×10^{3}	11000	Wieser et al. (2023)	Q	439

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
metaldehyde $C_8H_{16}O_4$ [108-62-3] GKKDCARASOJPNG-UHFFFAOYSA-N	1.9×10^{-1} 2.9×10^{-1}		HSDB (2015) Maniere et al. (2011)	V ?	 12, 166
diethyl carbitol $C_8H_{18}O_3$ (diethylene glycol diethyl ether) [112-36-7] RRQYJINTUHWNHW-UHFFFAOYSA-N	8.9×10^{1} 9.0×10^{1} 9.6×10^{-1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
2-[2-(2-ethoxyethoxy)ethoxy]ethanol $C_8H_{18}O_4$ (triethylene glycol monoethyl ether) [112-50-5] WFSMVVDJSNMRAR-UHFFFAOYSA-N	2.1×10^{8}		HSDB (2015)	Q	100
tetraethylene glycol $C_8H_{18}O_5$ [112-60-7] UWHCKJMYHZGTIT-UHFFFAOYSA-N	1.8×10^{13}		HSDB (2015)	Q	100
vanillin $C_8H_8O_3$ [121-33-5] MWOOGOJBHIARFG-UHFFFAOYSA-N	1.7×10^{3} 4.6×10^{3} 4.7×10^{3} 1.3×10^{3} 1.3×10^{3} 1.8×10^{3} 1.8×10^{3} 1.8×10^{3} 4.0×10^{3} 2.8×10^{2} 4.9×10^{3} 3.1×10^{2} 1.2×10^{5} 1.3×10^{3}	6800	Brockbank (2013) Duchowicz et al. (2020) HSDB (2015) Yaws (2003) Yaws (2003) Dupeux et al. (2022) Dupeux et al. (2022) Abney (2021) Duchowicz et al. (2020) Gharagheizi et al. (2012) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Gharagheizi et al. (2010)	L V V X X Q Q Q Q Q Q Q Q Q	1 187 259 238 260 260 401 243, 244 245 246 247
ethylparaben $C_9H_{10}O_3$ [120-47-8] NUVBSKCKDOMJSU-UHFFFAOYSA-N	2.1×10^{3}		HSDB (2015)	Q	100
ethyl vanillin $C_9H_{10}O_3$ [121-32-4] CBOQJANXLMLOSS-UHFFFAOYSA-N	1.2×10^{4}		HSDB (2015)	V	

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-phenoxypropan-2-ol $C_9H_{12}O_2$ (propylene glycol phenyl ether) [770-35-4] IBLKWZIFZMJLFL-UHFFFAOYSA-N	3.4×10^{2}		HSDB (2015)	V	
triacetin $C_9H_{14}O_6$ [102-76-1] URAYPUMNDPQOKB-UHFFFAOYSA-N	8.0×10^{2} 8.2×10^{2} 2.7×10^{2} 2.0×10^{3} 2.5×10^{2} 6.2×10^{3}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010)	V V Q Q Q Q	187 243, 244 245 246
tripropylene glycol $C_9H_{20}O_4$ [24800-44-0] LCZVSXRMYJUNFX-UHFFFAOYSA-N	3.0×10^{9}		HSDB (2015)	Q	100
coumarin $C_9H_6O_2$ [91-64-5] ZYGHJZDHTFUPRJ-UHFFFAOYSA-N	9.9×10^{1} 1.0×10^{2} 1.3×10^{2} 5.1		Duchowicz et al. (2020) HSDB (2015) Dupeux et al. (2022) Duchowicz et al. (2020)	V V Q Q	187 260
4-ethylguaiacol $C_9H_{12}O_2$ (4-ethyl-2-methoxyphenol) [2785-89-9] CHWNEIVBYREQRF-UHFFFAOYSA-N	5.5		McFall et al. (2020)	Q	476
4-methylsyringol $C_9H_{12}O_3$ [6638-05-7] ZFBNNSOJNZBLLS-UHFFFAOYSA-N	3.8×10^{1}		McFall et al. (2020)	Q	476
acetovanillone $C_9H_{10}O_3$ (apocynin) [498-02-2] DFYRUELUNQRZTB-UHFFFAOYSA-N	6.3×10^{3}		McFall et al. (2020)	Q	476
syringaldehyde $C_9H_{10}O_4$ [134-96-3] KCDXJAYRVLXPFO-UHFFFAOYSA-N	3.7×10^{5}		McFall et al. (2020)	Q	476
5-(1-propenyl)-1,3-benzodioxole $C_{10}H_{10}O_2$ (isosafrole) [120-58-1] VHVOLFRBFDOUSH-UHFFFAOYSA-N	2.7×10^{-4}		HSDB (2015)	Q	100

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
safrole $C_{10}H_{10}O_2$ [94-59-7] ZMQAAUBTXCXRIC-UHFFFAOYSA-N	1.1		HSDB (2015)	Q	100
5-propyl-1,3-benzodioxole $C_{10}H_{12}O_2$ (dihydrosafrole) [94-58-6] MYEIDJPOUKASEC-UHFFFAOYSA-N	8.2×10^{-1}		HSDB (2015)	Q	100
2-methoxy-4-(1-propenyl)phenol $C_{10}H_{12}O_2$ (isoeugenol) [97-54-1] BJIOGJUNALELMI-UHFFFAOYSA-N	2.7 1.7×10^{1}		HSDB (2015) McFall et al. (2020)	V Q	 476
p-cresyl glycidyl ether $C_{10}H_{12}O_2$ [26447-14-3] CUFXMPWHOWYNSO-UHFFFAOYSA-N	1.3×10^{1}		HSDB (2015)	Q	100
4-(4-hydroxyphenyl)-2-butanone $C_{10}H_{12}O_2$ (raspberry ketone) [5471-51-2] NJGBTKGETPDVIK-UHFFFAOYSA-N	1.8×10^{4}		HSDB (2015)	Q	449
guaifenesin $C_{10}H_{14}O_4$ [93-14-1] HSRJKNPTNIJEKV-UHFFFAOYSA-N	2.2×10^{5}		HSDB (2015)	Q	100
RO5R4O2H $C_{10}H_{18}O_7$ YORZXZYHORHTRW-UHFFFAOYSA-N	3.6×10^{10}	24000	Wieser et al. (2023)	Q	439
levomenthol $C_{10}H_{20}O$ (*L*-menthol) [2216-51-5] NOOLISFMXDJSKH-AEJSXWLSSA-N	6.6×10^{-1}		HSDB (2015)	Q	100
diethylene glycol hexyl ether $C_{10}H_{22}O_3$ [112-59-4] GZMAAYIALGURDQ-UHFFFAOYSA-N	5.7×10^{2} 5.8×10^{2} 1.0×10^{2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-[2-(2-butoxyethoxy)ethoxy]ethanol $C_{10}H_{22}O_4$ (triethylene glycol monobutyl ether) [143-22-6] COBPKKZHLDDMTB-UHFFFAOYSA-N	1.0×10^{8}		HSDB (2015)	Q	100
4-propylguaiacol $C_{10}H_{14}O_2$ (2-methoxy-4-propylphenol) [2785-87-7] PXIKRTCSSLJURC-UHFFFAOYSA-N	4.3 4.2		McFall et al. (2020) McFall et al. (2020)	M Q	 476
vanillyl ethyl ether $C_{10}H_{14}O_3$ (4-(ethoxymethyl)-2-methoxyphenol) [13184-86-6] KOCVACNWDMSLBM-UHFFFAOYSA-N	4.1×10^{2} 4.8×10^{2}		McFall et al. (2020) McFall et al. (2020)	M Q	 476
4-ethylsyringol $C_{10}H_{14}O_3$ [14059-92-8] PJWDIHUFLXQRFF-UHFFFAOYSA-N	3.0×10^{1}		McFall et al. (2020)	Q	476
guaiacylacetone $C_{10}H_{12}O_3$ (1-(4-hydroxy-3-methoxyphenyl)-2-propanone) [2503-46-0] LFVCJQWZGDLHSD-UHFFFAOYSA-N	1.2×10^{4} 1.1×10^{4}		McFall et al. (2020) McFall et al. (2020)	M Q	 476
acetosyringone $C_{10}H_{12}O_4$ [2478-38-8] OJOBTAOGJIWAGB-UHFFFAOYSA-N	5.0×10^{5}		McFall et al. (2020)	Q	476
coniferylaldehyde $C_{10}H_{10}O_3$ [458-36-6] UCZOBXQKIUMJDZ-UHFFFAOYSA-N	4.4×10^{4}		McFall et al. (2020)	Q	476
4-methoxy-6-(2-propenyl)-1,3-benzodioxole $C_{11}H_{12}O_3$ (myristicin) [607-91-0] BNWJOHGLIBDBOB-UHFFFAOYSA-N	1.8×10^{1}		HSDB (2015)	Q	100

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
butylparaben $C_{11}H_{14}O_3$ [94-26-8] QFOHBWFCKVYLES-UHFFFAOYSA-N	1.2×10^{3}		HSDB (2015)	Q	100
2-*tert*-butyl-4-methoxyphenol $C_{11}H_{16}O_2$ (butylated hydroxyanisole) [25013-16-5] MRBKEAMVRSLQPH-UHFFFAOYSA-N	8.4		HSDB (2015)	Q	100
3-hydroxy-2-naphthalenecarboxylic acid	7.0×10^{3}		HSDB (2015)	Q	100
$C_{11}H_8O_3$	7.2×10^{3}		Zhang et al. (2010)	Q	288, 289
[92-70-6]	1.2×10^{4}		Zhang et al. (2010)	Q	288, 290
ALKYHXVLJMQRLQ-UHFFFAOYSA-N	3.8×10^{5}		Zhang et al. (2010)	Q	288, 291
	8.2×10^{3}		Zhang et al. (2010)	Q	288, 292
4-propylsyringol $C_{11}H_{16}O_3$ [6766-82-1] YHEWWEXPVKCVFY-UHFFFAOYSA-N	2.2×10^{1}		McFall et al. (2020)	Q	476
zingerone	1.2×10^{4}		McFall et al. (2020)	M	
$C_{11}H_{14}O_3$	8.4×10^{3}		McFall et al. (2020)	Q	476
(vanillylacetone) [122-48-5] OJYLAHXKWMRDGS-UHFFFAOYSA-N					
allylsyringol $C_{11}H_{14}O_3$ [5438-54-0] IYIVYBWBUQPWAU-UHFFFAOYSA-N	6.3×10^{2}		McFall et al. (2020)	Q	476
4-propenylsyringol $C_{11}H_{14}O_3$ [6635-22-9] YFHOHYAUMDHSBX-UHFFFAOYSA-N	1.1×10^{3}		McFall et al. (2020)	Q	476
propionylsyringol $C_{11}H_{14}O_4$ [5650-43-1] CXCPJZXJNRBTGF-UHFFFAOYSA-N	3.8×10^{5}		McFall et al. (2020)	Q	476
sinapylaldehyde $C_{11}H_{12}O_4$ [4206-58-0] CDICDSOGTRCHMG-ONEGZZNKSA-N	3.1×10^{6}		McFall et al. (2020)	Q	476

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
arbutin $C_{12}H_{16}O_7$ [497-76-7] BJRNKVDFDLYUGJ-RMPHRYRLSA-N	8.2×10^{13}		HSDB (2015)	Q	100
butopyronoxyl $C_{12}H_{18}O_4$ (indalone) [532-34-3] OKIJSNGRQAOIGZ-UHFFFAOYSA-N	2.1×10^{2}		HSDB (2015)	Q	100
diethylene glycol bis(methacrylate) $C_{12}H_{18}O_5$ [2358-84-1] XFCMNSHQOZQILR-UHFFFAOYSA-N	1.2×10^{4}		HSDB (2015)	Q	100
dikegulac $C_{12}H_{18}O_7$ [18467-77-1] FWCBATIDXGJRMF-FLNNQWSLSA-N	5.2×10^{10}		HSDB (2015)	Q	100
propofol $C_{12}H_{18}O$ [2078-54-8] OLBCVFGFOZPWHH-UHFFFAOYSA-N	4.7		HSDB (2015)	Q	100
lactitol $C_{12}H_{24}O_{11}$ [585-86-4] VQHSOMBJVWLPSR-JVCRWLNRSA-N	1.2×10^{16}		HSDB (2015)	Q	100
maltitol $C_{12}H_{24}O_{11}$ [585-88-6] VQHSOMBJVWLPSR-WUJBLJFYSA-N	2.3×10^{15}		HSDB (2015)	Q	100
naphthalic anhydride $C_{12}H_6O_3$ [81-84-5] GRSMWKLPSNHDHA-UHFFFAOYSA-N	1.6×10^{1}		HSDB (2015)	Q	100
methoxsalen $C_{12}H_8O_4$ (8-methoxypsoralen) [298-81-7] QXKHYNVANLEOEG-UHFFFAOYSA-N	2.5×10^{2}		HSDB (2015)	Q	100
syringylacetone $C_{12}H_{16}O_4$ [112468-41-4] NULBEPOZYDYWOV-UHFFFAOYSA-N	1.2×10^{6} 5.7×10^{4}		McFall et al. (2020) McFall et al. (2020)	M Q	 476

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
butyrylsyringol $C_{12}H_{16}O_4$ [69271-91-6] QFHXMVPZYYMTCS-UHFFFAOYSA-N	2.9×10^{5}		McFall et al. (2020)	Q	476
bisphenol F $C_{13}H_{12}O_2$ [620-92-8] PXKLMJQFEQBVLD-UHFFFAOYSA-N	1.9×10^{6}		HSDB (2015)	Q	449
ibuprofen $C_{13}H_{18}O_2$ [15687-27-1] HEFNNWSXXWATRW-UHFFFAOYSA-N	6.6×10^{1} 2.0×10^{2}		HSDB (2015) Abraham et al. (2019)	V Q	
trinexapac-ethyl $C_{13}H_{16}O_5$ [95266-40-3] RVKCCVTVZORVGD-QXMHVHEDSA-N	5.1 7.6×10^{5} 1.9×10^{3}		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	187 166
benzoyl peroxide $C_{14}H_{10}O_4$ [94-36-0] OMPJBNCRMGITSC-UHFFFAOYSA-N	2.8 2.8 1.1×10^{2} 4.1×10^{2} 4.3×10^{3}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	100 288, 289 288, 290 288, 291 288, 292
oxybenzone $C_{14}H_{12}O_3$ (2-hydroxy-4-methoxybenzophenone) [131-57-7] DXGLGDHPHMLXJC-UHFFFAOYSA-N	6.6×10^{2}		HSDB (2015)	Q	100
resveratrol $C_{14}H_{12}O_3$ [501-36-0] LUKBXSAWLPMMSZ-OWOJBTEDSA-N	7.0×10^{10}		HSDB (2015)	Q	449
pindone $C_{14}H_{14}O_3$ [83-26-1] RZKYEQDPDZUERB-UHFFFAOYSA-N	1.1×10^{6}		HSDB (2015)	Q	100
1,1'-[oxybis(methylene)]bisbenzene $C_{14}H_{14}O$ (dibenzyl ether) [103-50-4] MHDVGSVTJDSBDK-UHFFFAOYSA-N	1.5 3.7×10^{-1} 3.1×10^{-1} 1.2×10^{2} 3.6		Duchowicz et al. (2020) Dupeux et al. (2022) Duchowicz et al. (2020) HSDB (2015) Modarresi et al. (2007)	V Q Q Q Q	187 260 100 68

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
butanoic acid, 3,3-bis((1,1-dimethylethyl)dioxy)-, ethyl ester	5.0		Zhang et al. (2010)	Q	288, 289
$C_{14}H_{28}O_6$	7.0×10^{-3}		Zhang et al. (2010)	Q	288, 290
[55794-20-2]	1.3×10^{2}		Zhang et al. (2010)	Q	288, 291
HARQWLDROVMFJE-UHFFFAOYSA-N	2.4×10^{2}		Zhang et al. (2010)	Q	288, 292
1-hydroxy-9,10-anthracenedione	1.4×10^{3}		Duchowicz et al. (2020)	V	187
$C_{14}H_8O_3$	1.4×10^{3}		HSDB (2015)	V	
(1-hydroxyanthraquinone)	3.5×10^{3}		Duchowicz et al. (2020)	Q	
[129-43-1]					
BTLXPCBPYBNQNR-UHFFFAOYSA-N					
danthron	1.8×10^{5}		HSDB (2015)	Q	100
$C_{14}H_8O_4$					
(1,8-dihydroxyanthraquinone)					
[117-10-2]					
QBPFLULOKWLNNW-UHFFFAOYSA-N					
bisphenol A	2.5×10^{5}		HSDB (2015)	V	
$C_{15}H_{16}O_2$					
[80-05-7]					
IISBACLAFKSPIT-UHFFFAOYSA-N					
atractylenolide III	1.0×10^{3}		HSDB (2015)	Q	100
$C_{15}H_{20}O_3$					
[73030-71-4]					
FBMORZZOJSDNRQ-GLQYFDAESA-N					
deoxynivalenol	4.9×10^{8}		HSDB (2015)	Q	449
$C_{15}H_{20}O_6$					
[51481-10-8]					
LINOMUASTDIRTM-WHNKEALZSA-N					
nivalenol	1.4×10^{10}		HSDB (2015)	Q	100
$C_{15}H_{20}O_7$					
[23282-20-4]					
UKOTXHQERFPCBU-UHFFFAOYSA-N					
tributyrin	1.0×10^{3}		HSDB (2015)	Q	100
$C_{15}H_{26}O_6$					
[60-01-5]					
UYXTWWCETRIEDR-UHFFFAOYSA-N					
diosmetin	3.3×10^{12}		HSDB (2015)	Q	449
$C_{16}H_{12}O_6$					
[520-34-3]					
MBNGWHIJMBWFHU-UHFFFAOYSA-N					

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
shikonin $C_{16}H_{16}O_5$ [517-89-5] NEZONWMXZKDMKF-SNVBAGLBSA-N	1.2×10^{9}		HSDB (2015)	Q	449
2,2-bis(4-hydroxyphenyl)butane $C_{16}H_{18}O_2$ (bisphenol B) [77-40-7] HTVITOHKHWFJKO-UHFFFAOYSA-N	8.2×10^{5}		HSDB (2015)	Q	449
ethyl 3,3-bis(*tert*-amylperoxy)butyrate	2.9		Zhang et al. (2010)	Q	288, 289
$C_{16}H_{32}O_6$	3.7×10^{-3}		Zhang et al. (2010)	Q	288, 290
[67567-23-1]	3.0×10^{1}		Zhang et al. (2010)	Q	288, 291
NICWAKGKDIAMOD-UHFFFAOYSA-N	1.5×10^{2}		Zhang et al. (2010)	Q	288, 292
aflatoxin B1 $C_{17}H_{12}O_6$ [1162-65-8] OQIQSTLJSLGHID-UHFFFAOYSA-N	7.0×10^{7}		HSDB (2015)	Q	100
aflatoxin G1 $C_{17}H_{12}O_7$ [1165-39-5] XWIYFDMXXLINPU-UHFFFAOYSA-N	2.0×10^{7}		HSDB (2015)	Q	100
aflatoxin B2 $C_{17}H_{14}O_6$ [7220-81-7] WWSYXEZEXMQWHT-UHFFFAOYSA-N	3.3×10^{9}		HSDB (2015)	Q	100
aflatoxin G2 $C_{17}H_{14}O_7$ [7241-98-7] WPCVRWVBBXIRMA-UHFFFAOYSA-N	9.0×10^{8}		HSDB (2015)	Q	100
bisphenol C $C_{17}H_{20}O_2$ [79-97-0] YMTYZTXUZLQUSF-UHFFFAOYSA-N	9.0×10^{5}		HSDB (2015)	Q	449
PR-toxin $C_{17}H_{20}O_6$ [56299-00-4] GSPFUBNBRPVALJ-VIEAGMIOSA-N	1.6×10^{8}		HSDB (2015)	Q	100
fusarenon X $C_{17}H_{22}O_8$ [23255-69-8] XGCUCFKWVIWWNW-UHFFFAOYSA-N	2.1×10^{11}		HSDB (2015)	Q	100

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dihydrotanshinone I $C_{18}H_{14}O_3$ [87205-99-0] HARGZZNYNSYSGJ-JTQLQIEISA-N	7.6×10^{4}		HSDB (2015)	Q	100
diethylstilbestrol $C_{18}H_{20}O_2$ [56-53-1] RGLYKWWBQGJZGM-ISLYRVAYSA-N	1.7×10^{2}		HSDB (2015)	Q	100
laminarin $C_{18}H_{32}O_{16}$ [9008-22-4] DBTMGCOVALSLOR-AWHOAIGYSA-N	$>2.9\times10^{6}$		Maniere et al. (2011)	?	73, 166
estrone $C_{18}H_{22}O_2$ [53-16-7] DNXHEGUUPJUMQT-UHFFFAOYSA-N	2.6×10^{4}		HSDB (2015)	Q	100
estradiol $C_{18}H_{24}O_2$ [50-28-2] VOXZDWNPVJITMN-AWDGRILASA-N	2.7×10^{5}		HSDB (2015)	Q	100
estriol $C_{18}H_{24}O_3$ [50-27-1] PROQIPRRNZUXQM-PVGHXWSTSA-N	7.6×10^{6}		HSDB (2015)	Q	100
nandrolone $C_{18}H_{26}O_2$ [434-22-0] NPAGDVCDWIYMMC-SVXFNXITSA-N	3.7×10^{3}		HSDB (2015)	Q	100
diofenolan $C_{18}H_{20}O_4$ [63837-33-2] ZDOOQPFIGYHZFV-UHFFFAOYSA-N	1.5×10^{2} 1.2×10^{3} 1.5×10^{2}		Duchowicz et al. (2020) Duchowicz et al. (2020) MacBean (2012a)	V Q ?	187
dicumarol $C_{19}H_{12}O_6$ [66-76-2] DOBMPNYZJYQDGZ-UHFFFAOYSA-N	7.0×10^{7}		HSDB (2015)	Q	100
coumatetralyl $C_{19}H_{16}O_3$ [5836-29-3] ULSLJYXHZDTLQK-UHFFFAOYSA-N	1.7×10^{8}		HSDB (2015)	V	

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
warfarin $C_{19}H_{16}O_4$ [81-81-2] PJVWKTKQMONHTI-UHFFFAOYSA-N	3.7×10^{4} 3.6×10^{2}		HSDB (2015) Mackay et al. (2006d)	V V	
tanshinone II $C_{19}H_{18}O_3$ [568-72-9] HYXITZLLTYIPOF-UHFFFAOYSA-N	2.0×10^{3}		HSDB (2015)	Q	100
gibberellic acid $C_{19}H_{22}O_6$ [77-06-5] IXORZMNAPKEEDV-UHFFFAOYSA-N	6.2×10^{9} 1.3×10^{6}		HSDB (2015) Maniere et al. (2011)	Q ?	100 166
prallethrin $C_{19}H_{24}O_3$ [23031-36-9] SMKRKQBMYOFFMU-UHFFFAOYSA-N	6.2		HSDB (2015)	V	
testolactone $C_{19}H_{24}O_3$ [968-93-4] BPEWUONYVDABNZ-LHXSAFEUSA-N	1.6×10^{2}		HSDB (2015)	Q	100
androstenedione $C_{19}H_{26}O_2$ [63-05-8] AEMFNILZOJDQLW-JRCHKSGSSA-N	2.7×10^{2}		HSDB (2015)	Q	100
diacetoxyscirpenol $C_{19}H_{26}O_7$ [2270-40-8] AUGQEEXBDZWUJY-UHFFFAOYSA-N	1.0×10^{11}		HSDB (2015)	Q	449
testosterone $C_{19}H_{28}O_2$ [58-22-0] MUMGGOZAMZWBJJ-JZJKZLICSA-N	2.8×10^{3}		HSDB (2015)	Q	100
5α-androst-16-en-4-one $C_{19}H_{28}O$ (androstenone) [18339-16-7] HFVMLYAGWXSTQI-QYXZOKGRSA-N	3.4×10^{-2}		Amoore and Buttery (1978)	M	
oxandrolone $C_{19}H_{30}O_3$ [53-39-4] QSLJIVKCVHQPLV-WPMSWULFSA-N	4.3×10^{2}		HSDB (2015)	Q	100

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
piperonyl butoxide $C_{19}H_{30}O_5$ [51-03-6] FIPWRIJSWJWJAI-UHFFFAOYSA-N	1.1×10^{5}		HSDB (2015)	Q	100
methoprene $C_{19}H_{34}O_3$ [40596-69-8] NFGXHKASABOEEW-LDRANXPESA-N	1.4		HSDB (2015)	V	
fluorescein $C_{20}H_{12}O_5$ [2321-07-5] GNBHRKFJIUUOQI-UHFFFAOYSA-N	1.1×10^{11}		HSDB (2015)	Q	100
phenolphthalein $C_{20}H_{14}O_4$ [77-09-8] KJFMBFZCATUALV-UHFFFAOYSA-N	1.1×10^{10}		HSDB (2015)	Q	100
avobenzone $C_{20}H_{22}O_3$ [70356-09-1] XNEFYCZVKIDDMS-UHFFFAOYSA-N	4.9×10^{4}		HSDB (2015)	Q	449
ethinyl estradiol $C_{20}H_{24}O_2$ [57-63-6] BFPYWIDHMRZLRN-UHFFFAOYSA-N	1.2×10^{6}		HSDB (2015)	Q	100
norethynodrel $C_{20}H_{26}O_2$ [68-23-5] ICTXHFFSOAJUMG-CEVCPLMDSA-N	7.6×10^{3}		HSDB (2015)	Q	100
norethindrone $C_{20}H_{26}O$ [68-22-4] VIKNJXKGJWUCNN-BROHZWGRSA-N	1.7×10^{4}		HSDB (2015)	Q	100
methandrostenolone $C_{20}H_{28}O_2$ [72-63-9] XWALNWXLMVGSFR-NSDIEPNESA-N	4.5×10^{3}		HSDB (2015)	Q	100
cinerin I $C_{20}H_{28}O_3$ [25402-06-6] FMTFEIJHMMQUJI-FPLPWBNLSA-N	1.0×10^{1}		HSDB (2015)	Q	100

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
17-methyltestosterone $C_{20}H_{30}O_2$ [58-18-4] GCKMFJBGXUYNAG-NSDIEPNESA-N	2.1×10^{3}		HSDB (2015)	Q	100
drostanolone $C_{20}H_{32}O_2$ (dromostanolone) [58-19-5] IKXILDNPCZPPRV-UHFFFAOYSA-N	1.2×10^{3}		HSDB (2015)	Q	100
curcumin $C_{21}H_{20}O_6$ [458-37-7] VFLDPWHFBUODDF-FCXRPNKRSA-N	1.4×10^{16}		HSDB (2015)	Q	100
bisphenol A diglycidyl ether $C_{21}H_{24}O_4$ [1675-54-3] LCFVJGUPQDGYKZ-UHFFFAOYSA-N	2.2×10^{5}		HSDB (2015)	Q	100
mestranol $C_{21}H_{26}O_2$ [72-33-3] IMSSROKUHAOUJS-ALAWOQLPSA-N	2.2×10^{3}		HSDB (2015)	Q	100
prednisone $C_{21}H_{26}O_5$ [53-03-2] XOFYZVNMUHMLCC-NUBBXXJJSA-N	3.5×10^{4}		HSDB (2015)	Q	100
norgestrel $C_{21}H_{28}O_2$ [6533-00-2] WWYNJERNGUHSAO-ZUHHCLADSA-N	1.3×10^{4}		HSDB (2015)	Q	100
levonorgestrel $C_{21}H_{28}O_2$ [797-63-7] WWYNJERNGUHSAO-XUDSTZEESA-N	1.3×10^{4}		HSDB (2015)	Q	100
pyrethrin I $C_{21}H_{28}O_3$ [121-21-1] ROVGZAWFACYCSP-CMDGGOBGSA-N	1.3×10^{1} 2.2×10^{-1} 8.4×10^{-1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
cinerin II $C_{21}H_{28}O_5$ [121-20-0] SHCRDCOTRILILT-WOBDGSLYSA-N	1.1×10^{4}		HSDB (2015)	Q	100

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
prednisolone $C_{21}H_{28}O_5$ [50-24-8] OIGNJSKKLXVSLS-UHFFFAOYSA-N	3.7×10^{2}		HSDB (2015)	Q	100
dronabinol $C_{21}H_{30}O_2$ (delta 9-tetrahydrocannabinol) [1972-08-3] CYQFCXCEBYINGO-UHFFFAOYSA-N	4.1×10^{1}		HSDB (2015)	Q	100
progesterone $C_{21}H_{30}O_2$ [57-83-0] RJKFOVLPORLFTN-UHFFFAOYSA-N	1.5×10^{2}		HSDB (2015)	Q	100
hydrocortisone $C_{21}H_{30}O_5$ [50-23-7] JYGXADMDTFJGBT-NDNUHCHRSA-N	1.7×10^{2}		HSDB (2015)	Q	100
calusterone $C_{21}H_{32}O_2$ [17021-26-0] IVFYLRMMHVYGJH-UHFFFAOYSA-N	1.6×10^{3}		HSDB (2015)	Q	100
oxymetholone $C_{21}H_{32}O_3$ [434-07-1] ICMWWNHDUZJFDW-RCXBLOTCSA-N	6.6×10^{3}		HSDB (2015)	Q	100
resmethrin $C_{22}H_{26}O_3$ [10453-86-8] VEMKTZHHVJILDY-UHFFFAOYSA-N	4.7×10^{-2} 7.6×10^{1} 2.2×10^{-1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
pyrethrin II $C_{22}H_{28}O_5$ [121-29-9] VJFUPGQZSXIULQ-VKTMSVCMSA-N	4.5×10^{2} 4.5×10^{2} 3.8×10^{2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
methylprednisolone $C_{22}H_{30}O_5$ [83-43-2] VHRSUDSXCMQTMA-UHFFFAOYSA-N	2.7×10^{2}		HSDB (2015)	Q	100
medroxyprogesterone $C_{22}H_{32}O_3$ [520-85-4] FRQMUZJSZHZSGN-HBNHAYAOSA-N	7.6×10^{2}		HSDB (2015)	Q	100

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dimethirimol $C_{23}H_{24}O_5$ [5221-53-4] VNKCZJKGJAEOCW-WXUKJITCSA-N	$>2.3\times10^{10}$		MacBean (2012a)	?	
rotenone $C_{23}H_{22}O_6$ [83-79-4] JUVIOZPCNVVQFO-UHFFFAOYSA-N	8.8×10^{7}		HSDB (2015)	Q	100
phenothrin $C_{23}H_{26}O_3$ [26002-80-2] SBNFWQZLDJGRLK-UHFFFAOYSA-N	1.5		MacBean (2012b)	X	352
spiromesifen $C_{23}H_{30}O_4$ [283594-90-1] GOLXNESZZPUPJE-UHFFFAOYSA-N	1.8×10^{-2}		HSDB (2015)	V	
digoxigenin $C_{23}H_{34}O_5$ [1672-46-4] SHIBSTMRCDJXLN-KCZCNTNESA-N	4.3×10^{5}		HSDB (2015)	Q	100
annatto $C_{24}H_{28}O_4$ [1393-63-1] ZVKOASAVGLETCT-LRRSNBNMSA-N	1.5×10^{11}		HSDB (2015)	Q	100
acequinocyl $C_{24}H_{32}O_4$ [57960-19-7] QDRXWCAVUNHOGA-UHFFFAOYSA-N	1.0×10^{1} 1.0×10^{1}		HSDB (2015) Maniere et al. (2011)	V ?	 242, 166
T-2 mycotoxin $C_{24}H_{34}O_9$ [21259-20-1] SSHHYBPAMCLKRH-UHFFFAOYSA-N	1.8×10^{12}		HSDB (2015)	Q	100
milk thistle extract $C_{25}H_{22}O_{10}$ [84604-20-6] SEBFKMXJBCUCAI-VGHNRKBZSA-N	6.2×10^{17}		HSDB (2015)	Q	100
simvastatin $C_{25}H_{38}O_5$ [79902-63-9] RYMZZMVNJRMUDD-UHFFFAOYSA-N	3.5×10^{4}		HSDB (2015)	Q	100

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
calcitriol $C_{27}H_{44}O_3$ (1,25-dihydroxycholecalciferol) [32222-06-3] GMRQFYUYWCNGIN-NKMMMXOESA-N	3.2×10^{1}		HSDB (2015)	Q	100
paricalcitol $C_{27}H_{44}O_3$ [131918-61-1] BPKAHTKRCLCHEA-UBFJEZKGSA-N	2.6×10^{1}		HSDB (2015)	Q	100
cholecalciferol $C_{27}H_{44}O$ [67-97-0] QYSXJUFSXHHAJI-SMGPGMQOSA-N	4.3×10^{-2}		HSDB (2015)	Q	100
cholesterol $C_{27}H_{46}O$ [57-88-5] HVYWMOMLDIMFJA-VUDDDUNTSA-N	5.8×10^{-2}		HSDB (2015)	Q	100
ergosterol $C_{28}H_{44}O$ [57-87-4] DNVPQKQSNYMLRS-CVGROQQCSA-N	6.2×10^{-2}		HSDB (2015)	Q	100
dihydrotachysterol $C_{28}H_{46}O$ [67-96-9] DTSXXSAWQHPLEF-GFVAUXBKSA-N	2.7×10^{-2}		HSDB (2015)	Q	100
etoposide $C_{29}H_{32}O_{13}$ [33419-42-0] VJJPUSNTGOMMGY-KWGSHVRASA-N	5.8×10^{24}		HSDB (2015)	Q	100
stigmasterol $C_{29}H_{48}O$ [83-48-7] HCXVJBMSMIARIN-BASBAMEESA-N	3.8×10^{-2}		HSDB (2015)	Q	100
pseudohypericin $C_{30}H_{16}O_9$ [55954-61-5] YXBUQQDFTYOHQI-UHFFFAOYSA-N	5.5×10^{23}		HSDB (2015)	Q	100
gossypol $C_{30}H_{30}O_8$ [303-45-7] QBKSWRVVCFFDOT-UHFFFAOYSA-N	4.3×10^{22}		HSDB (2015)	Q	100

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
maslinic acid $C_{30}H_{48}O_4$ [4373-41-5] MDZKJHQSJHYOHJ-LLICELPBSA-N	2.8×10^{5}		HSDB (2015)	Q	449
milbemectin $C_{31}H_{44}O_7$ [51596-10-2] ZLBGSRMUSVULIE-GSMJGMFJSA-N	6.5×10^{2} 3.9×10^{2}		Maniere et al. (2011) Maniere et al. (2011)	? ?	242, 166 242, 166
difenacoum $C_{31}H_{24}O_3$ [56073-07-5] FVQITOLOYMWVFU-UHFFFAOYSA-N	7.0×10^{6}		HSDB (2015)	Q	449
nonoxynol 9 $C_{33}H_{60}O_{10}$ [26571-11-9] FBWNMEQMRUMQSO-UHFFFAOYSA-N	1.8×10^{16}		HSDB (2015)	Q	100
azadirachtin $C_{35}H_{44}O_{16}$ [11141-17-6] FTNJWQUOZFUQQJ-GWTPYEAISA-N	3.5×10^{19}		HSDB (2015)	V	
monensin $C_{36}H_{62}O_{11}$ [17090-79-8] GAOZTHIDHYLHMS-LXKLZWMJSA-N	4.9×10^{18}		HSDB (2015)	Q	100
gossyplure $C_{36}H_{64}O_4$ [50933-33-0] BXJHOKLLMOYSRQ-QOXWLJPHSA-N	6.6×10^{-2}		HSDB (2015)	V	
capsanthin $C_{40}H_{56}O_3$ [465-42-9] VYIRVAXUEZSDNC-RDJLEWNRSA-N	3.4×10^{2}		HSDB (2015)	Q	100
heptamaloxyloglucan $C_{40}H_{70}O_{33}$ [870721-81-6] RAUODYOTTYNEJP-RQESCVSBSA-N	4.2×10^{13}		Maniere et al. (2011)	?	12, 166
digitoxin $C_{41}H_{64}O_{13}$ [71-63-6] WDJUZGPOPHTGOT-UCKSZOHFSA-N	7.6×10^{19}		HSDB (2015)	Q	100

Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
digoxin $C_{41}H_{64}O_{14}$ [20830-75-5] LTMHDMANZUZIPE-PUGKRICDSA-N	2.1×10^{21}		HSDB (2015)	Q	100
pyrethrum $C_{43}H_{56}O_8$ [8003-34-7] VXSIXFKKSNGRRO-YWUDCVDHSA-N	1.5×10^{1} 1.4×10^{4} 1.3×10^{1}		HSDB (2015) Maniere et al. (2011) Maniere et al. (2011)	Q ? ?	100 166 166
punicalagin $C_{48}H_{28}O_{30}$ [65995-63-3] SKNLUADAGHCXKF-UHFFFAOYSA-N	5.5×10^{10}		HSDB (2015)	Q	100
abamectin $C_{48}H_{72}O_{14}$ [71751-41-2] RRZXIRBKKLTSOM-IGNCFFBFSA-N	7.0×10^{3} $>3.7\times10^{2}$		HSDB (2015) Maniere et al. (2011)	V ?	 12, 166
notoginsenoside R1 $C_{48}H_{84}O_{18}$ [80418-24-2] ZBXDHDDTAIOMHK-UWGJVBKGSA-N	6.6×10^{25}		HSDB (2015)	Q	100
triolein $C_{57}H_{104}O_6$ [122-32-7] PHYFQTYBJUILEZ-IUPFWZBJSA-N	1.0×10^{-2}		HSDB (2015)	Q	449
tristearin $C_{57}H_{110}O_6$ [555-43-1] DCXXMTOCNZCJGO-UHFFFAOYSA-N	7.0×10^{-3}		HSDB (2015)	Q	100

A4 Organic species with nitrogen (N)

A4.1 Amines (C, H, N)

Table A4.1: Amines (C, H, N)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyanamide CH_2N_2 [420-04-2] XZMCDFZZKTWFGF-UHFFFAOYSA-N	3.7×10^{4}		HSDB (2015)	V	
methylhydrazine CH_6N_2 [60-34-4] HDZGCSFEDULWCS-UHFFFAOYSA-N	3.3		HSDB (2015)	V	
methanamine CH_3NH_2 (methylamine) [74-89-5] BAVYZALUXZFZLV-UHFFFAOYSA-N	8.9×10^{-1}		Burkholder et al. (2019)	L	
	8.9×10^{-1}		Burkholder et al. (2015)	L	
	3.5×10^{-1}	2600	Wilhelm et al. (1977)	L	
	8.9×10^{-1}		Christie and Crisp (1967)	M	
	1.1		Yaws (2003)	X	238
	7.4×10^{-1}		Keshavarz et al. (2022)	Q	
	6.2		Duchowicz et al. (2020)	Q	
	1.1		Gharagheizi et al. (2010)	Q	247
	1.2		Hilal et al. (2008)	Q	
	2.3		Modarresi et al. (2007)	Q	68
		5000	Kühne et al. (2005)	Q	
	9.2×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	1.1		English and Carroll (2001)	Q	231, 232
	6.1×10^{-1}		Katritzky et al. (1998)	Q	
	5.6×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	8.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	8.9×10^{-1}		Mackay et al. (2006d)	?	
		3200	Kühne et al. (2005)	?	
	8.8×10^{-1}		Abraham et al. (1990)	?	
		5400	Abraham (1984)	?	21
	1.4		Bone et al. (1983)	?	66
ethanamine $C_2H_5NH_2$ (ethylamine) [75-04-7] QUSNBJAOOMFDIB-UHFFFAOYSA-N	8.0×10^{-1}		Burkholder et al. (2019)	L	
	8.0×10^{-1}		Burkholder et al. (2015)	L	
	8.4×10^{-1}		Brockbank (2013)	L	
	3.5×10^{-1}	3600	Wilhelm et al. (1977)	L	
	8.0×10^{-1}		Christie and Crisp (1967)	M	
	9.9×10^{-1}		Butler and Ramchandani (1935)	M	
	3.0×10^{-1}		Hwang et al. (1992)	V	
	1.0		Keshavarz et al. (2022)	Q	
	2.2		Duchowicz et al. (2020)	Q	300
	9.7×10^{-1}		Li et al. (2014)	Q	242
	7.9×10^{-1}		Hilal et al. (2008)	Q	
	1.7		Modarresi et al. (2007)	Q	68

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.3×10^{-1}		Yao et al. (2002)	Q	230
	9.5×10^{-1}		English and Carroll (2001)	Q	231, 232
	4.7×10^{-1}		Katritzky et al. (1998)	Q	
	4.6×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	2.4		Russell et al. (1992)	Q	280
	1.3		Suzuki et al. (1992)	Q	233
	8.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	9.9×10^{-1}		Mackay et al. (2006d)	?	
	3.8×10^{-1}		Yaws (1999)	?	21, 12
	8.0×10^{-1}		Abraham et al. (1990)	?	
		6500	Abraham (1984)	?	21
1H-1,2,4-triazole $C_2H_3N_3$ [288-88-0] NSPMIYGKQJPBQR-UHFFFAOYSA-N	6.6		HSDB (2015)	Q	100
dicyandiamide $C_2H_4N_4$ (cyanoguanidine) [461-58-5] QGBSISYHAICWAH-UHFFFAOYSA-N	4.3×10^{4}		HSDB (2015)	Q	100
ethylenimine C_2H_5N [151-56-4] NOWKCMXCCJGMRR-UHFFFAOYSA-N	8.2×10^{-1}		Duchowicz et al. (2020)	V	187
	8.2×10^{-1}		HSDB (2015)	V	
	2.9×10^{1}		Duchowicz et al. (2020)	Q	
1,2-dimethylhydrazine $C_2H_8N_2$ [540-73-8] DIIIISSCIXVANO-UHFFFAOYSA-N	1.8		HSDB (2015)	V	
1,1-dimethylhydrazine $C_2H_8N_2$ [57-14-7] RHUYHJGZWVXEHW-UHFFFAOYSA-N	7.6×10^{-1}		HSDB (2015)	V	
1-propanamine $C_3H_7NH_2$ (propylamine) [107-10-8] WGYKZJWCGVVSQN-UHFFFAOYSA-N	6.6×10^{-1}		Burkholder et al. (2019)	L	
	6.6×10^{-1}		Burkholder et al. (2015)	L	
	6.7×10^{-1}		Brockbank (2013)	L	
	5.6×10^{-1}	6400	Leng et al. (2015a)	M	
	5.0×10^{-1}		Altschuh et al. (1999)	M	
	6.6×10^{-1}		Christie and Crisp (1967)	M	
	7.8×10^{-1}		Butler and Ramchandani (1935)	M	
	6.6×10^{-1}	6700	Plyasunov et al. (2001)	T	
	1.4		Keshavarz et al. (2022)	Q	
	2.3		Duchowicz et al. (2020)	Q	185
	4.8×10^{-1}		Hilal et al. (2008)	Q	

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.1		Modarresi et al. (2007)	Q	68
	6.7×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.6×10^{-1}		Yao et al. (2002)	Q	230
	5.2×10^{-1}		Katritzky et al. (1998)	Q	
	3.6×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.6		Russell et al. (1992)	Q	280
	1.0		Suzuki et al. (1992)	Q	233
	6.7×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	7.8×10^{-1}		Mackay et al. (2006d)	?	
	3.9×10^{-1}		Yaws (1999)	?	21
	6.7×10^{-1}		Abraham et al. (1990)	?	
		6700	Abraham (1984)	?	21
2-propanamine	2.2×10^{-1}		Duchowicz et al. (2020)	V	187
C_3H_9N	2.2×10^{-1}		Hilal et al. (2008)	C	
(isopropylamine)	8.9×10^{-1}		Duchowicz et al. (2020)	Q	
[75-31-0]	2.1×10^{-1}		Hilal et al. (2008)	Q	
JJWLVOIRVHMVIS-UHFFFAOYSA-N	2.4		Modarresi et al. (2007)	Q	68
	2.3×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	1.6×10^{-1}		Yao et al. (2002)	Q	230
	3.1×10^{-1}		Katritzky et al. (1998)	Q	
	1.3×10^{-1}		Yaws (1999)	?	21, 12
propanedinitrile	7.5×10^{1}		Duchowicz et al. (2020)	V	187
$C_3H_2N_2$	2.0×10^{1}		Duchowicz et al. (2020)	Q	
(malononitrile)	7.8×10^{2}		HSDB (2015)	Q	100
[109-77-3]	2.0×10^{1}		Gharagheizi et al. (2012)	Q	
CUONGYYJJVDODC-UHFFFAOYSA-N	6.3×10^{1}		Yaws (1999)	?	21, 12
2-methylaziridine	9.9×10^{-1}		Duchowicz et al. (2020)	V	187
C_3H_7N	1.2×10^{1}		Duchowicz et al. (2020)	Q	
[75-55-8]	1.2		Yaffe et al. (2003)	Q	249, 250
OZDGMOYKSFPLSE-UHFFFAOYSA-N	1.5		Katritzky et al. (1998)	Q	
1,2-diaminopropane	1.4×10^{3}	7400	Nguyen (2013)	M	11
$C_3H_{10}N_2$					
[78-90-0]					
AOHJOMMDDJHIJH-UHFFFAOYSA-N					
1-butanamine	5.6×10^{-1}		Burkholder et al. (2019)	L	
$C_4H_9NH_2$	5.6×10^{-1}		Burkholder et al. (2015)	L	
(butylamine)	5.4×10^{-1}		Brockbank (2013)	L	
[109-73-9]	5.6×10^{-1}		Altschuh et al. (1999)	M	
HQABUPZFAYXKJW-UHFFFAOYSA-N	5.2×10^{-1}		Rytting et al. (1978)	M	
	5.6×10^{-1}		Christie and Crisp (1967)	M	
	6.5×10^{-1}		Butler and Ramchandani (1935)	M	
	2.2×10^{-1}		Hwang et al. (1992)	V	
	4.5×10^{-1}		Amoore and Buttery (1978)	V	
	3.7×10^{-1}		Yaws (2003)	X	259

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.6×10^{-1}		Yaws (2003)	X	238
	2.1×10^{-1}		Dupeux et al. (2022)	Q	260
	1.2×10^{-1}		Keshavarz et al. (2022)	Q	
	2.3		Duchowicz et al. (2020)	Q	300
	6.5×10^{-1}		Li et al. (2014)	Q	242
	4.0×10^{-1}		Gharagheizi et al. (2010)	Q	247
	2.9×10^{-1}		Hilal et al. (2008)	Q	
	1.5		Modarresi et al. (2007)	Q	68
	5.2×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.4×10^{-1}		Yao et al. (2002)	Q	230
	7.3×10^{-1}		English and Carroll (2001)	Q	231, 232
	4.0×10^{-1}		Katritzky et al. (1998)	Q	
	2.8×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.1		Russell et al. (1992)	Q	280
	7.9×10^{-1}		Suzuki et al. (1992)	Q	233
	5.7×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	6.6×10^{-1}		Mackay et al. (2006d)	?	
	2.2×10^{-1}		Yaws (1999)	?	21
	5.2×10^{-1}		Abraham et al. (1990)	?	
		7100	Abraham (1984)	?	21
2-butanamine	4.0×10^{-1}	7700	Kish et al. (2013)	M	550
$C_4H_{11}N$	6.5×10^{-2}		Duchowicz et al. (2020)	V	187
(*sec*-butylamine)	6.5×10^{-2}		Hilal et al. (2008)	C	
[13952-84-6]	9.1×10^{-1}		Duchowicz et al. (2020)	Q	
BHRZNVHARXXAHW-UHFFFAOYSA-N	1.6×10^{-1}		Hilal et al. (2008)	Q	
	1.7		Modarresi et al. (2007)	Q	68
	2.2×10^{-1}		Katritzky et al. (1998)	Q	
2-methyl-1-propanamine	7.3×10^{-1}		Duchowicz et al. (2020)	V	187
$C_4H_{11}N$	7.2×10^{-1}		Hilal et al. (2008)	C	
(isobutylamine)	9.1×10^{-1}		Duchowicz et al. (2020)	Q	
[78-81-9]	2.4×10^{-1}		Hilal et al. (2008)	Q	
KDSNLYIMUZNERS-UHFFFAOYSA-N	2.0		Modarresi et al. (2007)	Q	68
	5.2×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	1.5×10^{-1}		Yao et al. (2002)	Q	230, 268
	3.9×10^{-1}		Katritzky et al. (1998)	Q	
	4.4×10^{-1}		Yaws (1999)	?	21, 12
2-methyl-2-propanamine	2.8×10^{-1}		Duchowicz et al. (2020)	V	187
$C_4H_{11}N$	2.8×10^{-1}		Hilal et al. (2008)	C	
(*tert*-butylamine)	4.0×10^{-1}		Duchowicz et al. (2020)	Q	
[75-64-9]	5.0×10^{-2}		Hilal et al. (2008)	Q	
YBRBMKDOPFTVDT-UHFFFAOYSA-N	1.0×10^{-1}		Modarresi et al. (2007)	Q	68
	2.9×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.1×10^{-1}		Katritzky et al. (1998)	Q	

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dimethylethylamine $C_4H_{11}N$ [598-56-1] DAZXVJBJRMWXJP-UHFFFAOYSA-N	1.1×10^{-1} 9.0×10^{-2} 1.1×10^{-1}		Yaws (2003) Ghargheizi et al. (2012) Ghargheizi et al. (2010)	X Q Q	238 247
2-propylguanidine $C_4H_{11}N_3$ [462-25-9] BWMDMTSNSXYYSP-UHFFFAOYSA-N	4.1×10^{4}		Ebert et al. (2023)	?	367
1,2-diethylhydrazine $C_4H_{12}N_2$ [1615-80-1] YCBOYOYVDOUXLH-UHFFFAOYSA-N	8.2×10^{1}		HSDB (2015)	Q	100
N-(2-aminoethyl)-1,2-ethanediamine $C_4H_{13}N_3$ (diethylenetriamine) [111-40-0] RPNUMPOLZDHAAY-UHFFFAOYSA-N	9.9×10^{8}		HSDB (2015)	Q	100
butanedinitrile $C_4H_4N_2$ [110-61-2] IAHFWCOBPZCAEA-UHFFFAOYSA-N	8.7×10^{2} 1.5×10^{3} 1.5×10^{3} 4.0×10^{3} 2.6×10^{1} 3.9×10^{3}	7000	Plyasunov et al. (2006) Duchowicz et al. (2020) HSDB (2015) Yaws (2003) Duchowicz et al. (2020) Gharagheizi et al. (2010)	L V V X Q Q	 187 238, 12 247
2-methyl-1H-imidazole $C_4H_6N_2$ [693-98-1] LXBGSDVWAMZHDD-UHFFFAOYSA-N	8.1×10^{2} 1.8×10^{3} 1.1×10^{3} 2.2		Du et al. (2017) Du et al. (2017) Du et al. (2017) HSDB (2015)	M Q Q Q	480 551 100
4-methyl-1H-imidazole $C_4H_6N_2$ [822-36-6] XLSZMDLNRCVEIJ-UHFFFAOYSA-N	2.4		HSDB (2015)	Q	100
N-methyl-1,3-propanediamine $C_4H_{12}N_2$ (3-(methylamino)propylamine) [6291-84-5] QHJABUZHRJTCAR-UHFFFAOYSA-N	1.4×10^{3} 2.1×10^{3}	7600 8800	Nguyen (2013) Kim et al. (2008)	M M	11 552

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-pentanamine	4.3×10^{-1}		Brockbank (2013)	L	
$C_5H_{11}NH_2$	4.0×10^{-1}		Rytting et al. (1978)	M	
(1-pentylamine)	3.1×10^{-1}		Amoore and Buttery (1978)	M	
[110-58-7]	4.0×10^{-1}		Christie and Crisp (1967)	M	
DPBLXKKOBLCELK-UHFFFAOYSA-N	1.7×10^{-1}		Keshavarz et al. (2022)	Q	
	2.4		Duchowicz et al. (2020)	Q	300
	1.6×10^{-1}		Hilal et al. (2008)	Q	
	1.2		Modarresi et al. (2007)	Q	68
	4.0×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	5.6×10^{-1}		English and Carroll (2001)	Q	231, 261
	4.0×10^{-1}		Katritzky et al. (1998)	Q	
	2.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	7.2×10^{-1}		Russell et al. (1992)	Q	360
	1.5×10^{-1}		Suzuki et al. (1992)	Q	233
	4.1×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	4.0×10^{-1}		Abraham et al. (1990)	?	
		7500	Abraham (1984)	?	21
3-methyl-1-butanamine	3.2×10^{-1}		Yaws (2003)	X	238
$C_5H_{13}N$	3.1×10^{-1}		Gharagheizi et al. (2010)	Q	247
[107-85-7]	2.2×10^{-1}		Hilal et al. (2008)	Q	
BMFVGAAISNGQNM-UHFFFAOYSA-N					
1,2-dimethylpropylamine	4.0×10^{-1}		Yaws (2003)	X	238
$C_5H_{13}N$	3.8×10^{-1}		Gharagheizi et al. (2010)	Q	247
[598-74-3]					
JOZZAIIGWFLONA-UHFFFAOYSA-N					
dimethylpropylamine	7.9×10^{-2}		Yaws (2003)	X	238
$C_5H_{13}N$	5.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[926-63-6]	9.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
ZUHZZVMEUAUWHY-UHFFFAOYSA-N					
dimethylisopropylamine	7.9×10^{-2}		Yaws (2003)	X	238
$C_5H_{13}N$	1.2×10^{-1}		Gharagheizi et al. (2010)	Q	247
[996-35-0]					
VMOWKUTXPNPTEN-UHFFFAOYSA-N					
ethylpropylamine	1.7×10^{-1}		Yaws (2003)	X	238
$C_5H_{13}N$	1.6×10^{-1}		Gharagheizi et al. (2010)	Q	247
[20193-20-8]					
XCVNDBIXFPGMIW-UHFFFAOYSA-N					
ethylisopropylamine	1.8×10^{-1}		Yaws (2003)	X	238
$C_5H_{13}N$	1.8×10^{-1}		Gharagheizi et al. (2010)	Q	247
[19961-27-4]					
RIVIDPPYRINTTH-UHFFFAOYSA-N					

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyldiethylamine $C_5H_{13}N$ [616-39-7] GNVRJGIVDSQCOP-UHFFFAOYSA-N	7.9×10^{-2} 1.1×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
2-methylpiperazine $C_5H_{12}N_2$ [109-07-9] JOMNTHCQHJPVAZ-UHFFFAOYSA-N	5.0×10^{3}	9200	Nguyen (2013)	M	11
1-hexanamine $C_6H_{13}NH_2$ (hexylamine) [111-26-2] BMVXCPBXGZKUPN-UHFFFAOYSA-N	3.5×10^{-1} 3.2×10^{-1} 3.7×10^{-1} 1.0×10^{-1} 2.3×10^{-1} 2.4 1.4×10^{-1} 3.7×10^{-1} 1.0 3.2×10^{-1} 9.2×10^{-2} 4.3×10^{-1} 3.3×10^{-1} 1.8×10^{-1} 3.4×10^{-1} 4.6×10^{-1} 3.7×10^{-1} 1.0×10^{-1} 3.2×10^{-1} 7900		Brockbank (2013) Rytting et al. (1978) Christie and Crisp (1967) Yaws (2003) Keshavarz et al. (2022) Duchowicz et al. (2020) Gharagheizi et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Yaffe et al. (2003) Yao et al. (2002) English and Carroll (2001) Katritzky et al. (1998) Nirmalakhandan et al. (1997) Russell et al. (1992) Suzuki et al. (1992) Duchowicz et al. (2020) Yaws (1999) Abraham et al. (1990) Abraham (1984)	L M M X Q Q Q Q Q Q Q Q Q Q Q Q ? ? ? ?	 238 185 247 68 249, 250 230, 268 231, 275 280 233 186, 21 21 21
2-hexanamine $C_6H_{15}N$ [5329-79-3] WGBBUURBHXLGFM-UHFFFAOYSA-N	1.9×10^{-1} 1.5×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
3-hexanamine $C_6H_{15}N$ [16751-58-9] HQLZFBUAULNEGP-UHFFFAOYSA-N	1.8×10^{-1} 1.5×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
1-amino-2-methylpentane $C_6H_{15}N$ [13364-16-4] WNDXRJBYZOSNQO-UHFFFAOYSA-N	2.0×10^{-1} 1.8×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-amino-3-methylpentane $C_6H_{15}N$ [42245-37-4] JLAUIBFZZUVOBB-UHFFFAOYSA-N	2.0×10^{-1} 1.8×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
1-amino-4-methylpentane $C_6H_{15}N$ [5344-20-7] QVIAMKXOQGCYCV-UHFFFAOYSA-N	2.0×10^{-1} 1.8×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
2-amino-3-methylpentane $C_6H_{15}N$ [35399-81-6] ZFAGOADKDXXTSV-UHFFFAOYSA-N	1.7×10^{-1} 2.1×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
2-amino-4-methylpentane $C_6H_{15}N$ [108-09-8] UNBMPKNTYKDYCG-UHFFFAOYSA-N	2.3×10^{-1} 2.3×10^{-1} 3.6×10^{-1} 2.0×10^{-1} 3.2×10^{-1}		Yaws (2003) Keshavarz et al. (2022) Duchowicz et al. (2020) Gharagheizi et al. (2010) Duchowicz et al. (2020)	X Q Q Q ?	238 185 247 186, 21
3-amino-2-methylpentane $C_6H_{15}N$ [54287-41-1] JYNQKCFJPQEXSL-UHFFFAOYSA-N	1.7×10^{-1} 2.1×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
1-amino-2-ethylbutane $C_6H_{15}N$ [617-79-8] MGWAGIQQTULHGU-UHFFFAOYSA-N	1.8×10^{-1} 1.8×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
1-amino-2,2-dimethylbutane $C_6H_{15}N$ [41781-17-3] PZVPOYBHOPRJNP-UHFFFAOYSA-N	2.1×10^{-1} 2.0×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
1-amino-2,3-dimethylbutane $C_6H_{15}N$ [66553-05-7] GBMSZXWHMSSBGP-UHFFFAOYSA-N	2.5×10^{-1} 2.2×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
1-amino-3,3-dimethylbutane $C_6H_{15}N$ [15673-00-4] GPWHFPWZAPOYNO-UHFFFAOYSA-N	1.6×10^{-1} 2.0×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
2-amino-3,3-dimethylbutane $C_6H_{15}N$ [3850-30-4] DXSUORGKJZADET-UHFFFAOYSA-N	2.4×10^{-1} 2.4×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dimethylbutylamine $C_6H_{15}N$ [927-62-8] DJEQZVQFEPKLOY-UHFFFAOYSA-N	8.9×10^{-2} 4.8×10^{-2} 6.7×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
dimethyl-*sec*-butylamine $C_6H_{15}N$ [921-04-0] USSPHSVODLAWSA-UHFFFAOYSA-N	1.0×10^{-1} 1.2×10^{-1} 8.8×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
dimethyl-*tert*-butylamine $C_6H_{15}N$ [918-02-5] OXQMIXBVXHWDPX-UHFFFAOYSA-N	1.0×10^{-1} 9.0×10^{-2}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
ethylbutylamine $C_6H_{15}N$ [13360-63-9] QHCCDDQKNUYGNC-UHFFFAOYSA-N	1.3×10^{-1} 1.2×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
ethylisobutylamine $C_6H_{15}N$ [13205-60-2] FNLUJDLKYOWMMF-UHFFFAOYSA-N	1.5×10^{-1} 1.2×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
ethyl-*sec*-butylamine $C_6H_{15}N$ [21035-44-9] KFYKZKISJBGVMR-UHFFFAOYSA-N	1.5×10^{-1} 1.3×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
methyl-1,1-dimethylpropylamine $C_6H_{15}N$ [2978-64-5] BUJFTKPQXSIZFX-UHFFFAOYSA-N	1.1×10^{-1} 1.8×10^{-1} 1.4×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
methyl-1,2-dimethylpropylamine $C_6H_{15}N$ [34317-39-0] LJLWVVCWBURGCC-UHFFFAOYSA-N	1.2×10^{-1} 5.9×10^{-2} 1.4×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
methyl-2,2-dimethylpropylamine $C_6H_{15}N$ [26153-91-3] UQGXHNDRCRTZAC-UHFFFAOYSA-N	1.1×10^{-1} 1.1×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
methyl-1-methylbutylamine $C_6H_{15}N$ [51932-19-5] IPBXLJFBVNLKFE-UHFFFAOYSA-N	1.2×10^{-1} 8.7×10^{-2} 1.2×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methylethylpropylamine $C_6H_{15}N$ [4458-32-6] SMBYUOXUISCLCF-UHFFFAOYSA-N	1.1×10^{-1} 1.0×10^{-1} 8.2×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
methylethylisopropylamine $C_6H_{15}N$ [39198-07-7] UTLDDSNRFHWERZ-UHFFFAOYSA-N	1.1×10^{-1} 9.8×10^{-2}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
methylpentylamine $C_6H_{15}N$ [25419-06-1] UOIWOHLIGKIYFE-UHFFFAOYSA-N	1.2×10^{-1} 1.1×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
propylisopropylamine $C_6H_{15}N$ [21968-17-2] VLSTXUUYLIALPB-UHFFFAOYSA-N	1.4×10^{-1} 1.3×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
1,6-hexanediamine $C_6H_{16}N_2$ (hexamethylenediamine) [124-09-4] NAQMVNRVTILPCV-UHFFFAOYSA-N	1.0×10^{3} 3.1×10^{3}	5000	Nguyen (2013) HSDB (2015)	M Q	11 100
N,N'-methanetetraylbis-2-propanamine $C_7H_{14}N_2$ (1,3-diisopropylcarbodiimide) [693-13-0] BDNKZNFMNDZQMI-UHFFFAOYSA-N	9.9×10^{-3}		HSDB (2015)	Q	449
4-methyl-2-hexanamine $C_7H_{17}N$ [105-41-9] YAHRDLICUYEDAU-UHFFFAOYSA-N	2.3×10^{-1}		HSDB (2015)	Q	449
1-heptanamine $C_7H_{17}N$ (1-heptylamine) [111-68-2] WJYIASZWHGOTOU-UHFFFAOYSA-N	2.8×10^{-1} 2.4×10^{-1} 8.0×10^{-2} 8.3×10^{-2} 4.5×10^{-1} 9.6×10^{-1} 2.1×10^{-1} 3.3×10^{-1} 1.4×10^{-1} 2.4×10^{-1}		Brockbank (2013) Rytting et al. (1978) Yaws (2003) Gharagheizi et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Yaffe et al. (2003) English and Carroll (2001) Nirmalakhandan et al. (1997) Abraham et al. (1990)	L M X Q Q Q Q Q Q ?	 238 247 68 249, 273 231, 232

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
diethylisopropylamine $C_7H_{17}N$ [6006-15-1] ULWOJODHECIZAU-UHFFFAOYSA-N	7.7×10^{-2} 8.0×10^{-2}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
diethylpropylamine $C_7H_{17}N$ [4458-31-5] PQZTVWVYCLIIJY-UHFFFAOYSA-N	7.7×10^{-2} 1.5×10^{-1} 7.3×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
dimethyl-1,1-dimethylpropylamine $C_7H_{17}N$ [57757-60-5] CUHMMDPUXJFCNB-UHFFFAOYSA-N	6.3×10^{-2} 6.5×10^{-2}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
dimethyl-1,2-dimethylpropylamine $C_7H_{17}N$ [66225-38-5] FWBCYOHCOBOARU-UHFFFAOYSA-N	6.9×10^{-2} 5.7×10^{-2} 7.8×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
dimethyl-2,2-dimethylpropylamine $C_7H_{17}N$ [10076-31-0] FUIRUFXAVIHAQB-UHFFFAOYSA-N	6.3×10^{-2} 1.8×10^{-2} 5.8×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
dimethyl-2-methylbutylamine $C_7H_{17}N$ [66225-39-6] BHMZPPHMQJHCHQ-UHFFFAOYSA-N	7.1×10^{-2} 2.4×10^{-2} 6.0×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
dimethyl-3-methylbutylamine $C_7H_{17}N$ [2315-43-7] KOOQJINBDNZUTB-UHFFFAOYSA-N	7.2×10^{-2} 3.5×10^{-2} 5.6×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
dimethylpentylamine $C_7H_{17}N$ [26153-88-8] IDFANOPDMXWIOP-UHFFFAOYSA-N	5.3×10^{-2} 4.1×10^{-2} 5.0×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
dimethyl-2-pentylamine $C_7H_{17}N$ [57303-85-2] LSTZYJQJHGEVKH-UHFFFAOYSA-N	7.7×10^{-2} 6.6×10^{-2} 6.0×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
dimethyl-3-pentylamine $C_7H_{17}N$ [18636-94-7] SUEKSPIQGIMSQM-UHFFFAOYSA-N	7.0×10^{-2} 5.5×10^{-2} 6.5×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethylpentylamine	8.6×10^{-2}		Yaws (2003)	X	238
$C_7H_{17}N$	5.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[17839-26-8]	9.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
ICVFPLUSMYSIFO-UHFFFAOYSA-N					
methyldiisopropylamine	7.1×10^{-2}		Yaws (2003)	X	238
$C_7H_{17}N$	7.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
[10342-97-9]					
ISRXMEYARGEVIU-UHFFFAOYSA-N					
methyldipropylamine	7.5×10^{-2}		Yaws (2003)	X	238
$C_7H_{17}N$	5.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[3405-42-3]	6.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
UVBMZKBIZUWTLV-UHFFFAOYSA-N					
methylethylbutylamine	7.2×10^{-2}		Yaws (2003)	X	238
$C_7H_{17}N$	8.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[66225-40-9]	6.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
WOLFCKKMHUVEPN-UHFFFAOYSA-N					
methylethylisobutylamine	7.8×10^{-2}		Yaws (2003)	X	238
$C_7H_{17}N$	4.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[60247-14-5]	6.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
QQWXQKMVASVXCI-UHFFFAOYSA-N					
methylethyl-*sec*-butylamine	8.2×10^{-2}		Yaws (2003)	X	238
$C_7H_{17}N$	7.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
[66225-41-0]					
HAFZSBASGRZPLA-UHFFFAOYSA-N					
methylethyl-*tert*-butylamine	7.0×10^{-2}		Yaws (2003)	X	238
$C_7H_{17}N$	7.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
[52841-28-8]					
BWWLCYLGZIWOHK-UHFFFAOYSA-N					
methylhexylamine	8.3×10^{-2}		Yaws (2003)	X	238
$C_7H_{17}N$	3.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[35161-70-7]	8.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
XJINZNWPEQMMBV-UHFFFAOYSA-N					
methylpropylisopropylamine	7.3×10^{-2}		Yaws (2003)	X	238
$C_7H_{17}N$	1.6×10^{-1}		Gharagheizi et al. (2012)	Q	
[66225-42-1]	7.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
OYQDUCLFZSKBCZ-UHFFFAOYSA-N					

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-octanamine	2.2×10^{-1}		Brockbank (2013)	L	
C_8H19N	1.9×10^{-1}		Rytting et al. (1978)	M	
(octylamine)	1.2×10^{-2}		Duchowicz et al. (2020)	V	187
[111-86-4]	2.4		Duchowicz et al. (2020)	Q	
IOQPZZOEVPZRBK-UHFFFAOYSA-N	1.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.3×10^{-1}		Hilal et al. (2008)	Q	
		7400	Kühne et al. (2005)	Q	
	2.1×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.5×10^{-1}		English and Carroll (2001)	Q	231, 232
	1.1×10^{-1}		Nirmalakhandan et al. (1997)	Q	
		6600	Kühne et al. (2005)	?	
	1.2×10^{-2}		Yaws (1999)	?	21
	1.9×10^{-1}		Abraham et al. (1990)	?	
2-ethyl-1-hexanamine	1.0×10^{-1}		Duchowicz et al. (2020)	V	187
$C_8H_{19}N$	9.4×10^{-1}		Duchowicz et al. (2020)	Q	
(2-ethylhexylamine)	3.7×10^{-1}		Hilal et al. (2008)	Q	
[104-75-6]	9.7×10^{-1}		Modarresi et al. (2007)	Q	68
LTHNHFOGQMKPOV-UHFFFAOYSA-N		7400	Kühne et al. (2005)	Q	
		7400	Kühne et al. (2005)	?	
diethylbutylamine	5.2×10^{-2}		Yaws (2003)	X	238
$C_8H_{19}N$	1.2×10^{-1}		Gharagheizi et al. (2012)	Q	
[4444-68-2]	5.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
ORSUTASIQKBEFU-UHFFFAOYSA-N					
dimethylhexylamine	3.4×10^{-2}		Yaws (2003)	X	238
$C_8H_{19}N$	3.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[4385-04-0]	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
QMHNQZGXPNCMCO-UHFFFAOYSA-N					
ethylhexylamine	6.2×10^{-2}		Yaws (2003)	X	238
$C_8H_{19}N$	4.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[20352-67-4]	7.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
WSTNFGAKGUERTC-UHFFFAOYSA-N					
methylheptylamine	6.2×10^{-2}		Yaws (2003)	X	238
$C_8H_{19}N$	2.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[36343-05-2]	7.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
LTGYRKOQQQWWAF-UHFFFAOYSA-N					
2,2'-azobis-(2-methylpropanenitrile)	2.4		Duchowicz et al. (2020)	V	187
$C_8H_{12}N_4$	8.0×10^{1}		Duchowicz et al. (2020)	Q	
[78-67-1]					
OZAIFHULBGXAKX-UHFFFAOYSA-N					

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
diethylpentylamine	4.0×10^{-2}		Yaws (2003)	X	238
$C_9H_{21}N$	8.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[2162-91-6]	4.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
YZULHOOBWDXEOT-UHFFFAOYSA-N					
dimethylheptylamine	2.5×10^{-2}		Yaws (2003)	X	238
$C_9H_{21}N$	2.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[5277-11-2]	3.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
LSICDRUYCNGRIF-UHFFFAOYSA-N					
ethylheptylamine	5.2×10^{-2}		Yaws (2003)	X	238
$C_9H_{21}N$	5.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-76-8]	6.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
IUZZLNVABCISOI-UHFFFAOYSA-N					
methyloctylamine	5.4×10^{-2}		Yaws (2003)	X	238
$C_9H_{21}N$	3.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[2439-54-5]	6.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
SEGJNMCIMOLEDM-UHFFFAOYSA-N					
nonylamine	5.9×10^{-2}		Yaws (2003)	X	238
$C_9H_{21}N$	2.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
[112-20-9]					
FJDUDHYHRVPMJZ-UHFFFAOYSA-N					
diethylhexylamine	3.3×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{23}N$	6.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[44979-90-0]	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
XHDKYWMKOLURNK-UHFFFAOYSA-N					
dimethyloctylamine	2.0×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{23}N$	4.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[7378-99-6]	2.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
UQKAOOAFEFCDGT-UHFFFAOYSA-N					
dipentylamine	5.3×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{23}N$	4.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[2050-92-2]	6.4×10^{-2}		Gharagheizi et al. (2010)	Q	247
JACMPVXHEARCBO-UHFFFAOYSA-N					
ethyloctylamine	5.2×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{23}N$	6.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[4088-36-2]	6.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
SDQCOADWEMMSGK-UHFFFAOYSA-N					
methylnonylamine	5.6×10^{-2}		Yaws (2003)	X	238
$C_{10}H_{23}N$	2.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[39093-27-1]	6.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
OZIXTIPURXIEMB-UHFFFAOYSA-N					

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
diethylheptylamine $C_{11}H_{25}N$ [26981-81-7] YUCNJMBRLIZNMO-UHFFFAOYSA-N	2.3×10^{-2} 1.1×10^{-1} 2.7×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
dimethylnonylamine $C_{11}H_{25}N$ [17373-27-2] AMAADDMFZSZCNT-UHFFFAOYSA-N	1.5×10^{-2} 3.7×10^{-2} 2.2×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
diethyloctylamine $C_{12}H_{27}N$ [4088-37-3] BVUGARXRRGZONH-UHFFFAOYSA-N	2.3×10^{-2} 2.6×10^{-2}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
dihexylamine $C_{12}H_{27}N$ [143-16-8] PXSXRABJBXYMFT-UHFFFAOYSA-N	1.3×10^{-1} 8.9×10^{-2}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
dimethyldecylamine $C_{12}H_{27}N$ [1120-24-7] YWWNNLPSZSEZNZ-UHFFFAOYSA-N	1.6×10^{-2} 4.3×10^{-2} 2.2×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
methylundecylamine $C_{12}H_{27}N$ [66553-53-5] JCJFBKCQLFMABE-UHFFFAOYSA-N	1.3×10^{-1} 8.8×10^{-2}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
diethylnonylamine $C_{13}H_{29}N$ [45124-35-4] IBTOMDSHMLGUHA-UHFFFAOYSA-N	3.1×10^{-2} 1.2×10^{-1} 2.8×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
dimethylundecylamine $C_{13}H_{29}N$ [17373-28-3] MMWFTWUMBYZIRZ-UHFFFAOYSA-N	2.7×10^{-2} 4.6×10^{-2} 2.6×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
ethylundecylamine $C_{13}H_{29}N$ [59570-04-6] LKVBHKWFYHKTSM-UHFFFAOYSA-N	1.4×10^{-1} 1.2×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
methyldodecylamine $C_{13}H_{29}N$ [7311-30-0] OMEMQVZNTDHENJ-UHFFFAOYSA-N	1.5×10^{-1} 1.4×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
diethyldecylamine $C_{14}H_{31}N$ [6308-94-7] UFFQZCPLBHYOFV-UHFFFAOYSA-N	4.2×10^{-2} 3.5×10^{-2}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
diheptylamine $C_{14}H_{31}N$ [2470-68-0] NJWMENBYMFZACG-UHFFFAOYSA-N	1.7×10^{-1} 2.7×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
ethyldodecylamine $C_{14}H_{31}N$ [35902-57-9] LWIPGCTWFZCIKX-UHFFFAOYSA-N	1.8×10^{-1} 2.3×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
methyltridecylamine $C_{14}H_{31}N$ [45165-81-9] XMRPIOZXPHTSCE-UHFFFAOYSA-N	2.0×10^{-1} 2.8×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	238 247
tripentylamine $C_{15}H_{33}N$ [621-77-2] OOHAUGDGCWURIT-UHFFFAOYSA-N	6.7×10^{-2} 3.1×10^{-2} 7.1×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	238 247
1-tridecanamine $C_{13}H_{29}N$ [2869-34-3] ABVVEAHYODGCLZ-UHFFFAOYSA-N	9.0×10^{-2}		Altschuh et al. (1999)	M	
dimethylamine $(CH_3)_2NH$ [124-40-3] ROSDSFDQCJNGOL-UHFFFAOYSA-N	5.5×10^{-1} 5.5×10^{-1} 6.2×10^{-1} 3.0×10^{-1} 5.6×10^{-1} 5.8×10^{-1} 6.8×10^{-2} 1.8 5.6×10^{-1} 6.0×10^{-1} 8.0×10^{-1} 6.7×10^{-1} 4.7×10^{-1} 5.4×10^{-1} 3.7×10^{-1} 8.0×10^{-1} 5.6×10^{-1} 5.6×10^{-1} 5.7×10^{-1}	 4000 6400 	Burkholder et al. (2019) Burkholder et al. (2015) Brockbank (2013) Wilhelm et al. (1977) Christie and Crisp (1967) Bagno et al. (1991) Keshavarz et al. (2022) Duchowicz et al. (2020) Li et al. (2014) Hilal et al. (2008) Modarresi et al. (2007) Yaffe et al. (2003) Katritzky et al. (1998) Nirmalakhandan et al. (1997) Russell et al. (1992) Suzuki et al. (1992) Duchowicz et al. (2020) Mackay et al. (2006d) Abraham et al. (1990)	L L L L M T Q Q Q Q Q Q Q Q Q Q ? ? ?	 475 185 242 68 249, 273 280 405, 233 186, 21

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
diethylamine	3.8×10^{-1}		Burkholder et al. (2019)	L	
$(C_2H_5)_2NH$	3.8×10^{-1}		Burkholder et al. (2015)	L	
[109-89-7]	3.7×10^{-1}		Brockbank (2013)	L	
HPNMFZURTQLUMO-UHFFFAOYSA-N	3.9×10^{-1}		Christie and Crisp (1967)	M	
	4.1×10^{-1}	7700	Bagno et al. (1991)	T	475
	2.9×10^{-1}		Yaws (2003)	X	259
	1.3	10000	Goldstein (1982)	X	299
	5.2×10^{-2}		Dupeux et al. (2022)	Q	260
	1.2×10^{-1}		Keshavarz et al. (2022)	Q	
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	2.5×10^{-1}		Modarresi et al. (2007)	Q	68
	5.2×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	2.5×10^{-1}		Yao et al. (2002)	Q	230
	3.1×10^{-1}		English and Carroll (2001)	Q	231, 232
	1.5×10^{-1}		Katritzky et al. (1998)	Q	
	1.5×10^{-1}		Russell et al. (1992)	Q	360
	4.7×10^{-1}		Suzuki et al. (1992)	Q	233
	3.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	3.8×10^{-1}		Mackay et al. (2006d)	?	
	1.4×10^{-1}		Yaws (1999)	?	21
	1.5×10^{-1}		Yaws and Yang (1992)	?	21
	3.9×10^{-1}		Abraham et al. (1990)	?	
dipropylamine	2.0×10^{-1}		Burkholder et al. (2019)	L	
$(C_3H_7)_2NH$	2.0×10^{-1}		Burkholder et al. (2015)	L	
[142-84-7]	2.1×10^{-1}		Brockbank (2013)	L	
WEHWNAOGRSTTBQ-UHFFFAOYSA-N	1.2×10^{-1}	8900	Leng et al. (2015a)	M	
	1.9×10^{-1}		Christie and Crisp (1967)	M	
	2.3×10^{-1}		Keshavarz et al. (2022)	Q	
	2.2×10^{-1}		Duchowicz et al. (2020)	Q	
	7.0×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.1×10^{-1}		Hilal et al. (2008)	Q	
	2.7×10^{-1}		Modarresi et al. (2007)	Q	68
		6900	Kühne et al. (2005)	Q	
	2.1×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	9.6×10^{-2}		Yao et al. (2002)	Q	230
	1.9×10^{-1}		English and Carroll (2001)	Q	231, 261
	1.1×10^{-1}		Katritzky et al. (1998)	Q	
	2.3×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	2.8×10^{-1}		Suzuki et al. (1992)	Q	233
	1.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		8100	Kühne et al. (2005)	?	
	1.1×10^{-1}		Yaws (1999)	?	21, 553
	1.9×10^{-1}		Abraham et al. (1990)	?	
			Betterton (1992)	W	554

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-methylpropanamine $C_4H_{11}N$ [627-35-0] GVWISOJSERXQBM-UHFFFAOYSA-N	1.9×10^{-1}		Hilal et al. (2008)	Q	
N-methyl-2-propanamine $C_4H_{11}N$ [4747-21-1] XHFGWHUWQXTGAT-UHFFFAOYSA-N	1.6×10^{-1} 1.4×10^{-1}		Gharagheizi et al. (2012) Hilal et al. (2008)	Q Q	
N-(1-methylethyl)-2-propanamine $C_6H_{15}N$ (diisopropylamine) [108-18-9] UAOMVDZJSHZZME-UHFFFAOYSA-N	1.0×10^{-1} 1.3×10^{-1} 3.3×10^{-2} 1.4×10^{-1} 6.2×10^{-2} 4.1×10^{-1} 9.7×10^{-2} 9.5×10^{-2} 6.7×10^{-2} 1.8×10^{-1} 9.2×10^{-2}	 6900 8600 	Duchowicz et al. (2020) Yaws (2003) Duchowicz et al. (2020) Gharagheizi et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Kühne et al. (2005) Yaffe et al. (2003) English and Carroll (2001) Katritzky et al. (1998) Nirmalakhandan et al. (1997) Kühne et al. (2005) Abraham et al. (1990)	V X Q Q Q Q Q Q Q Q Q ? ?	187 238 247 68 249, 250 231, 275
N,N-dipropyl-1-propanamine $C_9H_{21}N$ (tripropylamine) [102-69-2] YFTHZRPMJXBUME-UHFFFAOYSA-N	2.6×10^{-2} 2.6×10^{-2} 2.6×10^{-2} 2.6×10^{-2} 5.1×10^{-2} 3.6×10^{-2} 4.4×10^{-2} 6.7×10^{-2} 1.3×10^{-2} 2.7×10^{-2} 2.1×10^{-2} 4.2×10^{-2} 2.6×10^{-2}		Duchowicz et al. (2020) HSDB (2015) Yaws (2003) Hilal et al. (2008) Duchowicz et al. (2020) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Yaffe et al. (2003) Yao et al. (2002) Katritzky et al. (1998) Yaws (1999)	V V X C Q Q Q Q Q Q Q Q ?	187 238 247 68 249, 250 230 21
N-methyl-1-butanamine $C_5H_{13}N$ (N-methylbutylamine) [110-68-9] QCOGKXLOEWLIDC-UHFFFAOYSA-N	1.3×10^{-1} 5.7×10^{-2} 1.4×10^{-1} 1.1×10^{-1} 	 6600 5000	Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Hilal et al. (2008) Kühne et al. (2005) Kühne et al. (2005)	X Q Q Q Q ?	238 247

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dibutylamine	1.3×10^{-1}		Brockbank (2013)	L	
$(C_4H_9)_2NH$	1.0		Altschuh et al. (1999)	M	
[111-92-2]	1.1×10^{-1}		Christie and Crisp (1967)	M	
JQVDAXLFBXTEQA-UHFFFAOYSA-N	1.2×10^{-1}		Mackay et al. (2006d)	V	
	1.2×10^{-1}		Mackay et al. (1995)	V	
	7.0×10^{-2}		Yaws (2003)	X	238
	4.1×10^{-1}		Keshavarz et al. (2022)	Q	
	2.2×10^{-1}		Duchowicz et al. (2020)	Q	300
	4.5×10^{-2}		Gharagheizi et al. (2012)	Q	
	7.6×10^{-2}		Gharagheizi et al. (2010)	Q	247
	2.4×10^{-1}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Modarresi et al. (2007)	Q	68
		7600	Kühne et al. (2005)	Q	
	9.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	6.2×10^{-2}		Yao et al. (2002)	Q	230
	1.2×10^{-1}		English and Carroll (2001)	Q	231, 232
	8.8×10^{-2}		Katritzky et al. (1998)	Q	
	1.4×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.6×10^{-1}		Suzuki et al. (1992)	Q	233
	1.1×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		7400	Kühne et al. (2005)	?	
	7.0×10^{-2}		Yaws (1999)	?	21
	9.7×10^{-2}		Abraham et al. (1990)	?	
diisobutylamine	1.8×10^{-2}		Duchowicz et al. (2020)	V	187
$C_8H_{19}N$	4.3×10^{-2}		Yaws (2003)	X	238
[110-96-3]	3.4×10^{-2}		Duchowicz et al. (2020)	Q	
NJBCRXCAPCODGX-UHFFFAOYSA-N	6.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
	1.5×10^{-1}		Modarresi et al. (2007)	Q	68
		7600	Kühne et al. (2005)	Q	
	1.8×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.5×10^{-2}		Katritzky et al. (1998)	Q	
		7300	Kühne et al. (2005)	?	
bis-(1-methylpropyl)-amine		7600	Kühne et al. (2005)	Q	
$C_8H_{19}N$		7000	Kühne et al. (2005)	?	
(di-*sec*-butylamine)					
[626-23-3]					
OBYVIBDTOCAXSN-UHFFFAOYSA-N					
tetraethylenepentamine	3.3×10^{14}		HSDB (2015)	Q	100
$C_8H_{23}N_5$					
[112-57-2]					
FAGUFWYHJQFNRV-UHFFFAOYSA-N					

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N,N-di-2-propenyl-2-propen-1-amine	3.9×10^{-2}	7500	Brockbank (2013)	L	1
$C_9H_{15}N$	3.8×10^{-2}		Duchowicz et al. (2020)	V	187
(triallylamine)	3.8×10^{-2}		HSDB (2015)	V	
[102-70-5]	2.2		Duchowicz et al. (2020)	Q	
VPYJNCGUESNPMV-UHFFFAOYSA-N					
trimethylamine	9.9×10^{-2}		Burkholder et al. (2019)	L	
$(CH_3)_3N$	9.9×10^{-2}		Burkholder et al. (2015)	L	
[75-50-3]	8.4×10^{-2}	6300	Leng et al. (2015a)	M	
GETQZCLCWQTVFV-UHFFFAOYSA-N	9.4×10^{-1}	4200	Tsuji et al. (1990)	M	63
	7.6×10^{-2}		Amoore and Buttery (1978)	M	
	9.5×10^{-2}		Christie and Crisp (1967)	M	
	9.8×10^{-2}		Amoore and Buttery (1978)	V	
	1.0×10^{-1}		Hayer et al. (2022)	Q	20
	9.2×10^{-2}		Keshavarz et al. (2022)	Q	
	1.3		Duchowicz et al. (2020)	Q	
	3.7×10^{-2}		Hilal et al. (2008)	Q	
	3.3×10^{-2}		Modarresi et al. (2007)	Q	68
	9.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	8.4×10^{-2}		English and Carroll (2001)	Q	231, 232
	1.6×10^{-1}		Katritzky et al. (1998)	Q	
	4.7×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	6.4×10^{-2}		Russell et al. (1992)	Q	280
	1.2×10^{-1}		Suzuki et al. (1992)	Q	233
	9.5×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	1.5×10^{-1}		Mackay et al. (2006d)	?	
	9.0×10^{-2}		Abraham et al. (1990)	?	
triethylamine	6.6×10^{-2}		Burkholder et al. (2019)	L	
$(C_2H_5)_3N$	6.6×10^{-2}		Burkholder et al. (2015)	L	
[121-44-8]	9.3×10^{-2}		Brockbank (2013)	L	
ZMANZCXQSJIPKH-UHFFFAOYSA-N	5.0×10^{-2}	8300	Leng et al. (2015b)	M	
	6.6×10^{-2}		Christie and Crisp (1967)	M	
	7.1×10^{-2}		Mackay et al. (2006d)	V	
	7.1×10^{-2}		Mackay et al. (1995)	V	
	8.6×10^{-2}		Yaws (2003)	X	259
	8.5×10^{-2}		Yaws (2003)	X	238
	5.0×10^{-3}		Dupeux et al. (2022)	Q	260
	9.2×10^{-3}		Hayer et al. (2022)	Q	20
	2.3×10^{-1}		Keshavarz et al. (2022)	Q	
	5.1×10^{-2}		Duchowicz et al. (2020)	Q	300
	6.7×10^{-2}		Li et al. (2014)	Q	242
	9.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
	8.6×10^{-2}		Hilal et al. (2008)	Q	
	2.3×10^{-2}		Modarresi et al. (2007)	Q	68
		6700	Kühne et al. (2005)	Q	

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.1×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	7.8×10^{-2}		Yao et al. (2002)	Q	230
	1.3×10^{-1}		English and Carroll (2001)	Q	231, 232
	8.8×10^{-2}		Katritzky et al. (1998)	Q	
	3.3×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	3.1×10^{-2}		Russell et al. (1992)	Q	280
	6.1×10^{-2}		Suzuki et al. (1992)	Q	233
	6.6×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		9000	Kühne et al. (2005)	?	
	8.5×10^{-2}		Yaws (1999)	?	21
	9.2×10^{-2}		Abraham et al. (1990)	?	
tributylamine	3.7×10^{-1}	8700	Brockbank (2013)	L	
$C_{12}H_{27}N$	4.0×10^{-1}		Altschuh et al. (1999)	M	
[102-82-9]	6.2×10^{-2}		Duchowicz et al. (2020)	V	187
IMFACGCPASFAPR-UHFFFAOYSA-N	4.0×10^{-5}		Mackay et al. (2006d)	V	
	4.0×10^{-5}		Mackay et al. (1995)	V	
	4.9×10^{-2}		Yaws (2003)	X	238
	5.2×10^{-2}		Duchowicz et al. (2020)	Q	
	2.9×10^{-2}		Gharagheizi et al. (2010)	Q	247
		8700	Kühne et al. (2005)	Q	
		7500	Kühne et al. (2005)	?	
	6.1×10^{-2}		Yaws (1999)	?	21
N,N-dimethyl-1-dodecanamine	>4.0		Altschuh et al. (1999)	M	
$C_{14}H_{31}N$	4.6×10^{-2}		Yaws (2003)	X	238
[112-18-5]	2.0×10^{-3}		HSDB (2015)	Q	100
YWFWDNVOPHGWMX-UHFFFAOYSA-N	4.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
ethylenediamine	1.8×10^{3}	6700	Nguyen (2013)	M	11
$H_2NCH_2CH_2NH_2$	5.8×10^{3}		Westheimer and Ingraham (1956)	M	
[107-15-3]	1.5×10^{2}	9200	Cabani et al. (1978)	T	
PIICEJLVQHRZGT-UHFFFAOYSA-N	6.7×10^{3}		Keshavarz et al. (2022)	Q	
	2.2×10^{3}		Duchowicz et al. (2020)	Q	
	5.6×10^{3}		Hilal et al. (2008)	Q	
	1.4×10^{4}		Modarresi et al. (2007)	Q	68
	6.2×10^{2}		Yao et al. (2002)	Q	230
	5.7×10^{3}		Duchowicz et al. (2020)	?	186, 21
	2.3×10^{2}		Yaws (1999)	?	21, 12
2-propen-1-amine	1.0	5400	Leng et al. (2015a)	M	
C_3H_7N	5.4×10^{-1}		Duchowicz et al. (2020)	V	187
(allylamine)	5.4×10^{-1}		HSDB (2015)	V	
[107-11-9]	5.4×10^{-1}		Hilal et al. (2008)	C	
VVJKKWFAADXIJK-UHFFFAOYSA-N	7.7		Duchowicz et al. (2020)	Q	
	2.4		Hilal et al. (2008)	Q	
	4.4		Modarresi et al. (2007)	Q	68

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
di-2-propenylamine	3.3×10^{-1}		Duchowicz et al. (2020)	V	187
$C_6H_{11}N$	3.3×10^{-1}		HSDB (2015)	V	
(diallylamine)	2.6		Duchowicz et al. (2020)	Q	
[124-02-7]		7200	Kühne et al. (2005)	Q	
DYUWTXWIYMHBQS-UHFFFAOYSA-N		8000	Kühne et al. (2005)	?	
hexamethyleneimine	1.6	8200	Cabani et al. (1971a)	T	
$(CH_2)_6NH$	1.0		Keshavarz et al. (2022)	Q	
[111-49-9]	1.3×10^{1}		Duchowicz et al. (2020)	Q	185
ZSIQJIWKELUFRJ-UHFFFAOYSA-N	6.4		Hilal et al. (2008)	Q	
	3.5×10^{-1}		Modarresi et al. (2007)	Q	68
	1.2		Suzuki et al. (1992)	Q	233
	4.3×10^{-1}		Meylan and Howard (1991)	Q	
	1.6		Duchowicz et al. (2020)	?	186, 21
cyclohexanamine	2.2	7500	Brockbank (2013)	L	1
$C_6H_{13}N$	2.4		Altschuh et al. (1999)	M	
(cyclohexylamine)	2.2	7800	Bernauer et al. (2006)	V	1
[108-91-8]	9.4×10^{-1}		Amoore and Buttery (1978)	V	
PAFZNILMFXTMIY-UHFFFAOYSA-N	3.3		Keshavarz et al. (2022)	Q	
	7.3		Duchowicz et al. (2020)	Q	300
	6.7×10^{-1}		Hilal et al. (2008)	Q	
	4.2		Modarresi et al. (2007)	Q	68
	9.5×10^{-1}		English and Carroll (2001)	Q	231, 232
	1.2		Nirmalakhandan et al. (1997)	Q	
	2.4		Duchowicz et al. (2020)	?	186, 21
	9.5×10^{-1}		Abraham et al. (1990)	?	
3-methylcyclohexylamine	1.1		Hilal et al. (2008)	Q	
$C_7H_{15}N$					
[6850-35-7]					
JYDYHSHPBDZRPU-UHFFFAOYSA-N					
N-ethylcyclohexanamine		7200	Kühne et al. (2005)	Q	
$C_8H_{17}N$		6500	Kühne et al. (2005)	?	
(N-ethylcyclohexylamine)					
[5459-93-8]					
AGVKXDPPPSLISR-UHFFFAOYSA-N					
N,N-dimethylcyclohexylamine	4.2×10^{-1}		Altschuh et al. (1999)	M	
$C_8H_{17}N$	4.1×10^{-1}		Keshavarz et al. (2022)	Q	
[98-94-2]	1.4		Duchowicz et al. (2020)	Q	300
SVYKKECYCPFKGB-UHFFFAOYSA-N	5.1×10^{-1}		Hilal et al. (2008)	Q	
	8.5×10^{-2}		Modarresi et al. (2007)	Q	68
		7000	Kühne et al. (2005)	Q	
	4.2×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		8500	Kühne et al. (2005)	?	

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexamethylenetetramine	6.2×10^{3}		HSDB (2015)	V	
$C_6H_{12}N_4$	6.1×10^{-5}		Zhang et al. (2010)	Q	288, 289
[100-97-0]	5.8×10^{5}		Zhang et al. (2010)	Q	288, 290
VKYKSIONXSXAKP-UHFFFAOYSA-N	9.2×10^{2}		Zhang et al. (2010)	Q	288, 291
	5.4×10^{7}		Zhang et al. (2010)	Q	288, 292
	1.3×10^{4}		Hilal et al. (2008)	Q	
	5.8×10^{3}		Modarresi et al. (2007)	Q	68
1-decanamine	2.6×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{10}H_{23}N$	1.5×10^{-1}		Yaws et al. (2001)	X	352
[2016-57-1]	2.4		Duchowicz et al. (2020)	Q	
MHZGKXUYDGKKIU-UHFFFAOYSA-N					
N-cyclohexylcyclohexanamine	1.8×10^{-1}		HSDB (2015)	Q	100
$C_{12}H_{23}N$					
(dicyclohexylamine)					
[101-83-7]					
XBPCUCUWBYBCDP-UHFFFAOYSA-N					
1-dodecanamine	3.7×10^{-2}		HSDB (2015)	Q	100
$C_{12}H_{27}N$					
[124-22-1]					
JRBPAEWTRLWTQC-UHFFFAOYSA-N					
1-octadecanamine	1.0×10^{-2}		HSDB (2015)	Q	100
$C_{18}H_{39}N$					
[124-30-1]					
REYJJPSVUYRZGE-UHFFFAOYSA-N					
N,N-dioctyl-1-octanamine	7.0×10^{-4}		HSDB (2015)	Q	100
$C_{24}H_{51}N$					
(tri-N-octylamine)					
[1116-76-3]					
XTAZYLNFDRKIHJ-UHFFFAOYSA-N					
aminobenzene	4.9	6800	Brockbank (2013)	L	1
C_6H_7N	4.4		Chao et al. (2017)	M	
(aniline)	5.2		Altschuh et al. (1999)	M	
[62-53-3]	1.2		Heal et al. (1995)	M	375
PAYRUJLWNCNPSJ-UHFFFAOYSA-N	5.0		Jayasinghe et al. (1992)	M	
	1.1		Dallos et al. (1983)	M	555
	4.4		Chao et al. (2017)	V	
	4.6	6500	Bernauer et al. (2006)	V	1
	6.0		Mackay et al. (2006d)	V	
	6.0		Schüürmann (2000)	V	
	7.1×10^{-5}		Lide and Frederikse (1995)	V	
	6.0		Mackay et al. (1995)	V	
	5.5		Hwang et al. (1992)	V	
	3.4		Yoshida et al. (1983)	V	
	5.8		Yaws (2003)	X	259

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.1×10^{-5}		Howard (1989)	X	366
	5.7		Yaws (2003)	X	238
	8.2×10^{-2}		Howard (1989)	X	414
	2.4		Dupeux et al. (2022)	Q	260
	3.3		Keshavarz et al. (2022)	Q	
	5.1		Duchowicz et al. (2020)	Q	300
	1.8×10^{1}		Gharagheizi et al. (2012)	Q	
	5.5		Gharagheizi et al. (2010)	Q	247
	5.1		Hilal et al. (2008)	Q	
	4.2		Modarresi et al. (2007)	Q	68
		6200	Kühne et al. (2005)	Q	
	4.8		Yaffe et al. (2003)	Q	249, 250
	2.4		Yao et al. (2002)	Q	230
	3.0		Katritzky et al. (1998)	Q	
	4.9		Duchowicz et al. (2020)	?	186, 21
	8.2×10^{-2}		Mackay et al. (2006d)	?	
		7100	Kühne et al. (2005)	?	
	5.8		Yaws (1999)	?	21
	4.3		Abraham et al. (1990)	?	
benzylamine C_7H_9N [100-46-9] WGQKYBSKWIADBV-UHFFFAOYSA-N	7.1×10^{-1}		Yao et al. (2002)	Q	230
	3.4×10^{-1}		Yaws (1999)	?	21
2-methylbenzenamine C_7H_9N (2-methylaniline; *o*-toluidine) [95-53-4] RNVCVTLRINQCPJ-UHFFFAOYSA-N	4.8	7100	Brockbank (2013)	L	
	3.0		Chao et al. (2017)	M	
	5.0		Altschuh et al. (1999)	M	
	4.0		Chao et al. (2017)	V	
	1.1×10^{1}		Mackay et al. (2006d)	V	
	4.1		Schüürmann (2000)	V	
	1.1×10^{1}		Mackay et al. (1995)	V	
	1.1×10^{1}		Mackay et al. (1995)	V	
	3.4		Yoshida et al. (1983)	V	
	4.6		Abraham et al. (1994a)	R	
	4.1		Yaws (2003)	X	238
	3.0×10^{-1}		Keshavarz et al. (2022)	Q	
	2.7		Duchowicz et al. (2020)	Q	300
	3.3		Gharagheizi et al. (2012)	Q	
	4.4		Gharagheizi et al. (2010)	Q	247
	3.1		Hilal et al. (2008)	Q	
	1.0		Modarresi et al. (2007)	Q	68
	1.6		Yao et al. (2002)	Q	230
	4.0		English and Carroll (2001)	Q	231, 232
	4.4		Katritzky et al. (1998)	Q	
	2.0		Nirmalakhandan et al. (1997)	Q	
	5.0		Duchowicz et al. (2020)	?	186, 21
	4.1		Yaws (1999)	?	21

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methylbenzenamine	5.6	7200	Brockbank (2013)	L	
C_7H_9N	3.2		Chao et al. (2017)	M	
(3-methylaniline; *m*-toluidine)	5.9		Altschuh et al. (1999)	M	
[108-44-1]	3.9		Chao et al. (2017)	V	
JJYPMNFTHPTTDI-UHFFFAOYSA-N	3.9		Mackay et al. (2006d)	V	
	3.9		Mackay et al. (1995)	V	
	5.1		Yaws (2003)	X	238, 12
	4.5		Keshavarz et al. (2022)	Q	
	2.7		Duchowicz et al. (2020)	Q	300
	4.7		Gharagheizi et al. (2012)	Q	
	4.4		Gharagheizi et al. (2010)	Q	247
	4.8		Hilal et al. (2008)	Q	
	3.9		Modarresi et al. (2007)	Q	68
	1.5		Yao et al. (2002)	Q	230
	6.4		Katritzky et al. (1998)	Q	
	5.9		Duchowicz et al. (2020)	?	186, 21
	3.5		Yaws (1999)	?	21, 12
4-methylbenzenamine	2.9	4400	Brockbank (2013)	L	
C_7H_9N	4.4		Chao et al. (2017)	M	
(4-methylaniline; *p*-toluidine)	1.3×10^{1}		Altschuh et al. (1999)	M	
[106-49-0]	4.4		Jayasinghe et al. (1992)	M	
RZXMPPFPUUCRFN-UHFFFAOYSA-N	1.5		Mackay et al. (2006d)	V	
	1.5		Mackay et al. (1995)	V	
	1.6		Yoshida et al. (1983)	V	
	5.0		Abraham et al. (1994a)	R	
	4.5		Keshavarz et al. (2022)	Q	
	2.7		Duchowicz et al. (2020)	Q	
	3.9		Gharagheizi et al. (2012)	Q	
	5.3		Hilal et al. (2008)	Q	
	5.0		Modarresi et al. (2007)	Q	68
	4.0		English and Carroll (2001)	Q	231, 232
	6.1		Katritzky et al. (1998)	Q	
	2.0		Nirmalakhandan et al. (1997)	Q	
	4.9		Duchowicz et al. (2020)	?	186, 21
2-ethylaniline	2.6	7300	Brockbank (2013)	L	1, 556
$C_8H_{11}N$	2.7		HSDB (2015)	Q	100
(*o*-ethylaniline)		7200	Kühne et al. (2005)	Q	
[578-54-1]		7500	Kühne et al. (2005)	?	
MLPVBIWIRCKMJV-UHFFFAOYSA-N					
4-ethylaniline	3.1		Mackay et al. (2006d)	V	
$C_8H_{11}N$	3.1		Mackay et al. (1995)	V	
(*p*-ethylaniline)		6900	Kühne et al. (2005)	Q	
[589-16-2]		8100	Kühne et al. (2005)	?	
HRXZRAXKKNUKRF-UHFFFAOYSA-N					

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4-dimethylbenzenamine	2.8	7700	Brockbank (2013)	L	1
$C_8H_{11}N$	2.4		Mackay et al. (2006d)	V	
(2,4-dimethylaniline; 2,4-xylidine)	1.4×10^{-1}		Schüürmann (2000)	V	
[95-68-1]	2.4		Mackay et al. (1995)	V	
CZZZABOKJQXEBO-UHFFFAOYSA-N	3.9		HSDB (2015)	Q	100
		7200	Kühne et al. (2005)	Q	
		7400	Kühne et al. (2005)	?	
3,4-dimethylbenzenamine	5.3		Jayasinghe et al. (1992)	M	
$C_8H_{11}N$	6.0		Keshavarz et al. (2022)	Q	
(3,4-dimethylaniline; 3,4-xylidine)	1.4		Duchowicz et al. (2020)	Q	
[95-64-7]	6.7		Hilal et al. (2008)	Q	
DOLQYFPDPKPQSS-UHFFFAOYSA-N	1.6		Modarresi et al. (2007)	Q	68
	9.0		Katritzky et al. (1998)	Q	
	5.3		Duchowicz et al. (2020)	?	186, 21
2,5-dimethylbenzenamine	2.3		Duchowicz et al. (2020)	V	187
$C_8H_{11}N$	1.4		Duchowicz et al. (2020)	Q	
(2,5-dimethylaniline; 2,5-xylidine)	3.9		HSDB (2015)	Q	100
[95-78-3]	7.7×10^{-1}		Modarresi et al. (2007)	Q	68
VOWZNBNDMFLQGM-UHFFFAOYSA-N		7200	Kühne et al. (2005)	Q	
		7700	Kühne et al. (2005)	?	
2,6-dimethylbenzenamine	3.9		Duchowicz et al. (2020)	V	187
$C_8H_{11}N$	3.9		HSDB (2015)	V	
(2,6-dimethylaniline; 2,6-xylidine)	5.8×10^{-2}		Mackay et al. (2006d)	V	
[87-62-7]	5.8×10^{-2}		Mackay et al. (1995)	V	
UFFBMTHBGFGIHF-UHFFFAOYSA-N	2.7		Abraham et al. (1994a)	R	
	2.9×10^{-1}		Duchowicz et al. (2020)	Q	
	3.3		Hilal et al. (2008)	Q	
	1.7×10^{1}		Modarresi et al. (2007)	Q	68
		7500	Kühne et al. (2005)	Q	
	2.1		English and Carroll (2001)	Q	231, 232
	4.2		Katritzky et al. (1998)	Q	
	1.4		Nirmalakhandan et al. (1997)	Q	
		7600	Kühne et al. (2005)	?	
2,4,5-trimethylbenzenamine	3.9		Jayasinghe et al. (1992)	M	
$C_9H_{13}N$	5.5×10^{-1}		Keshavarz et al. (2022)	Q	
(2,4,5-trimethylaniline)	7.3×10^{-1}		Duchowicz et al. (2020)	Q	185
[137-17-7]	6.0		Hilal et al. (2008)	Q	
BMIPMKQAAJKBKP-UHFFFAOYSA-N	3.5×10^{-1}		Modarresi et al. (2007)	Q	68
	4.0		Duchowicz et al. (2020)	?	186, 21
2-(1-methylethyl)-benzenamine		7500	Kühne et al. (2005)	Q	
$C_9H_{13}N$		6400	Kühne et al. (2005)	?	
(2-isopropylaniline)					
[643-28-7]					
YKOLZVXSPGIIBJ-UHFFFAOYSA-N					

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,6-diethylbenzenamine	8.8		Duchowicz et al. (2020)	V	187
$C_{10}H_{15}N$	9.0		HSDB (2015)	V	
(2,6-diethylaniline)	3.0×10^{-1}		Duchowicz et al. (2020)	Q	
[579-66-8]	9.0×10^{-1}		Hilal et al. (2008)	Q	
FOYHNROGBXVLLX-UHFFFAOYSA-N	6.8		Modarresi et al. (2007)	Q	68
	8.8		Yaffe et al. (2003)	Q	249, 250
	5.0		Katritzky et al. (1998)	Q	
	8.8		Yaws (1999)	?	21, 404
1,2-benzenediamine	1.4×10^{3}		Duchowicz et al. (2020)	V	187
$C_6H_8N_2$	1.4×10^{3}		HSDB (2015)	V	
(*o*-phenylenediamine)	7.6×10^{1}		Schüürmann (2000)	V	
[95-54-5]	1.0×10^{2}		Yaws (2003)	X	238, 557
GEYOCULIXLDCMW-UHFFFAOYSA-N	2.9×10^{3}		Duchowicz et al. (2020)	Q	
	1.2×10^{2}		Gharagheizi et al. (2012)	Q	
	1.0×10^{2}		Gharagheizi et al. (2010)	Q	247
	1.2×10^{3}		Hilal et al. (2008)	Q	
1,3-benzenediamine	7.9×10^{3}		Duchowicz et al. (2020)	V	187
$C_6H_8N_2$	7.6×10^{3}		HSDB (2015)	V	
(*m*-phenylenediamine)	1.3×10^{4}		Schüürmann (2000)	V	
[108-45-2]	6.9×10^{3}		Yaws (2003)	X	238
WZCQRUWWHSTZEM-UHFFFAOYSA-N	2.8×10^{3}		Duchowicz et al. (2020)	Q	
	2.8×10^{2}		Gharagheizi et al. (2012)	Q	
	2.2×10^{3}		Gharagheizi et al. (2010)	Q	247
	1.1×10^{5}		Hilal et al. (2008)	Q	
	3.7×10^{4}		Modarresi et al. (2007)	Q	68
1,4-benzenediamine	7.1×10^{2}		Yaws (2003)	X	238, 80
$C_6H_8N_2$	1.5×10^{4}		HSDB (2015)	Q	100
(*p*-phenylenediamine)	1.7×10^{2}		Gharagheizi et al. (2012)	Q	
[106-50-3]	2.2×10^{3}		Gharagheizi et al. (2010)	Q	247
CBCKQZAAMUWICA-UHFFFAOYSA-N					
2-methyl-1,3-benzenediamine	1.3×10^{4}		HSDB (2015)	Q	100
$C_7H_{10}N_2$					
[823-40-5]					
RLYCRLGLCUXUPO-UHFFFAOYSA-N					
2-methyl-1,4-benzenediamine	1.3×10^{4}		HSDB (2015)	Q	100
$C_7H_{10}N_2$					
[95-70-5]					
OBCSAIDCZQSFQH-UHFFFAOYSA-N					
3-methyl-1,2-benzenediamine	1.0×10^{4}		HSDB (2015)	Q	100
$C_7H_{10}N_2$					
(2,3-diaminotoluene)					
[2687-25-4]					
AXNUJYHFQHQZBE-UHFFFAOYSA-N					

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methyl-1,3-benzenediamine $C_7H_{10}N_2$ (toluene-2,4-diamine) [95-80-7] VOZKAJLKRJDJLL-UHFFFAOYSA-N	1.0×10^{4}		HSDB (2015)	Q	100
3,5-diaminotoluene $C_7H_{10}N_2$ [108-71-4] LVNDUJYMLJDECN-UHFFFAOYSA-N	1.3×10^{4}		HSDB (2015)	Q	547
phenylhydrazine $C_6H_8N_2$ [100-63-0] HKOOXMFOFWEVGF-UHFFFAOYSA-N	2.2×10^{3}		Duchowicz et al. (2020)	V	187
	3.4×10^{2}		HSDB (2015)	V	
	9.6		Duchowicz et al. (2020)	Q	
	6.9×10^{2}		Hilal et al. (2008)	Q	
	8.3×10^{3}		Modarresi et al. (2007)	Q	68
(methylamino)-benzene C_7H_9N (N-methylaniline) [100-61-8] AFBPFSWMIHJQDM-UHFFFAOYSA-N	8.7×10^{-1}		HSDB (2015)	V	
	8.7×10^{-1}		Schüürmann (2000)	V	
	1.1		Abraham et al. (1994a)	R	
	3.0×10^{-1}		Keshavarz et al. (2022)	Q	
	3.7		Duchowicz et al. (2020)	Q	300
	1.5		Hilal et al. (2008)	Q	
	5.7×10^{-1}		Modarresi et al. (2007)	Q	68
	6.1×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	2.0		Yao et al. (2002)	Q	230
	7.3×10^{-1}		English and Carroll (2001)	Q	231, 232
	4.5		Katritzky et al. (1998)	Q	
	2.7		Nirmalakhandan et al. (1997)	Q	
	1.1		Duchowicz et al. (2020)	?	186, 21
	8.7×10^{-1}		Yaws (1999)	?	21
(ethylamino)-benzene $C_8H_{11}N$ (N-ethylaniline) [103-69-5] OJGMBLNIHDZDGS-UHFFFAOYSA-N	8.1×10^{-1}	7900	Brockbank (2013)	L	1, 558
	1.0		Altschuh et al. (1999)	M	
	4.1×10^{-1}		Keshavarz et al. (2022)	Q	
	1.3		Duchowicz et al. (2020)	Q	185
	6.2×10^{-1}		HSDB (2015)	Q	100
	7.0×10^{-1}		Hilal et al. (2008)	Q	
	9.5×10^{-1}		Modarresi et al. (2007)	Q	68
		7100	Kühne et al. (2005)	Q	
	6.1×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	3.1		Katritzky et al. (1998)	Q	
	1.0		Duchowicz et al. (2020)	?	186, 21
		7600	Kühne et al. (2005)	?	

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(dimethylamino)-benzene	1.7×10^{-1}		HSDB (2015)	V	
$C_8H_{11}N$	8.5×10^{-2}		Mackay et al. (2006d)	V	
(N,N-dimethylaniline)	8.5×10^{-2}		Mackay et al. (1995)	V	
[121-69-7]	1.3×10^{-1}		Meylan and Howard (1991)	V	
JLTDJTHDQAWBAV-UHFFFAOYSA-N	1.6×10^{-1}		Yoshida et al. (1983)	V	
	9.9×10^{-2}		Hilal et al. (2008)	Q	
	1.0×10^{-1}		Modarresi et al. (2007)	Q	68
		6900	Kühne et al. (2005)	Q	
	1.4×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.5		Katritzky et al. (1998)	Q	
	2.4		Nirmalakhandan et al. (1997)	Q	
	1.1		Meylan and Howard (1991)	Q	
		6300	Kühne et al. (2005)	?	
	9.7×10^{-2}		Yaws (1999)	?	21
	1.4×10^{-1}		Abraham et al. (1990)	?	
benzeneethanamine	1.2×10^{1}		HSDB (2015)	Q	100
$C_8H_{11}N$					
(2-phenylethylamine)					
[64-04-0]					
BHHGXPLMPWCGHP-UHFFFAOYSA-N					
2,3-dimethylbenzenamine	3.9		HSDB (2015)	Q	100
$C_8H_{11}N$					
(2,3-xylidine)					
[87-59-2]					
VVAKEQGKZNKUSU-UHFFFAOYSA-N					
3,5-dimethylbenzenamine	3.9		HSDB (2015)	Q	100
$C_8H_{11}N$					
[108-69-0]					
MKARNSWMMBGSHX-UHFFFAOYSA-N					
dimethylaniline	3.9		HSDB (2015)	Q	100
$C_8H_{11}N$					
(xylidine)					
[1300-73-8]					
CDULGHZNHURECF-UHFFFAOYSA-N					
phenelzine	2.9×10^{3}		HSDB (2015)	Q	100
$C_8H_{12}N_2$					
[51-71-8]					
RMUCZJUITONUFY-UHFFFAOYSA-N					
N,N-dimethyl-1,4-benzenediamine	3.3×10^{2}		HSDB (2015)	Q	100
$C_8H_{12}N_2$					
[99-98-9]					
BZORFPDSXLZWJF-UHFFFAOYSA-N					

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4,6-trimethylbenzenamine $C_9H_{13}N$ (2,4,6-trimethylaniline) [88-05-1] KWVPRPSXBZNOHS-UHFFFAOYSA-N	3.7		HSDB (2015)	Q	100
N-ethyl-3-methylbenzenamine $C_9H_{13}N$ [102-27-2] GUYMMHOQXYZMJQ-UHFFFAOYSA-N	1.6		HSDB (2015)	Q	100
N-(1-methylethyl)benzenamine $C_9H_{13}N$ [768-52-5] FRCFWPVMFJMNDP-UHFFFAOYSA-N	1.3		HSDB (2015)	Q	100
2-ethyl-6-methylbenzenamine	3.2		Zhang et al. (2010)	Q	288, 289
$C_9H_{13}N$	2.1		Zhang et al. (2010)	Q	288, 290
[24549-06-2]	1.0		Zhang et al. (2010)	Q	288, 291
JJVKJJNCIILLRP-UHFFFAOYSA-N	8.4×10^{-1}		Zhang et al. (2010)	Q	288, 292
N,N-dimethylbenzylamine		7700	Kühne et al. (2005)	Q	
$C_9H_{13}N$		7700	Kühne et al. (2005)	?	
[103-83-3]					
XXBDWLFCJWSEKW-UHFFFAOYSA-N					
N,N,4-trimethylbenzenamine	2.0×10^{-1}		Duchowicz et al. (2020)	V	187
$C_9H_{13}N$	1.1×10^{-1}		Duchowicz et al. (2020)	Q	
[99-97-8]	1.4×10^{-1}		Hilal et al. (2008)	Q	
GYVGXEWAOAAJEU-UHFFFAOYSA-N	4.0×10^{-2}		Modarresi et al. (2007)	Q	68
N,N'-di-*tert*-butylethylenediamine	3.6×10^{2}		Zhang et al. (2010)	Q	288, 289
$C_{10}H_{24}N_2$	2.3		Zhang et al. (2010)	Q	288, 290
[4062-60-6]	9.9×10^{-1}		Zhang et al. (2010)	Q	288, 291
KGHYGBGIWLNFAV-UHFFFAOYSA-N	1.2×10^{1}		Zhang et al. (2010)	Q	288, 292
(diethylamino)-benzene	6.7×10^{-2}	6700	Brockbank (2013)	L	
$C_{10}H_{15}N$	5.1×10^{-2}		Duchowicz et al. (2020)	V	187
(N,N-diethylaniline)	5.2×10^{-2}		HSDB (2015)	V	
[91-66-7]	4.6×10^{-1}		Mackay et al. (2006d)	V	
GGSUCNLOZRCGPQ-UHFFFAOYSA-N	4.6×10^{-1}		Mackay et al. (1995)	V	
	2.4×10^{-2}		Duchowicz et al. (2020)	Q	
	9.9×10^{-2}		Hilal et al. (2008)	Q	
	6.0×10^{-2}		Modarresi et al. (2007)	Q	68
		7600	Kühne et al. (2005)	Q	
	2.4		Katritzky et al. (1998)	Q	
		5800	Kühne et al. (2005)	?	
	5.2		Yaws (1999)	?	21, 559

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-naphthylamine	1.6×10^{2}		Altschuh et al. (1999)	M	
$C_{10}H_9N$	2.1×10^{1}		HSDB (2015)	V	
[134-32-7]	8.8×10^{1}		Abraham et al. (1994a)	R	
RUFPHBVGCFYCNW-UHFFFAOYSA-N	6.2×10^{2}		Keshavarz et al. (2022)	Q	
	2.0×10^{1}		Duchowicz et al. (2020)	Q	185
	3.0×10^{1}		Hilal et al. (2008)	Q	
	8.3×10^{1}		Modarresi et al. (2007)	Q	68
	1.2×10^{2}		English and Carroll (2001)	Q	231, 232
	4.6×10^{2}		Nirmalakhandan et al. (1997)	Q	
	8.9×10^{1}		Duchowicz et al. (2020)	?	186, 21
2-naphthylamine	1.2×10^{2}		Abraham et al. (1994a)	R	
$C_{10}H_9N$	1.2×10^{2}		Keshavarz et al. (2022)	Q	
[91-59-8]	2.0×10^{1}		Duchowicz et al. (2020)	Q	300
JBIJLHTVPXGSAM-UHFFFAOYSA-N	8.0×10^{1}		Hilal et al. (2008)	Q	
	1.0×10^{2}		Modarresi et al. (2007)	Q	68
	1.2×10^{2}		English and Carroll (2001)	Q	231, 275
	4.5×10^{2}		Nirmalakhandan et al. (1997)	Q	
	1.2×10^{2}		Duchowicz et al. (2020)	?	186, 21
	1.2×10^{2}		HSDB (2015)	?	421
1,5-naphthalenediamine $C_{10}H_{10}N_2$ [2243-62-1] KQSABULTKYLFEV-UHFFFAOYSA-N	1.5×10^{5}		HSDB (2015)	Q	100
phentermine $C_{10}H_{15}N$ [122-09-8] DHHVAGZRUROJKS-UHFFFAOYSA-N	7.0		HSDB (2015)	Q	100
N,N-diethyl-1,4-benzenediamine $C_{10}H_{16}N_2$ [93-05-0] QNGVNLMMEQUVQK-UHFFFAOYSA-N	1.9×10^{2}		HSDB (2015)	Q	100
3,5-diethyltoluene-2,6-diamine	6.2×10^{3}		Zhang et al. (2010)	Q	288, 289
$C_{11}H_{18}N_2$	6.9×10^{3}		Zhang et al. (2010)	Q	288, 290
[2095-01-4]	6.1×10^{1}		Zhang et al. (2010)	Q	288, 291
RQEOBXYYEPMCPJ-UHFFFAOYSA-N	2.1×10^{2}		Zhang et al. (2010)	Q	288, 292
2,4-diethyl-6-methylbenzene-1,3-diamine	6.2×10^{3}		Zhang et al. (2010)	Q	288, 289
$C_{11}H_{18}N_2$	7.0×10^{3}		Zhang et al. (2010)	Q	288, 290
[2095-02-5]	6.2×10^{1}		Zhang et al. (2010)	Q	288, 291
PISLZQACAJMAIO-UHFFFAOYSA-N	2.1×10^{2}		Zhang et al. (2010)	Q	288, 292

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
diphenylamine	3.7		Duchowicz et al. (2020)	V	187
$C_{12}H_{11}N$	3.7		HSDB (2015)	V	
[122-39-4]	2.9×10^{1}		Mackay et al. (2006d)	V	
DMBHHRLKUKUOEG-UHFFFAOYSA-N	2.9×10^{1}		Mackay et al. (1995)	V	
	3.5		Meylan and Howard (1991)	V	
	1.5		Yaws (2003)	X	238, 12
	3.5		Howard et al. (1991)	X	414
	4.1×10^{1}		Duchowicz et al. (2020)	Q	
	1.5		Gharagheizi et al. (2010)	Q	247
	3.0		Hilal et al. (2008)	Q	
	9.4		Meylan and Howard (1991)	Q	
benzidine	2.2×10^{6}		Mackay et al. (2006d)	V	
$C_{12}H_{12}N_2$	2.6×10^{5}		Lide and Frederikse (1995)	V	
[92-87-5]	2.2×10^{6}		Mackay et al. (1995)	V	
HFACYLZERDEVSX-UHFFFAOYSA-N	2.5×10^{1}		Mackay et al. (1995)	C	
	1.9×10^{5}		HSDB (2015)	Q	100
1,1-diphenylhydrazine	2.4×10^{2}		HSDB (2015)	Q	100
$C_{12}H_{12}N_2$					
[530-50-7]					
YHYKLKNNBYLTQY-UHFFFAOYSA-N					
1,2-diphenylhydrazine	2.1×10^{1}		Duchowicz et al. (2020)	V	187
$C_{12}H_{12}N_2$	2.1×10^{1}		HSDB (2015)	V	
(N,N'-bianiline)			Mackay et al. (2006d)	V	560
[122-66-7]	2.9×10^{3}		Mackay et al. (1995)	V	
YBQZXXMEJHZYMB-UHFFFAOYSA-N	2.3×10^{2}		Duchowicz et al. (2020)	Q	
4-(phenylazo)-benzenamine	1.1×10^{5}		HSDB (2015)	Q	100
$C_{12}H_{11}N_3$	9.3×10^{2}		Gharagheizi et al. (2012)	Q	
(4-aminoazobenzene)	1.9×10^{3}		Zhang et al. (2010)	Q	288, 289
[60-09-3]	3.2×10^{3}		Zhang et al. (2010)	Q	288, 290
QPQKUYVSJWQSDY-UHFFFAOYSA-N	7.3×10^{5}		Zhang et al. (2010)	Q	288, 291
	3.4×10^{2}		Zhang et al. (2010)	Q	288, 292
azobenzene	7.3×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{12}H_{10}N_2$	7.0×10^{-1}		HSDB (2015)	V	
[103-33-3]	2.6		Duchowicz et al. (2020)	Q	
DMLAVOWQYNRWNQ-UHFFFAOYSA-N					
2-aminobiphenyl	6.6×10^{1}		HSDB (2015)	Q	100
$C_{12}H_{11}N$					
[90-41-5]					
TWBPWBPGNQWFSJ-UHFFFAOYSA-N					

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-aminobiphenyl $C_{12}H_{11}N$ [92-67-1] DMVOXQPQNTYEKQ-UHFFFAOYSA-N	6.6×10^{1}		HSDB (2015)	Q	100
N-phenyl-1,4-benzenediamine	1.5×10^{3}		Yaws (2003)	X	238
$C_{12}H_{12}N_2$	2.7×10^{4}		HSDB (2015)	Q	100
(p-aminodiphenylamine)	5.9×10^{2}		Gharagheizi et al. (2012)	Q	
[101-54-2]	3.6×10^{3}		Gharagheizi et al. (2010)	Q	247
ATGUVEKSASEFFO-UHFFFAOYSA-N					
2-fluorenamine $C_{13}H_{11}N$ [153-78-6] CFRFHWQYWJMEJN-UHFFFAOYSA-N	2.7×10^{2}		HSDB (2015)	Q	547
4,4'-methylenebisbenzenamine $C_{13}H_{14}N_2$ [101-77-9] YBRVSVVVWCFQMG-UHFFFAOYSA-N	1.9×10^{5}		HSDB (2015)	V	
2-anthracenamine $C_{14}H_{11}N$ [613-13-8] YCSBALJAGZKWFF-UHFFFAOYSA-N	3.3×10^{1}		HSDB (2015)	Q	547
3,3'-dimethylbenzidine $C_{14}H_{16}N_2$ [119-93-7] NUIURNJTPRWVAP-UHFFFAOYSA-N	1.6×10^{5}		HSDB (2015)	Q	449
N,N-dimethyl-4-(phenylazo)-benzenamine	1.4×10^{3}		HSDB (2015)	V	
$C_{14}H_{15}N_3$	4.2×10^{1}		Zhang et al. (2010)	Q	288, 289
[60-11-7]	4.1×10^{1}		Zhang et al. (2010)	Q	288, 290
JCYPECIVGRXBMO-UHFFFAOYSA-N	8.2×10^{1}		Zhang et al. (2010)	Q	288, 291
	1.0×10^{1}		Zhang et al. (2010)	Q	288, 292
o-aminoazotoluene	3.1×10^{2}		Duchowicz et al. (2020)	V	187
$C_{14}H_{15}N_3$	3.8×10^{2}		Duchowicz et al. (2020)	Q	
[97-56-3]					
PFRYFZZSECNQOL-UHFFFAOYSA-N					
N-ethyl-N-phenylbenzenemethanamine	1.1		Zhang et al. (2010)	Q	288, 289
$C_{15}H_{17}N$	1.1		Zhang et al. (2010)	Q	288, 290
[92-59-1]	4.6×10^{-1}		Zhang et al. (2010)	Q	288, 291
HSZCJVZRHXPCIA-UHFFFAOYSA-N	6.7		Zhang et al. (2010)	Q	288, 292

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-(1-methylethyl)-N'-phenyl-1,4-benzenediamine $C_{15}H_{18}N_2$ (4-(iso-propylamino)diphenylamine) [101-72-4] OUBMGJOQLXMSNT-UHFFFAOYSA-N	7.0×10^3		HSDB (2015)	Q	100
4,4'-methylene-bis-(N-methylaniline) $C_{15}H_{18}N_2$ [1807-55-2] ZMVMYBGDGJLCHV-UHFFFAOYSA-N	3.4×10^4		HSDB (2015)	Q	100
C.I. Food Yellow 10 $C_{16}H_{13}N_3$ [85-84-7] KLCDQSGLLRINHY-UHFFFAOYSA-N	1.9×10^4		HSDB (2015)	Q	100
3,3',5,5'-tetramethylbenzidine $C_{16}H_{20}N_2$ [54827-17-7] UAIUNKRWKOVEES-UHFFFAOYSA-N	1.3×10^5		HSDB (2015)	Q	100
N-phenyl-1-naphthalenamine $C_{16}H_{13}N$ [90-30-2] XQVWYOYUZDUNRW-UHFFFAOYSA-N	7.0×10^1 9.7×10^1 4.6×10^1 1.2×10^1 2.8×10^2		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	V Q Q Q Q	 288, 289 288, 290 288, 291 288, 292
yellow OB $C_{17}H_{15}N_3$ [131-79-3] BWLVSYUUKOQICP-FMQUCBEESA-N	1.8×10^4		HSDB (2015)	Q	100
auramine $C_{17}H_{21}N_3$ [492-80-8] JPIYZTWMUGTEHX-UHFFFAOYSA-N	1.2×10^2		HSDB (2015)	V	
benzphetamine $C_{17}H_{21}N$ [156-08-1] YXKTVDFXDRQTKV-UHFFFAOYSA-N	2.3×10^1		HSDB (2015)	Q	100

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,4'-methylenebis(N,N-dimethylbenzenamine) $C_{17}H_{22}N_2$ (bis(p-dimethylamino)phenylmethane) [101-61-1] JNRLEMMIVRBKJE-UHFFFAOYSA-N	8.2×10^{1}		HSDB (2015)	Q	100
phencyclidine $C_{17}H_{25}N$ [77-10-1] JTJMJGYZQZDUJJ-UHFFFAOYSA-N	1.8		HSDB (2015)	Q	100
N,N'-diphenyl-1,4-benzenediamine $C_{18}H_{16}N_2$ [74-31-7] UTGQNNCQYDRXCH-UHFFFAOYSA-N	4.7×10^{4}		HSDB (2015)	Q	100
N-(1,3-dimethylbutyl)-N'-phenyl-1,4-phenylenediamine	2.9×10^{3}		Zhang et al. (2010)	Q	288, 289
$C_{18}H_{24}N_2$	3.9×10^{2}		Zhang et al. (2010)	Q	288, 290
[793-24-8]	3.9×10^{1}		Zhang et al. (2010)	Q	288, 291
ZZMVLMVFYMGSMY-UHFFFAOYSA-N	2.3×10^{3}		Zhang et al. (2010)	Q	288, 292
amitraz	1.0		MacBean (2012b)	X	352
$C_{19}H_{23}N_3$	1.3		Keshavarz et al. (2022)	Q	
[33089-61-1]	1.4×10^{2}		Duchowicz et al. (2020)	Q	
QXAITBQSYVNQDR-UHFFFAOYSA-N	2.1×10^{1}		Modarresi et al. (2007)	Q	68
	1.0		Duchowicz et al. (2020)	?	186, 21
N,N'-bis(1-ethyl-3-methylpentyl)-1,4-benzenediamine	5.8×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_{22}H_{40}N_2$	5.8		Zhang et al. (2010)	Q	288, 290
[139-60-6]	1.8		Zhang et al. (2010)	Q	288, 291
JUHXTONDLXIGGK-UHFFFAOYSA-N	1.9×10^{1}		Zhang et al. (2010)	Q	288, 292
p,*p*'-benzylidenebis(N,N-dimethylaniline) $C_{23}H_{26}N_2$ (leucomalachite green) [129-73-7] WZKXBGJNNCGHIC-UHFFFAOYSA-N	1.0×10^{3}		HSDB (2015)	Q	100
N-phenyl-N-(2,4,4-trimethyl-2-pentanyl)-1-naphthalenamine	6.4×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{24}H_{29}N$	9.7×10^{-1}		Zhang et al. (2010)	Q	288, 290
[51772-35-1]	9.0×10^{-1}		Zhang et al. (2010)	Q	288, 291
SNWVRVDHQRBBFG-UHFFFAOYSA-N	1.1×10^{1}		Zhang et al. (2010)	Q	288, 292

Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tris(2-ethylhexyl)amine	7.0×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_{24}H_{51}N$	1.2×10^{-2}		Zhang et al. (2010)	Q	288, 290
[1860-26-0]	6.1×10^{-6}		Zhang et al. (2010)	Q	288, 291
BZUDVELGTZDOIG-UHFFFAOYSA-N	3.7×10^{-4}		Zhang et al. (2010)	Q	288, 292
4,4',4"-methylidyne-tris(N,N-dimethylbenzenamine)	6.4×10^{4}		Zhang et al. (2010)	Q	288, 289
$C_{25}H_{31}N_3$	3.1×10^{4}		Zhang et al. (2010)	Q	288, 290
(Leucocrystal violet)	3.5×10^{2}		Zhang et al. (2010)	Q	288, 291
[603-48-5]	1.1×10^{6}		Zhang et al. (2010)	Q	288, 292
OAZWDJGLIYNYMU-UHFFFAOYSA-N					
N-phenylbenzenamide	8.2×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{30}H_{47}N$	4.7×10^{-1}		Zhang et al. (2010)	Q	288, 290
[68608-79-7]	1.5×10^{-1}		Zhang et al. (2010)	Q	288, 291
FSPSHPMYFQHGQD-UHFFFAOYSA-N	2.9×10^{-1}		Zhang et al. (2010)	Q	288, 292
4,4',4"-methanetriyltris(N,N-diethylaniline)	9.0×10^{4}		Zhang et al. (2010)	Q	288, 289
$C_{31}H_{43}N_3$	7.0×10^{5}		Zhang et al. (2010)	Q	288, 290
[68814-02-8]	1.7×10^{3}		Zhang et al. (2010)	Q	288, 291
HOGMPEULJBVHLZ-UHFFFAOYSA-N	1.5×10^{6}		Zhang et al. (2010)	Q	288, 292

A4.2 Heterocycles with nitrogen (C, H, N)

Table A4.2: Heterocycles with nitrogen (C, H, N)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
amitrole $C_2H_4N_4$ [61-82-5] KLSJWNVTNUYHDU-UHFFFAOYSA-N	4.5×10^{7} 4.5×10^{7} 6.1×10^{9} 1.5×10^{3}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Duchowicz et al. (2020)	V V V Q	187
azetidine C_3H_7N [503-29-7] HONIICLYMWZJFZ-UHFFFAOYSA-N	4.8		Ebert et al. (2023)	?	367
imidazole $C_3H_4N_2$ [288-32-4] RAXXELZNTBOGNW-UHFFFAOYSA-N	3.3×10^{3} 2.1×10^{3} 3.1×10^{3}		Du et al. (2017) Du et al. (2017) Du et al. (2017)	M Q Q	480 551
1,3,5-triazine-2,4,6-triamine $C_3H_6N_6$ [108-78-1] JDSHMPZPIAZGSV-UHFFFAOYSA-N	5.5×10^{8} 5.2×10^{7} 6.7×10^{8} 5.8×10^{9} 8.4×10^{8}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	V Q Q Q Q	 288, 289 288, 290 288, 291 288, 292
pyrrolidine C_4H_8NH [123-75-1] RWRDLPDLKQPQOW-UHFFFAOYSA-N	4.2 4.2 1.8 1.3×10^{1} 6.0 5.3×10^{-1} 4.1 8.4×10^{-1} 2.0 4.1	 7600 	Amoore and Buttery (1978) Cabani et al. (1971a) Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Yaffe et al. (2003) Katritzky et al. (1998) Suzuki et al. (1992) Duchowicz et al. (2020)	V T Q Q Q Q Q Q Q ?	 300 68 249, 250 233 186, 21
1-pyrroline C_4H_7N [5724-81-2] ZVJHJDDKYZXRJI-UHFFFAOYSA-N	1.6		Amoore and Buttery (1978)	M	
3-pyrroline C_4H_7N [109-96-6] JVQIKJMSUIMUDI-UHFFFAOYSA-N	4.9		Amoore and Buttery (1978)	V	
1,4-diazacyclohexane $C_4H_{10}N_2$ (piperazine) [110-85-0] GLUUGHFHXGJENI-UHFFFAOYSA-N	4.5×10^{3} 1.0×10^{2}	7400 11000	Nguyen (2013) Cabani et al. (1975a)	M T	11

Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pyrrole	5.5×10^{-1}		Hawthorne et al. (1985)	M	
C_4H_5N	6.1×10^{-1}		Mackay et al. (2006d)	V	
(1H-pyrrole)	6.1×10^{-1}		Mackay et al. (1995)	V	
[109-97-7]	1.8		Keshavarz et al. (2022)	Q	
KAESVJOAVNADME-UHFFFAOYSA-N	4.1		Duchowicz et al. (2020)	Q	185
	7.2×10^{-1}		Hilal et al. (2008)	Q	
	8.6×10^{-1}		Modarresi et al. (2007)	Q	68
	5.4×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	4.2		Katritzky et al. (1998)	Q	
	5.5×10^{-1}		Duchowicz et al. (2020)	?	186, 21
1-methyl-1H-imidazole	6.9×10^{1}		Du et al. (2017)	M	480
$C_4H_6N_2$	3.4×10^{2}		Du et al. (2017)	Q	551
[616-47-7]	8.9×10^{1}		Du et al. (2017)	Q	
MCTWTZJPVLRJOU-UHFFFAOYSA-N	1.1×10^{2}		Hilal et al. (2008)	Q	
1,3-diazine	1.0×10^{1}		Hilal et al. (2008)	Q	
$C_4H_4N_2$					
[289-95-2]					
CZPWVGJYEJSRLH-UHFFFAOYSA-N					
N-methylpyrrolidine	3.3×10^{-1}	7600	Cabani et al. (1971a)	T	
$C_4H_8NCH_3$	1.7×10^{-1}		Keshavarz et al. (2022)	Q	
[120-94-5]	1.2		Duchowicz et al. (2020)	Q	185
AVFZOVWCLRSYKC-UHFFFAOYSA-N	2.2×10^{-1}		Hilal et al. (2008)	Q	
	5.6×10^{-2}		Modarresi et al. (2007)	Q	68
	3.2×10^{-1}		Suzuki et al. (1992)	Q	233
	3.3×10^{-1}		Duchowicz et al. (2020)	?	186, 21
piperidine	2.8	7900	Bernauer and Dohnal (2009)	M	
$C_5H_{10}NH$	2.0		Amoore and Buttery (1978)	V	
[110-89-4]	2.2	7900	Cabani et al. (1971a)	T	
NQRYJNQNLNOLGT-UHFFFAOYSA-N	2.5		Keshavarz et al. (2022)	Q	
	1.3×10^{1}		Duchowicz et al. (2020)	Q	300
	7.3		Hilal et al. (2008)	Q	
	1.0		Modarresi et al. (2007)	Q	68
	7.2×10^{-1}		Katritzky et al. (1998)	Q	
	6.7×10^{-1}		Russell et al. (1992)	Q	280
	1.5		Suzuki et al. (1992)	Q	233
	2.2		Duchowicz et al. (2020)	?	186, 21
2-ethylimidazole	7.6×10^{2}		Du et al. (2017)	M	480
$C_5H_8N_2$	1.4×10^{4}		Du et al. (2017)	Q	551
[1072-62-4]	8.2×10^{2}		Du et al. (2017)	Q	
PQAMFDRRWURCFQ-UHFFFAOYSA-N					

Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-dimethylimidazole	4.3×10^{1}		Du et al. (2017)	M	480
$C_5H_8N_2$	2.9×10^{2}		Du et al. (2017)	Q	551
[1739-84-0]	3.3×10^{1}		Du et al. (2017)	Q	
GIWQSPITLQVMSG-UHFFFAOYSA-N					
N-methylpiperazine	1.8×10^{3}	9900	Nguyen (2013)	M	11
$C_5H_{12}N_2$	2.0×10^{2}	11000	Cabani et al. (1975a)	T	
(1-methylpiperazine)					
[109-01-3]					
PVOAHINGSUIXLS-UHFFFAOYSA-N					
1-methyl-1H-pyrrole	9.0×10^{-3}		Hilal et al. (2008)	Q	
C_5H_7N					
[96-54-8]					
OXHNLMTVIGZXSG-UHFFFAOYSA-N					
pyridine	9.1×10^{-1}	4700	Brockbank (2013)	L	
C_5H_5N	1.1	6000	Bernauer and Dohnal (2009)	M	
[110-86-1]	4.6×10^{-2}	-2300	Dewulf et al. (1999)	M	
JUJWROOIHBZHMG-UHFFFAOYSA-N	9.8×10^{-1}		Welke et al. (1998)	M	
	5.5×10^{-1}		Chaintreau et al. (1995)	M	
	8.2×10^{-1}		Hawthorne et al. (1985)	M	
	1.1		Arnett and Chawla (1979)	M	561
	7.1×10^{-1}		Amoore and Buttery (1978)	M	
	1.1	5900	Andon et al. (1954)	M	338
	8.4×10^{-1}		Keshavarz et al. (2022)	Q	
	2.4×10^{-1}		Duchowicz et al. (2020)	Q	300
	1.1		Li et al. (2014)	Q	242
	7.5×10^{-1}		Hilal et al. (2008)	Q	
	6.4×10^{-1}		Modarresi et al. (2007)	Q	68
		6000	Kühne et al. (2005)	Q	
	1.2		Yaffe et al. (2003)	Q	249, 250
	1.3		Yao et al. (2002)	Q	230
	1.2		English and Carroll (2001)	Q	231, 232
	9.0×10^{-2}		Katritzky et al. (1998)	Q	
	1.8		Nirmalakhandan et al. (1997)	Q	
	3.3		Russell et al. (1992)	Q	280
	1.2		Suzuki et al. (1992)	Q	233
	9.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	1.1		Mackay et al. (2006d)	?	
		5400	Kühne et al. (2005)	?	
	1.1		Yaws (1999)	?	21
	8.9×10^{-1}		Yaws and Yang (1992)	?	21
	1.1		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	562

Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pyridine-d5 C_5D_5N [7291-22-7] JUJWROOIHBZHMG-RALIUCGRSA-N	4.2	10000	Hiatt (2013)	M	
4-aminopyridine $C_5H_6N_2$ [504-24-5] NUKYPUAOHBNCPY-UHFFFAOYSA-N	4.3×10^{4}		HSDB (2015)	V	
2-aminopyridine $C_5H_6N_2$ [504-29-0] ICSNLGPSRYBMBD-UHFFFAOYSA-N	3.9×10^{3}		HSDB (2015)	Q	100
2-methylpyrazine $C_4N_2H_3CH_3$ [109-08-0] CAWHJQAVHZEVTJ-UHFFFAOYSA-N	4.5		Buttery et al. (1971)	M	
	4.9		Keshavarz et al. (2022)	Q	
	6.8×10^{-1}		Duchowicz et al. (2020)	Q	185
	4.8		Hilal et al. (2008)	Q	
	4.9		Modarresi et al. (2007)	Q	68
	1.6×10^{2}		Katritzky et al. (1998)	Q	
	3.1		Nirmalakhandan et al. (1997)	Q	
	1.2		Russell et al. (1992)	Q	280
	4.5		Duchowicz et al. (2020)	?	186, 21
adenine $C_5H_5N_5$ [73-24-5] GFFGJBXGBJISGV-UHFFFAOYSA-N	1.3×10^{9}		Duchowicz et al. (2020)	V	187
	5.3×10^{5}		Duchowicz et al. (2020)	Q	
9-methyladenine $C_6H_7N_5$ [700-00-5] WRXCXOUDSPTXNX-UHFFFAOYSA-N	3.9×10^{6}		Ebert et al. (2023)	?	367
N-methylpiperidine $C_5H_{10}NCH_3$ [626-67-5] PAMIQIKDUOTOBW-UHFFFAOYSA-N	2.4×10^{-1}		Abraham et al. (1994a)	R	
	2.9×10^{-1}	7900	Cabani et al. (1971a)	T	
	2.3×10^{-1}		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	
	4.8×10^{-1}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	68
		6300	Kühne et al. (2005)	Q	
	3.0×10^{-1}		English and Carroll (2001)	Q	231, 232
	2.9×10^{-1}		Katritzky et al. (1998)	Q	
	2.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	9.9×10^{-2}		Russell et al. (1992)	Q	280
	2.5×10^{-1}		Suzuki et al. (1992)	Q	233
	2.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		6600	Kühne et al. (2005)	?	

Table A4.2: Heterocycles with nitrogen (C, H, N) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
triethylenediamine	3.1×10^{3}		Du et al. (2017)	M	480
$C_6H_{12}N_2$	8.9×10^{2}		Du et al. (2017)	Q	551
[280-57-9]	2.2×10^{3}		Du et al. (2017)	Q	
IMNIMPAHZVJRPE-UHFFFAOYSA-N					
2-ethyl-4-methylimidazole	2.8×10^{2}		Du et al. (2017)	M	480
$C_6H_{10}N_2$	1.4×10^{3}		Du et al. (2017)	Q	551
[931-36-2]	3.1×10^{2}		Du et al. (2017)	Q	
ULKLGIFJWFIQFF-UHFFFAOYSA-N					
3-(aminomethyl)pyridine	4.3×10^{2}		Du et al. (2017)	M	480
$C_6H_8N_2$	5.0×10^{2}		Du et al. (2017)	Q	551
[3731-52-0]	3.7×10^{2}		Du et al. (2017)	Q	
HDOUGSFASVGDCS-UHFFFAOYSA-N					
N,N'-dimethylpiperazine	2.0×10^{2}	11000	Nguyen (2013)	M	11
$C_6H_{14}N_2$	1.4×10^{2}	11000	Cabani et al. (1975a)	T	
(1,4-dimethylpiperazine)					
[106-58-1]					
RXYPXQSKLGGKOL-UHFFFAOYSA-N					
cyromazine	1.7×10^{8}		Duchowicz et al. (2020)	V	187
$C_6H_{10}N_6$	1.7×10^{8}		HSDB (2015)	V	
[66215-27-8]	1.3×10^{8}		Duchowicz et al. (2020)	Q	
LVQDKIWDGQRHTE-UHFFFAOYSA-N					
1H-benzotriazole	3.1×10^{1}		HSDB (2015)	V	
$C_6H_5N_3$					
(1,2,3-benzotriazole)					
[95-14-7]					
QRUDEWIWKLJBPS-UHFFFAOYSA-N					
1-piperazineethanamine	1.5×10^{7}		HSDB (2015)	Q	100
$C_6H_{15}N_3$					
(N-(2-aminoethyl)piperazine)					
[140-31-8]					
IMUDHTPIFIBORV-UHFFFAOYSA-N					
2-methylpyridine	9.8×10^{-1}	6300	Brockbank (2013)	L	
$C_5H_4NCH_3$	9.9×10^{-1}	6400	Andon et al. (1954)	M	338
(2-picoline; α-picoline)	1.1		Keshavarz et al. (2022)	Q	
[109-06-8]	8.0×10^{-2}		Duchowicz et al. (2020)	Q	
BSKHPKMHTQYZBB-UHFFFAOYSA-N	4.1×10^{-1}		Hilal et al. (2008)	Q	
	1.2		Modarresi et al. (2007)	Q	68
		6400	Kühne et al. (2005)	Q	
	1.0		Yaffe et al. (2003)	Q	249, 250
	1.0		Yao et al. (2002)	Q	230
	1.4×10^{2}		English and Carroll (2001)	Q	231, 232
	2.1		Katritzky et al. (1998)	Q	
	1.3		Nirmalakhandan et al. (1997)	Q	

Table A4.2: Heterocycles with nitrogen (C, H, N) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.8×10^{-1}		Suzuki et al. (1992)	Q	233
	9.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	9.9×10^{-1}		Mackay et al. (2006d)	?	
		6300	Kühne et al. (2005)	?	
	9.9×10^{-1}		Yaws (1999)	?	21
	3.4×10^{-1}		Yaws and Yang (1992)	?	21
	9.9×10^{-1}		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	562
3-methylpyridine	1.2	6400	Brockbank (2013)	L	
$C_5H_4NCH_3$	4.2×10^{-1}		Chaintreau et al. (1995)	M	
(3-picoline; β-picoline)	1.3	6300	Andon et al. (1954)	M	338
[108-99-6]	1.1		Keshavarz et al. (2022)	Q	
ITQTTZVARXURQS-UHFFFAOYSA-N	8.0×10^{-2}		Duchowicz et al. (2020)	Q	300
	8.8×10^{-1}		Hilal et al. (2008)	Q	
	8.5×10^{-1}		Modarresi et al. (2007)	Q	68
		6400	Kühne et al. (2005)	Q	
	1.0		Yaffe et al. (2003)	Q	249, 273
	1.3		Yao et al. (2002)	Q	230, 268
	9.5×10^{-1}		English and Carroll (2001)	Q	231, 232
	2.3		Katritzky et al. (1998)	Q	
	1.3		Nirmalakhandan et al. (1997)	Q	
	8.8×10^{-1}		Suzuki et al. (1992)	Q	233
	1.3		Duchowicz et al. (2020)	?	186, 21
	1.3		Mackay et al. (2006d)	?	
		6300	Kühne et al. (2005)	?	
	1.4		Yaws (1999)	?	21
	5.4×10^{-1}		Yaws and Yang (1992)	?	21
	1.3		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	562
4-methylpyridine	1.6	6500	Brockbank (2013)	L	
$C_5H_4NCH_3$	1.7	6500	Andon et al. (1954)	M	338
[108-89-4]	1.1		Keshavarz et al. (2022)	Q	
FKNQCJSGGFJEIZ-UHFFFAOYSA-N	8.0×10^{-2}		Duchowicz et al. (2020)	Q	185
	1.6		Li et al. (2014)	Q	242
	9.0×10^{-1}		Hilal et al. (2008)	Q	
	8.6×10^{-1}		Modarresi et al. (2007)	Q	68
		6400	Kühne et al. (2005)	Q	
	1.2		Yaffe et al. (2003)	Q	249, 273
	1.2		Yao et al. (2002)	Q	230
	1.1		English and Carroll (2001)	Q	231, 232
	2.4		Katritzky et al. (1998)	Q	
	1.3		Nirmalakhandan et al. (1997)	Q	
	2.1		Russell et al. (1992)	Q	280
	8.8×10^{-1}		Suzuki et al. (1992)	Q	233
	1.6		Duchowicz et al. (2020)	?	186, 21
	1.7		Mackay et al. (2006d)	?	

Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		6500	Kühne et al. (2005)	?	
	1.7		Yaws (1999)	?	21, 12
	1.6		Abraham et al. (1990)	?	
	1.4		Arnett and Chawla (1979)	?	561
			Staudinger and Roberts (2001)	W	562
3-cyanopyridine	3.6×10^{1}		Abraham et al. (1994a)	R	
$C_6H_4N_2$	1.9×10^{1}		Keshavarz et al. (2022)	Q	
[100-54-9]	5.4		Duchowicz et al. (2020)	Q	
GZPHSAQLYPIAIN-UHFFFAOYSA-N	3.6×10^{1}		HSDB (2015)	Q	100
	1.6×10^{1}		Hilal et al. (2008)	Q	
	1.1×10^{1}		Modarresi et al. (2007)	Q	68
	6.9×10^{1}		English and Carroll (2001)	Q	231, 232
	1.2×10^{2}		Nirmalakhandan et al. (1997)	Q	
	3.6×10^{1}		Duchowicz et al. (2020)	?	186, 21
4-cyanopyridine	1.1×10^{1}		Abraham et al. (1994a)	R	
$C_6H_4N_2$	1.9×10^{1}		Keshavarz et al. (2022)	Q	
[100-48-1]	5.4		Duchowicz et al. (2020)	Q	
GPHQHTOMRSGBNZ-UHFFFAOYSA-N	1.7×10^{1}		Hilal et al. (2008)	Q	
	1.0×10^{1}		Modarresi et al. (2007)	Q	68
	1.2×10^{2}		Nirmalakhandan et al. (1997)	Q	
	1.1×10^{1}		Duchowicz et al. (2020)	?	186, 21
2-ethylpyrazine	4.0		Buttery et al. (1971)	M	
$C_4N_2H_3(C_2H_5)$	6.5		Keshavarz et al. (2022)	Q	
[13925-00-3]	7.3×10^{-1}		Duchowicz et al. (2020)	Q	185
KVFIJIWMDBAGDP-UHFFFAOYSA-N	2.7		Hilal et al. (2008)	Q	
	3.4		Modarresi et al. (2007)	Q	68
	2.7		Nirmalakhandan et al. (1997)	Q	
	4.0		Duchowicz et al. (2020)	?	186, 21
2,5-dimethylpyrazine	7.1		Marin et al. (1999)	M	
$C_6H_8N_2$	5.5		Druaux et al. (1998)	M	
[123-32-0]	5.5		Marin et al. (1999)	V	
LCZUOKDVTBMCMX-UHFFFAOYSA-N	6.4		Marin et al. (1999)	Q	
2,6-dimethylpyrazine $C_6H_8N_2$ (3,5-dimethylpyrazine) [108-50-9] HJFZAYHYIWGLNL-UHFFFAOYSA-N	9.8×10^{-1}		Chaintreau et al. (1995)	M	
N-ethylpiperidine	3.9×10^{-1}		Hilal et al. (2008)	Q	
$C_7H_{15}N$		6600	Kühne et al. (2005)	Q	
(1-ethylpiperidine)		6600	Kühne et al. (2005)	?	
[766-09-6]					
HTLZVHNRZJPSMI-UHFFFAOYSA-N					

Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1H-benzimidazole $C_7H_6N_2$ [51-17-2] HYZJCKYKOHLVJF-UHFFFAOYSA-N	2.7×10^{1}		HSDB (2015)	Q	100
2-ethenylpyridine C_7H_7N (2-vinylpyridine) [100-69-6] KGIGUEBEKRSTEW-UHFFFAOYSA-N	7.0×10^{-1} 2.8×10^{-1} 2.7		Duchowicz et al. (2020) Duchowicz et al. (2020) HSDB (2015)	V Q Q	187 100
4-ethenylpyridine C_7H_7N (4-vinylpyridine) [100-43-6] KFDVPJUYSDEJTH-UHFFFAOYSA-N	1.2 2.8×10^{-1} 3.1		Duchowicz et al. (2020) Duchowicz et al. (2020) HSDB (2015)	V Q Q	187 100
2-ethylpyridine $C_5H_4NC_2H_5$ [100-71-0] NRGGMCIBEHEAIL-UHFFFAOYSA-N	6.0×10^{-1} 1.5 8.2×10^{-2} 2.9×10^{-1} 6.5×10^{-1} 6.1×10^{-1} 2.4 1.1 1.4 6.0×10^{-1} 6.0×10^{-1}	6700 6700 7900 	Andon et al. (1954) Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Kühne et al. (2005) Yaffe et al. (2003) Katritzky et al. (1998) Nirmalakhandan et al. (1997) Suzuki et al. (1992) Duchowicz et al. (2020) Kühne et al. (2005) Abraham et al. (1990) Staudinger and Roberts (2001)	M Q Q Q Q Q Q Q Q Q ? ? ? W	338 300 68 249, 250 233 186, 21 562
3-ethylpyridine $C_5H_4NC_2H_5$ [536-78-7] MFEIKQPHQINPRI-UHFFFAOYSA-N	9.5×10^{-1} 1.5 8.2×10^{-2} 6.7×10^{-1} 6.0×10^{-1} 1.0 2.9 1.1 1.4 9.5×10^{-1} 9.5×10^{-1}	6400 6700 6200 	Andon et al. (1954) Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Kühne et al. (2005) English and Carroll (2001) Katritzky et al. (1998) Nirmalakhandan et al. (1997) Suzuki et al. (1992) Duchowicz et al. (2020) Kühne et al. (2005) Abraham et al. (1990) Staudinger and Roberts (2001)	M Q Q Q Q Q Q Q Q Q ? ? ? W	338 68 231, 232 233 186, 21 562

Table A4.2: Heterocycles with nitrogen (C, H, N) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-ethylpyridine	1.2	6300	Andon et al. (1954)	M	338
$C_5H_4NC_2H_5$	1.5		Keshavarz et al. (2022)	Q	
[536-75-4]	8.2×10^{-2}		Duchowicz et al. (2020)	Q	300
VJXRKZJMGVSXPX-UHFFFAOYSA-N	1.2		Li et al. (2014)	Q	242
	7.0×10^{-1}		Hilal et al. (2008)	Q	
	5.7×10^{-1}		Modarresi et al. (2007)	Q	68
		6700	Kühne et al. (2005)	Q	
	1.2		Yaffe et al. (2003)	Q	249, 250
	1.0		English and Carroll (2001)	Q	231, 261
	2.9		Katritzky et al. (1998)	Q	
	1.1		Nirmalakhandan et al. (1997)	Q	
	1.4		Suzuki et al. (1992)	Q	233
	1.2		Duchowicz et al. (2020)	?	186, 21
		6300	Kühne et al. (2005)	?	
	1.2		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	562
2,3-dimethylpyridine	1.4	6900	Andon et al. (1954)	M	338
$C_5H_3N(CH_3)_2$	1.5		Keshavarz et al. (2022)	Q	
(2,3-lutidine)	2.7×10^{-2}		Duchowicz et al. (2020)	Q	185
[583-61-9]	6.2×10^{-1}		Hilal et al. (2008)	Q	
HPYNZHMRTTWQTB-UHFFFAOYSA-N	2.1×10^{-1}		Modarresi et al. (2007)	Q	68
		6200	Kühne et al. (2005)	Q	
	1.2		Yaffe et al. (2003)	Q	249, 273
	1.6		English and Carroll (2001)	Q	231, 275
	3.0		Katritzky et al. (1998)	Q	
	9.5×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.3		Suzuki et al. (1992)	Q	233
	1.4		Duchowicz et al. (2020)	?	186, 21
	1.4		Mackay et al. (2006d)	?	
		5800	Kühne et al. (2005)	?	
	1.4		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	562
2,4-dimethylpyridine	9.9×10^{-1}		Hawthorne et al. (1985)	M	
$C_5H_3N(CH_3)_2$	1.5	7100	Andon et al. (1954)	M	338
(2,4-lutidine)	1.5		Keshavarz et al. (2022)	Q	
[108-47-4]	2.7×10^{-2}		Duchowicz et al. (2020)	Q	
JYYNAJVZFGKDEQ-UHFFFAOYSA-N	1.5		Li et al. (2014)	Q	242
	5.1×10^{-1}		Hilal et al. (2008)	Q	
	2.9×10^{-1}		Modarresi et al. (2007)	Q	68
		6700	Kühne et al. (2005)	Q	
	1.5		Yaffe et al. (2003)	Q	249, 273
	1.8		English and Carroll (2001)	Q	231, 232
	3.1		Katritzky et al. (1998)	Q	
	9.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.7		Russell et al. (1992)	Q	280
	1.3		Suzuki et al. (1992)	Q	233

Table A4.2: Heterocycles with nitrogen (C, H, N) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	1.5		Duchowicz et al. (2020)	?	186, 21
	1.5		Mackay et al. (2006d)	?	
		6400	Kühne et al. (2005)	?	
	1.5		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	562
2,5-dimethylpyridine	1.1	7000	Andon et al. (1954)	M	338
$C_5H_3N(CH_3)_2$	1.5		Keshavarz et al. (2022)	Q	
(2,5-lutidine)	2.7×10^{-2}		Duchowicz et al. (2020)	Q	300
[589-93-5]	5.7×10^{-1}		Hilal et al. (2008)	Q	
XWKFPIODWVPXLX-UHFFFAOYSA-N	2.1×10^{-1}		Modarresi et al. (2007)	Q	68
		6700	Kühne et al. (2005)	Q	
	1.2		Yaffe et al. (2003)	Q	249, 250
	1.6		English and Carroll (2001)	Q	231, 232
	2.9		Katritzky et al. (1998)	Q	
	9.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.3		Suzuki et al. (1992)	Q	233
	1.2		Meylan and Howard (1991)	Q	
	1.1		Duchowicz et al. (2020)	?	186, 21
		6900	Kühne et al. (2005)	?	
	1.1		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	562
2,6-dimethylpyridine	9.2×10^{-1}	7300	Brockbank (2013)	L	
$C_5H_3N(CH_3)_2$	6.6×10^{-1}		Hawthorne et al. (1985)	M	
(2,6-lutidine)	9.5×10^{-1}	7300	Andon et al. (1954)	M	338
[108-48-5]	1.5		Keshavarz et al. (2022)	Q	
OISVCGZHLKNMSJ-UHFFFAOYSA-N	2.7×10^{-2}		Duchowicz et al. (2020)	Q	300
	4.5×10^{-1}		Hilal et al. (2008)	Q	
	6.8×10^{-1}		Modarresi et al. (2007)	Q	68
		6700	Kühne et al. (2005)	Q	
	1.6		English and Carroll (2001)	Q	231, 232
	2.4		Katritzky et al. (1998)	Q	
	9.5×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.3		Suzuki et al. (1992)	Q	233
	9.5×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	9.4×10^{-1}		Mackay et al. (2006d)	?	
		6600	Kühne et al. (2005)	?	
	9.5×10^{-1}		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	562
3,4-dimethylpyridine	2.7	6800	Andon et al. (1954)	M	338
$C_5H_3N(CH_3)_2$	1.5		Keshavarz et al. (2022)	Q	
(3,4-lutidine)	2.7×10^{-2}		Duchowicz et al. (2020)	Q	300
[583-58-4]	1.3		Hilal et al. (2008)	Q	
NURQLCJSMXZBPC-UHFFFAOYSA-N	3.8×10^{-1}		Modarresi et al. (2007)	Q	68
		6200	Kühne et al. (2005)	Q	
	2.7		Yaffe et al. (2003)	Q	249, 250

Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.4		English and Carroll (2001)	Q	231, 261
	2.8		Katritzky et al. (1998)	Q	
	9.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.3		Suzuki et al. (1992)	Q	233
	2.7		Duchowicz et al. (2020)	?	186, 21
		6400	Kühne et al. (2005)	?	
	2.7		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	562
3,5-dimethylpyridine	1.4	6800	Andon et al. (1954)	M	338
$C_5H_3N(CH_3)_2$	1.5		Keshavarz et al. (2022)	Q	
(3,5-lutidine)	2.7×10^{-2}		Duchowicz et al. (2020)	Q	185
[591-22-0]	9.7×10^{-1}		Hilal et al. (2008)	Q	
HWWYDZCSSYKIAD-UHFFFAOYSA-N	5.9×10^{-1}		Modarresi et al. (2007)	Q	68
		6700	Kühne et al. (2005)	Q	
	1.5		Yaffe et al. (2003)	Q	249, 250
	1.2		English and Carroll (2001)	Q	231, 232
	3.3		Katritzky et al. (1998)	Q	
	9.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.3		Suzuki et al. (1992)	Q	233
	1.4		Duchowicz et al. (2020)	?	186, 21
		6500	Kühne et al. (2005)	?	
	1.4		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	562
5-ethyl-2-methylpyridine	5.2×10^{-1}		Duchowicz et al. (2020)	V	187
$C_8H_{11}N$	5.2×10^{-1}		HSDB (2015)	V	
[104-90-5]	2.7×10^{-2}		Duchowicz et al. (2020)	Q	
NTSLROIKFLNUIJ-UHFFFAOYSA-N	8.6×10^{-1}		Zhang et al. (2010)	Q	288, 289
	3.8×10^{-1}		Zhang et al. (2010)	Q	288, 290
	7.0×10^{-1}		Zhang et al. (2010)	Q	288, 291
	6.2×10^{-2}		Zhang et al. (2010)	Q	288, 292
	4.4×10^{-1}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Modarresi et al. (2007)	Q	68
2,4,6-trimethylpyridine	1.1		Duchowicz et al. (2020)	V	187
$C_5H_2N(CH_3)_3$	1.1		HSDB (2015)	V	
(2,4,6-collidine)	5.7×10^{-2}		Mackay et al. (2006d)	V	
[108-75-8]	5.7×10^{-2}		Mackay et al. (1995)	V	
BWZVCCNYKMEVEX-UHFFFAOYSA-N	1.1		Hilal et al. (2008)	C	
	8.9×10^{-3}		Duchowicz et al. (2020)	Q	
	5.4×10^{-1}		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	68
		7100	Kühne et al. (2005)	Q	
	2.5		Katritzky et al. (1998)	Q	
		8600	Kühne et al. (2005)	?	

Table A4.2: Heterocycles with nitrogen (C, H, N) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
indole	1.9×10^{1}		Duchowicz et al. (2020)	V	187
C_8H_7N	1.9×10^{1}		HSDB (2015)	V	
[120-72-9]	7.1		Mackay et al. (2006d)	V	
SIKJAQJRHWYJAI-UHFFFAOYSA-N	7.1		Mackay et al. (1995)	V	
	1.6×10^{1}		Yaws (2003)	X	259
	1.6×10^{1}		Yaws (2003)	X	238, 12
	1.5×10^{1}		Howard and Meylan (1997)	X	448
	5.3		Dupeux et al. (2022)	Q	260
	1.6×10^{1}		Duchowicz et al. (2020)	Q	
	7.0×10^{1}		Gharagheizi et al. (2012)	Q	
	1.7×10^{1}		Gharagheizi et al. (2010)	Q	247
	9.0		Hilal et al. (2008)	Q	
	9.9		Yaws (1999)	?	21, 12
2-ethyl-3,5-dimethylpyrazine	2.9	8500	Wieland et al. (2015)	M	563
$C_8H_{12}N_2$					
[13925-07-0]					
JZBCTZLGKSYRSF-UHFFFAOYSA-N					
2-isobutylpyrazine	2.0		Buttery et al. (1971)	M	
$C_4N_2H_3C_4H_9$	1.2×10^{1}		Keshavarz et al. (2022)	Q	
[29460-92-2]	1.4		Nirmalakhandan et al. (1997)	Q	
YAIMUUJMEBJXAA-UHFFFAOYSA-N					
2-(1-methylpropyl)-pyrazine	1.6		Hilal et al. (2008)	Q	
$C_8H_{12}N_2$	2.2		Modarresi et al. (2007)	Q	68
[29460-93-3]					
NFFQZEXYZVZKNN-UHFFFAOYSA-N					
5-ethenyl-2-methylpyridine	2.2		HSDB (2015)	Q	100
C_8H_9N					
[140-76-1]					
VJOWMORERYNYON-UHFFFAOYSA-N					
4-(1,1-dimethylethyl)-pyridine	3.9×10^{-1}		Hilal et al. (2008)	Q	
$C_9H_{13}N$	7.5×10^{-1}		Abraham et al. (1990)	?	
(4-*tert*-butylpyridine)	7.5×10^{-1}	7000	Arnett and Chawla (1979)	?	561
[3978-81-2]					
YSHMQTRICHYLGF-UHFFFAOYSA-N					
nornicotine	7.2×10^{3}		HSDB (2015)	Q	449
$C_9H_{12}N_2$					
[494-97-3]					
MYKUKUCHPMASKF-UHFFFAOYSA-N					
2,4-diamino-6-phenyl-1,3,5-triazine	2.4×10^{5}		HSDB (2015)	Q	100
$C_9H_9N_5$					
[91-76-9]					
GZVHEAJQGPRDLQ-UHFFFAOYSA-N					

Table A4.2: Heterocycles with nitrogen (C, H, N) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-methylindole C_9H_9N [603-76-9] BLRHMMGNCXNXJL-UHFFFAOYSA-N	8.7		Ebert et al. (2023)	?	367
3-methylindole C_9H_9N (skatole) [83-34-1] ZFRKQXVRDFCRJG-UHFFFAOYSA-N	2.9×10^{-5} 4.7	-2500	Wetlaufer et al. (1964) HSDB (2015)	M V	
2,3-diethyl-5-methylpyrazine $C_9H_{14}N_2$ [18138-04-0] PSINWXIDJYEXLO-UHFFFAOYSA-N	8.1×10^{-1}		Roberts and Pollien (1997)	M	
benzo[*b*]pyridine C_9H_7N (quinoline) [91-22-5] SMWDFEZZVXVKRB-UHFFFAOYSA-N	5.9 5.8 3.8×10^{1} 3.8×10^{1} 6.0 3.9×10^{1} 6.4 3.7×10^{1} 9.3×10^{-1} 5.7×10^{1} 6.4 5.8 6.1 9.0 3.2×10^{-1} 3.4×10^{1} 1.4×10^{1} 6.5	 5400 7300 7300 	Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Mackay et al. (1995) Meylan and Howard (1991) Smith and Bomberger (1980) Abraham et al. (1994a) Goldstein (1982) Duchowicz et al. (2020) Gharagheizi et al. (2012) Hilal et al. (2008) Modarresi et al. (2007) Kühne et al. (2005) Yaffe et al. (2003) English and Carroll (2001) Katritzky et al. (1998) Nirmalakhandan et al. (1997) Meylan and Howard (1991) Kühne et al. (2005) Yaws (1999)	V V V V V V R X Q Q Q Q Q Q Q Q Q ? ?	187 24 299 68 249, 250 231, 232 21, 12
benzo[*c*]pyridine C_9H_7N (isoquinoline) [119-65-3] AWJUIBRHMBBTKR-UHFFFAOYSA-N	5.2×10^{-2} 5.2×10^{-2} 5.7 5.6 9.2 3.8		Mackay et al. (2006d) Mackay et al. (1995) Yaws (2003) Gharagheizi et al. (2010) Hilal et al. (2008) Yaws (1999)	V V X Q Q ?	 238, 12 247 21, 12
nicotine $C_{10}H_{14}N_2$ [54-11-5] SNICXCGAKADSCV-SNVBAGLBSA-N	3.3×10^{3}		HSDB (2015)	Q	100

Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2'-bipyridine $C_{10}H_8N_2$ [366-18-7] ROFVEXUMMXZLPA-UHFFFAOYSA-N	1.8×10^{4}		HSDB (2015)	Q	547
4,4'-bipyridine $C_{10}H_8N_2$ [553-26-4] MWVTWFVJZLCBMC-UHFFFAOYSA-N	3.9×10^{3} 1.7×10^{1}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
2-methylquinoline $C_{10}H_9N$ [91-63-4] SMUQFGGVLNAIOZ-UHFFFAOYSA-N	1.4×10^{1}		Ebert et al. (2023)	?	317
4-methylquinoline $C_{10}H_9N$ [491-35-0] MUDSDYNRBDKLGK-UHFFFAOYSA-N	1.3×10^{1}		HSDB (2015)	Q	100
MEIQX $C_{11}H_{11}N_5$ (2-amino-3,8-dimethylimidazo[4,5-f]quinoxaline) [77500-04-0] DVCCCQNKIYNAKB-UHFFFAOYSA-N	6.2×10^{7}		HSDB (2015)	Q	100
3-(phenylazo)-2,6-pyridinediamine $C_{11}H_{11}N_5$ (phenazopyridine) [94-78-0] QPFYXYFORQJZEC-UHFFFAOYSA-N	3.0×10^{9}		HSDB (2015)	Q	100
2-amino-9H-pyrido[2,3-b]indole $C_{11}H_9N_3$ [26148-68-5] FJTNLJLPLJDTRM-UHFFFAOYSA-N	2.5×10^{8}		HSDB (2015)	Q	100
carbazole $C_{12}H_9N$ [86-74-8] UJOBWOGCFQCDNV-UHFFFAOYSA-N	9.4×10^{1} 9.3×10^{1} 6.6×10^{-2} 6.6×10^{-2} 6.3×10^{-2} 2.0×10^{1} 6.3×10^{1} 1.1×10^{2} 8.5×10^{1}	4300 4300	Brockbank (2013) Odabasi et al. (2006) Mackay et al. (2006d) Mackay et al. (1995) Smith and Bomberger (1980) Keshavarz et al. (2022) Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	L M V V V Q Q Q ?	 24 100 186, 21

Table A4.2: Heterocycles with nitrogen (C, H, N) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
o-phenanthroline	1.1×10^{5}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_8N_2$	9.9×10^{3}		Zhang et al. (2010)	Q	288, 290
[66-71-7]	1.2×10^{5}		Zhang et al. (2010)	Q	288, 291
DGEZNRSVGBDHLK-UHFFFAOYSA-N	4.4×10^{2}		Zhang et al. (2010)	Q	288, 292
benzyladenine	1.1×10^{8}		HSDB (2015)	V	
$C_{12}H_{11}N_5$	1.1×10^{-1}		Maniere et al. (2011)	?	242, 166
[1214-39-7]					
NWBJYWHLCVSVIJ-UHFFFAOYSA-N					
diquat	2.8×10^{5}		Ebert et al. (2023)	?	319
$C_{12}H_{12}N_2$					
[2764-72-9]					
SYJFEGQWDCRVNX-UHFFFAOYSA-N					
MEIQ	2.5×10^{7}		HSDB (2015)	Q	100
$C_{12}H_{12}N_4$					
(2-amino-3,4-dimethylimidazo[4,5-f]quinoxaline)					
[77094-11-2]					
GMGWMIJIGUYNAY-UHFFFAOYSA-N					
pyrimethanil	3.4×10^{2}	15000	Feigenbrugel and Le Calvé (2021)	M	
$C_{12}H_{13}N_3$	2.8×10^{2}		Duchowicz et al. (2020)	V	187
[53112-28-0]	2.8×10^{2}		Tomlin (1998)	X	564, 12
ZLIBICFPKPWGIZ-UHFFFAOYSA-N	9.2×10^{2}		Duchowicz et al. (2020)	Q	
	3.9		HSDB (2015)	Q	100
	2.8×10^{2}		Maniere et al. (2011)	?	242, 166
paraquat	$>2.4\times10^{8}$		HSDB (2015)	V	
$C_{12}H_{14}N_2$					
[4685-14-7]					
INFDPOAKFNIJBF-UHFFFAOYSA-N					
N,N-dimethyltryptamine	1.5×10^{4}		HSDB (2015)	Q	100
$C_{12}H_{16}N_2$					
[61-50-7]					
DMULVCHRPCFFGV-UHFFFAOYSA-N					
benzo[*f*]quinoline	5.7×10^{1}		Duchowicz et al. (2020)	V	187
$C_{13}H_9N$			Mackay et al. (2006d)	V	560
[85-02-9]	1.0×10^{2}		Mackay et al. (1995)	V	
HCAUQPZEWLULFJ-UHFFFAOYSA-N	1.0×10^{2}		Smith and Bomberger (1980)	V	24
	3.6		Duchowicz et al. (2020)	Q	

Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,6-bis-(1,1-dimethylethyl)-pyridine	8.0×10^{-4}	6900	Arnett and Chawla (1979)	M	561
$C_{13}H_{21}N$	2.8×10^{-1}		Arnett and Chawla (1979)	V	565
(2,6-di-*tert*-butylpyridine)					
[585-48-8]					
UWKQJZCTQGMHKD-UHFFFAOYSA-N					
PHIP	3.5×10^{7}		HSDB (2015)	Q	100
$C_{13}H_{12}N_4$					
(2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine)					
[105650-23-5]					
UQVKZNNCIHJZLS-UHFFFAOYSA-N					
N,N'-diphenylguanidine	1.4×10^{6}		HSDB (2015)	Q	100
$C_{13}H_{13}N_3$					
[102-06-7]					
OWRCNXZUPFZXOS-UHFFFAOYSA-N					
acridine	3.3×10^{1}		Mackay et al. (2006d)	V	
$C_{13}H_9N$	3.3×10^{1}		Mackay et al. (1995)	V	
[260-94-6]	2.5×10^{1}		HSDB (2015)	Q	100
DZBUGLKDJFMEHC-UHFFFAOYSA-N					
phenanthridine	6.0×10^{2}		Duchowicz et al. (2020)	V	187
$C_{13}H_9N$	3.6		Duchowicz et al. (2020)	Q	
[229-87-8]					
RDOWQLZANAYVLL-UHFFFAOYSA-N					
mepanipyrim	6.0×10^{2}		Maniere et al. (2011)	?	242, 166
$C_{14}H_{13}N_3$					
[110235-47-7]					
CIFWZNRJIBNXRE-UHFFFAOYSA-N					
cyprodinil	1.2×10^{2}		Duchowicz et al. (2020)	V	187
$C_{14}H_{15}N_3$	1.2×10^{2}		HSDB (2015)	V	
[121552-61-2]	2.9×10^{3}		Duchowicz et al. (2020)	Q	
HAORKNGNJCEJBX-UHFFFAOYSA-N					
imiquimod	1.2×10^{7}		HSDB (2015)	Q	100
$C_{14}H_{16}N_4$					
[99011-02-6]					
DOUYETYNHWVLEO-UHFFFAOYSA-N					
ametoctradin	2.4×10^{6}		Maniere et al. (2011)	?	12, 166
$C_{15}H_{25}N_5$					
[865318-97-4]					
GGKQIOFASHYUJZ-UHFFFAOYSA-N					

Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ferimzone $C_{15}H_{18}N_4$ [89269-64-7] GOWLARCWZRESHU-UHFFFAOYSA-N	1.6×10^{5} 2.4×10^{2}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
benz[*c*]acridine $C_{17}H_{11}N$ [225-51-4] OAPPEBNXKAKQGS-UHFFFAOYSA-N	3.7×10^{2}		HSDB (2015)	Q	449
6-pentyl-1,2,3,4,7,8,9,10-octahydrophenanthridine $C_{18}H_{27}N$ [10594-03-3] FNUATPIDZQSFPD-UHFFFAOYSA-N	4.5×10^{-1} 2.0×10^{1} 6.2 2.2×10^{-2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
2-diphenylmethylpiperidine $C_{18}H_{21}N$ (desoxypipradrol) [519-74-4] RWTNXJXZVGHMGI-UHFFFAOYSA-N	6.6×10^{1}		HSDB (2015)	Q	100
fenpropidin $C_{19}H_{31}N$ [67306-00-7] MGNFYQILYYYUBS-UHFFFAOYSA-N	7.1×10^{2} 1.1×10^{2} 9.9×10^{-2} 9.5×10^{-2} 9.3×10^{-2}	6200	Feigenbrugel and Le Calvé (2021) Duchowicz et al. (2020) Tomlin (1998) Duchowicz et al. (2020) Maniere et al. (2011)	M V X Q ?	33 187 564, 12 166
N,N-bis(2-ethylhexyl)-1H-1,2,4-triazole-1-methanamine $C_{19}H_{38}N_4$ [91273-04-0] AVBBHCMDRGQBNW-UHFFFAOYSA-N	2.9×10^{1}		Ebert et al. (2023)	?	367
7H-dibenzo[*c*, *g*]carbazole $C_{20}H_{13}N$ [194-59-2] STJXCDGCXVZHDU-UHFFFAOYSA-N	2.1×10^{3} 4.0×10^{3}		Smith and Bomberger (1980) HSDB (2015)	V Q	24 100
porphyrin $C_{20}H_{14}N_4$ (porphin) [101-60-0] RKCAIXNGYQCCAL-YYOYBPFYSA-N	3.9×10^{5}		Abraham et al. (2019)	Q	
dibenz[*a*, *j*]acridine $C_{21}H_{13}N$ [224-42-0] ANUCHZVCBDOPOX-UHFFFAOYSA-N	5.2×10^{3}		HSDB (2015)	Q	100

Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dibenz[a, h]acridine $C_{21}H_{13}N$ [226-36-8] JNCSIWAONQTVCF-UHFFFAOYSA-N	5.2×10^{3}		HSDB (2015)	Q	100
1,3,5-tricyclohexylhexahydro-1,3,5-triazine	1.7×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{21}H_{39}N_3$	4.0×10^{5}		Zhang et al. (2010)	Q	288, 290
[6281-14-7]	1.2×10^{5}		Zhang et al. (2010)	Q	288, 291
ZLLRUEJANKJPQE-UHFFFAOYSA-N	1.5×10^{4}		Zhang et al. (2010)	Q	288, 292

A4.3 Nitriles (C, H, N)

Table A4.3: Nitriles (C, H, N)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyano radical CN [2074-87-5] JEVCWSUVFOYBFI-UHFFFAOYSA-N	7.8×10^{-4}	1400	Berdnikov and Bazhin (1970)	T	48
hydrogen cyanide	8.9×10^{-2}	8200	Burkholder et al. (2019)	L	
HCN	8.9×10^{-2}	8200	Burkholder et al. (2015)	L	
(hydrocyanic acid)	1.7×10^{-1}	4400	Yoo et al. (1986)	L	1
[74-90-8]	1.1×10^{-1}	5000	Edwards et al. (1978)	L	1
LELOWRISYMNNSU-UHFFFAOYSA-N	8.9×10^{-2}	8200	Ma et al. (2010a)	M	
	7.5×10^{-2}		Riveros et al. (1998)	M	12
	1.2×10^{-1}		Fredenhagen and Wellmann (1932b)	M	
	9.2×10^{-2}		Hine and Weimar (1965)	R	
	9.9×10^{-2}	4200	Edwards et al. (1975)	T	1
	7.6×10^{-2}	2900	Kotlik and Lebedeva (1974)	X	566
	7.4×10^{-2}		Gaffney and Senum (1984)	X	391, 493
	5.0×10^{-2}		Keshavarz et al. (2022)	Q	
	4.2×10^{-2}		Duchowicz et al. (2020)	Q	185
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Modarresi et al. (2007)	Q	68
	4.7		Katritzky et al. (1998)	Q	
	7.4×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	1.1×10^{-1}		Yaws (1999)	?	21
ethanenitrile	5.2×10^{-1}	4000	Burkholder et al. (2019)	L	
CH_3CN	5.2×10^{-1}	4000	Burkholder et al. (2015)	L	
(acetonitrile)	4.9×10^{-1}	4300	Brockbank (2013)	L	1
[75-05-8]	5.2×10^{-1}	4000	Sander et al. (2011)	L	
WEVYAHXRMPXWCK-UHFFFAOYSA-N	5.2×10^{-1}	4000	Sander et al. (2006)	L	
	3.8×10^{-1}	4200	Plyasunov et al. (2006)	L	
	5.0×10^{-1}	4100	Fogg and Sangster (2003)	L	
	5.1×10^{-1}	4000	Staudinger and Roberts (2001)	L	
	4.7×10^{-1}	3500	Arijs and Brasseur (1986)	L	
	6.0×10^{-1}	6300	Hiatt (2013)	M	
	5.2×10^{-1}	4000	Ji and Evans (2007)	M	
	4.9×10^{-1}		Bebahani et al. (2002)	M	
	3.2×10^{-1}	3300	Hovorka et al. (2002)	M	11
	3.4×10^{-1}		Welke et al. (1998)	M	
	5.3×10^{-1}	4100	Benkelberg et al. (1995)	M	
	4.6×10^{-1}		Li and Carr (1993)	M	
	8.2×10^{-2}		Yu (1992)	M	12
	4.8×10^{-1}	3900	Snider and Dawson (1985)	M	
	5.3×10^{-1}	4100	Hamm et al. (1984)	M	
	3.7×10^{-2}		Abraham and Acree (2007)	V	
	5.0×10^{-1}		Hwang et al. (1992)	V	

Table A4.3: Nitriles (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.9×10^{-1}		Hine and Weimar (1965)	R	
	2.9×10^{-1}		Gaffney and Senum (1984)	X	391
	4.7×10^{-1}		Hayer et al. (2022)	Q	20
	3.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	
	2.9×10^{-1}		Li et al. (2014)	Q	242
	7.7×10^{-1}		Hilal et al. (2008)	Q	
	3.7×10^{-1}		Modarresi et al. (2007)	Q	68
		4200	Kühne et al. (2005)	Q	
	2.9×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.9×10^{-1}		English and Carroll (2001)	Q	231, 232
	4.4		Katritzky et al. (1998)	Q	
	2.9×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	3.1×10^{-1}		Suzuki et al. (1992)	Q	233
	2.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	3.6×10^{-1}		Mackay et al. (2006d)	?	
		4300	Kühne et al. (2005)	?	
	4.9×10^{-1}		Yaws (1999)	?	21
	4.9×10^{-1}		Yaws and Yang (1992)	?	21
	2.9×10^{-1}		Abraham et al. (1990)	?	
propanenitrile	3.4×10^{-1}	4500	Brockbank (2013)	L	1
C_2H_5CN	2.4×10^{-1}	4800	Plyasunov et al. (2006)	L	
(propionitrile)	4.3×10^{-1}	6200	Hiatt (2013)	M	
[107-12-0]	3.3×10^{-1}	4600	Ji and Evans (2007)	M	
FVSKHRXBFJPNKK-UHFFFAOYSA-N	1.8×10^{-1}		Hovorka et al. (2002)	M	38
	2.5×10^{-1}		Li and Carr (1993)	M	
	1.9×10^{-1}		Hawthorne et al. (1985)	M	
	2.6×10^{-1}		Butler and Ramchandani (1935)	M	
	3.1×10^{-1}		Mackay et al. (2006d)	V	
	3.1×10^{-1}		Mackay et al. (1995)	V	
	1.7×10^{-1}		Howard (1990)	X	414
	3.5×10^{-1}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	
	5.0×10^{-1}		Hilal et al. (2008)	Q	
	2.6×10^{-1}		Modarresi et al. (2007)	Q	68
	2.9×10^{-1}		English and Carroll (2001)	Q	231, 232
	5.6×10^{-1}		Russell et al. (1992)	Q	280
	2.4×10^{-1}		Suzuki et al. (1992)	Q	233
	2.7×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	2.6×10^{-1}		Mackay et al. (2006d)	?	
	2.9×10^{-1}		Yaws (1999)	?	21
	2.7×10^{-1}		Abraham et al. (1990)	?	

Table A4.3: Nitriles (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
butanenitrile	1.8×10^{-1}	5100	Brockbank (2013)	L	1
C_3H_7CN	1.8×10^{-1}	5100	Plyasunov et al. (2006)	L	
(butyronitrile)	2.7×10^{-1}	5100	Ji and Evans (2007)	M	
[109-74-0]	1.3×10^{-1}		Ramachandran et al. (1996)	M	
KVNRLNFWIYMESJ-UHFFFAOYSA-N	1.9×10^{-1}		Li and Carr (1993)	M	
	1.4×10^{-1}		Hawthorne et al. (1985)	M	
	1.9×10^{-1}		Butler and Ramchandani (1935)	M	
	1.8×10^{-1}		Yaws (2003)	X	259
	1.8×10^{-1}		Yaws (2003)	X	238
	3.7×10^{-1}		Dupeux et al. (2022)	Q	260
	1.2×10^{-1}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.8×10^{-1}		Gharagheizi et al. (2010)	Q	247
	3.5×10^{-1}		Hilal et al. (2008)	Q	
	1.5×10^{-1}		Modarresi et al. (2007)	Q	68
		4900	Kühne et al. (2005)	Q	
	1.5×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	5.7×10^{-2}		English and Carroll (2001)	Q	231, 275
	1.9×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	5.4×10^{-1}		Russell et al. (1992)	Q	280
	1.9×10^{-1}		Suzuki et al. (1992)	Q	233
	1.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	1.9×10^{-1}		Mackay et al. (2006d)	?	
		4700	Kühne et al. (2005)	?	
	1.8×10^{-1}		Yaws (1999)	?	21
	1.9×10^{-1}		Abraham et al. (1990)	?	
2-methylpropanenitrile	1.1×10^{-1}	5200	Brockbank (2013)	L	
C_4H_7N	1.0×10^{-1}	4800	Plyasunov et al. (2006)	L	
(isobutyronitrile)	9.4×10^{-2}		Li and Carr (1993)	M	
[78-82-0]	1.8×10^{-1}		HSDB (2015)	Q	100
LRDFRRGEGBBSRN-UHFFFAOYSA-N	1.9×10^{-1}		Hilal et al. (2008)	Q	
		4900	Kühne et al. (2005)	Q	
		5100	Kühne et al. (2005)	?	
pentanenitrile	1.6×10^{-1}	6100	Brockbank (2013)	L	
C_4H_9CN	1.4×10^{-1}	5500	Plyasunov et al. (2006)	L	
(butyl cyanide; valeronitrile)	1.4×10^{-1}		Li and Carr (1993)	M	
[110-59-8]	1.6×10^{-1}		Amoore and Buttery (1978)	V	
RFFFKMOABOFIDF-UHFFFAOYSA-N	2.7×10^{-1}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	68
	1.5×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	4.1×10^{-2}		English and Carroll (2001)	Q	231, 232
	1.5×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	1.5×10^{-1}		Abraham et al. (1990)	?	

Table A4.3: Nitriles (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexanenitrile $C_6H_{11}N$ [628-73-9] AILKHAQXUAOOFU-UHFFFAOYSA-N	1.2×10^{-1} 2.3×10^{-1}		Plyasunov et al. (2006) Hilal et al. (2008)	L Q	
heptanenitrile $C_7H_{13}N$ [629-08-3] SDAXRHHPNYTELL-UHFFFAOYSA-N	1.6×10^{-1}		Hilal et al. (2008)	Q	
octanenitrile $C_8H_{15}N$ [124-12-9] YSIMAPNUZAVQER-UHFFFAOYSA-N	5.7×10^{-2} 1.3×10^{-1}		Plyasunov et al. (2006) Hilal et al. (2008)	L Q	
nonanenitrile $C_9H_{17}N$ [2243-27-8] PLZZPPHAMDJOSR-UHFFFAOYSA-N	1.0×10^{-1}		Hilal et al. (2008)	Q	
decanenitrile $C_{10}H_{19}N$ [1975-78-6] HBZDPWBWBJMYRY-UHFFFAOYSA-N	8.0×10^{-2}		Hilal et al. (2008)	Q	
undecanenitrile $C_{11}H_{21}N$ [2244-07-7] SZKKNEOUHLFYNA-UHFFFAOYSA-N	6.1×10^{-2}		Hilal et al. (2008)	Q	
cyclohexanecarbonitrile $C_7H_{11}N$ [766-05-2] VBWIZSYFQSOUFQ-UHFFFAOYSA-N	7.3×10^{-1}		Hilal et al. (2008)	Q	
ethanedinitrile C_2N_2 (cyanogen) [460-19-5] JMANVNJQNLATNU-UHFFFAOYSA-N	1.8×10^{-3} 1.8×10^{-3} 1.9×10^{-3} 1.9×10^{1} 1.8×10^{-3} 2.6×10^{-3} 2.9×10^{-2} 1.9×10^{-3} 1.8×10^{-3}		Duchowicz et al. (2020) HSDB (2015) Yaws (2003) Duchowicz et al. (2020) Gharagheizi et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Yaws (1999) Yaws and Yang (1992)	V V X Q Q Q Q ? ?	187 238, 12 247 68 21, 12 21, 12
pentanedinitrile $C_5H_6N_2$ [544-13-8] ZTOMUSMDRMJOTH-UHFFFAOYSA-N	7.8×10^{2}	7600	Plyasunov et al. (2006)	L	

Table A4.3: Nitriles (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexanedinitrile	1.5×10^{3}	8000	Plyasunov et al. (2006)	L	
$C_6H_8N_2$	8.2×10^{3}		Duchowicz et al. (2020)	V	187
(adiponitrile)	8.2×10^{3}		HSDB (2015)	V	
[111-69-3]	2.4×10^{2}		Mackay et al. (2006d)	V	
BTGRAWJCKBQKAO-UHFFFAOYSA-N	2.4×10^{2}		Mackay et al. (1995)	V	
	2.3×10^{1}		Duchowicz et al. (2020)	Q	
	2.2×10^{3}		Hilal et al. (2008)	Q	
2-methylpentanedinitrile	3.3×10^{2}		HSDB (2015)	Q	100
$C_6H_8N_2$					
[4553-62-2]					
FPPLREPCQJZDAQ-UHFFFAOYSA-N					
tetramethylbutanedinitrile	1.9×10^{2}		HSDB (2015)	Q	100
$C_8H_{12}N_2$					
[3333-52-6]					
ZVQXQPNJHRNGID-UHFFFAOYSA-N					
2-propenenitrile	1.0×10^{-1}	3900	Brockbank (2013)	L	
C_3H_3N	1.2×10^{-1}	6800	Hiatt (2013)	M	
(acrylonitrile)	7.6×10^{-2}		Hovorka et al. (2002)	M	38
[107-13-1]	3.1×10^{-2}		Welke et al. (1998)	M	
NLHHRLWOUZZQLW-UHFFFAOYSA-N	1.3×10^{-1}		Mackay et al. (2006d)	V	
	8.2×10^{-2}	3400	Fogg and Sangster (2003)	V	
	9.1×10^{-2}		Lide and Frederikse (1995)	V	
	1.3×10^{-1}		Mackay et al. (1995)	V	
	9.8×10^{-2}		Hwang et al. (1992)	V	
	1.1×10^{-1}	2800	Goldstein (1982)	X	299
	1.1×10^{-1}		Mackay et al. (1995)	C	
	1.1×10^{-1}		Ryan et al. (1988)	C	
	9.2×10^{-2}		Keshavarz et al. (2022)	Q	
	4.3×10^{-1}		Duchowicz et al. (2020)	Q	185
	2.2×10^{-2}		Hilal et al. (2008)	Q	
	4.6×10^{-1}		Modarresi et al. (2007)	Q	68
		3600	Kühne et al. (2005)	Q	
	7.2×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	9.0×10^{-2}		Mackay et al. (2006d)	?	
		3600	Kühne et al. (2005)	?	
	1.0×10^{-1}		Yaws (1999)	?	21, 12
2-butenenitrile	8.8×10^{-2}		Duchowicz et al. (2020)	V	187
C_4H_5N	1.5×10^{-1}		Duchowicz et al. (2020)	Q	
(crotononitrile)	2.7×10^{-1}		Modarresi et al. (2007)	Q	68
[4786-20-3]					
NKKMVIVFRUYPLQ-NSCUHMNNSA-N					

Table A4.3: Nitriles (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-butenenitrile C_4H_5N (vinylacetonitrile) [109-75-1] SJNALLRHIVGIBI-UHFFFAOYSA-N	2.0×10^{-1}	4900	Brockbank (2013)	L	
2-methyl-2-propene nitrile	3.6×10^{-2}	4200	Brockbank (2013)	L	1
C_4H_5N	5.4×10^{-2}	6700	Hiatt (2013)	M	
(methacrylonitrile)	4.0×10^{-2}		Duchowicz et al. (2020)	V	187
[126-98-7]	4.0×10^{-2}		HSDB (2015)	V	
GYCMBHHDWRMZGG-UHFFFAOYSA-N	1.2×10^{-1}		Duchowicz et al. (2020)	Q	
	1.7×10^{-2}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Modarresi et al. (2007)	Q	68
		4000	Kühne et al. (2005)	Q	
		4600	Kühne et al. (2005)	?	
benzenenitrile	3.5×10^{-1}	5600	Brockbank (2013)	L	1
C_6H_5CN	2.9×10^{-1}	5100	Lee et al. (2013)	M	
(benzonitrile)	1.9×10^{-1}		Duchowicz et al. (2020)	V	187
[100-47-0]	1.9×10^{-1}		HSDB (2015)	V	
JFDZBHWFFUWGJE-UHFFFAOYSA-N	1.9×10^{-1}		Mackay et al. (2006d)	V	
	3.9×10^{-1}		Schüürmann (2000)	V	
	1.9×10^{-1}		Mackay et al. (1995)	V	
	1.9×10^{-1}		Mackay et al. (1995)	V	
	5.0×10^{-1}		Abraham et al. (1994a)	R	
	2.3×10^{-1}		Duchowicz et al. (2020)	Q	
	1.3×10^{-1}		Li et al. (2014)	Q	242
	2.4×10^{-1}		Hilal et al. (2008)	Q	
	6.7×10^{-1}		Modarresi et al. (2007)	Q	68
		5900	Kühne et al. (2005)	Q	
	5.2×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.3		Katritzky et al. (1998)	Q	
	1.5×10^{-1}		Nirmalakhandan et al. (1997)	Q	
		6400	Kühne et al. (2005)	?	
	9.6×10^{-1}		Yaws (1999)	?	21, 417
	1.8×10^{-2}		Yaws and Yang (1992)	?	21, 417
	4.1×10^{-1}		Abraham et al. (1990)	?	
2-pyridinecarbonitrile $C_6H_4N_2$ [100-70-9] FFNVQNRYTPFDDP-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	100
3,3'-iminobispropanenitrile $C_6H_9N_3$ [111-94-4] SBAJRGRUGUQKAF-UHFFFAOYSA-N	2.0×10^{6}		HSDB (2015)	Q	100

Table A4.3: Nitriles (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methylbenzonitrile C_8H_7N (*o*-tolunitrile) [529-19-1] NWPNXBQSRGKSJB-UHFFFAOYSA-N	7.6×10^{-1}		Schüürmann (2000)	V	
3-methylbenzonitrile	1.7×10^{-1}		Zhang et al. (2010)	Q	288, 289
C_8H_7N	3.4×10^{-1}		Zhang et al. (2010)	Q	288, 290
(*m*-tolunitrile)	8.8×10^{-1}		Zhang et al. (2010)	Q	288, 291
[620-22-4]	1.8×10^{-1}		Zhang et al. (2010)	Q	288, 292
BOHCMQZJWOGWTA-UHFFFAOYSA-N					
benzeneacetonitrile	1.1	6800	Brockbank (2013)	L	
C_8H_7N	7.0×10^{-2}		HSDB (2015)	V	
(phenylacetonitrile)	1.0×10^{1}		Hilal et al. (2008)	Q	
[140-29-4]		6200	Kühne et al. (2005)	Q	
SUSQOBVLVYHIEX-UHFFFAOYSA-N		5100	Kühne et al. (2005)	?	
1,2-benzenedicarbonitrile $C_8H_4N_2$ [91-15-6] XQZYPMVTSDWCCE-UHFFFAOYSA-N	2.0×10^{1}		HSDB (2015)	Q	100
3,7-dimethyl-2,6-octadienenitrile $C_{10}H_{15}N$ (geranyl nitrile) [5146-66-7] HLCSDJLATUNSSI-JXMROGBWSA-N	2.9×10^{-2}		Helburn et al. (2008)	M	
2,2'-azobis(2-methylbutyronitrile)	4.5×10^{4}		Zhang et al. (2010)	Q	288, 289
$C_{10}H_{16}N_4$	9.2×10^{1}		Zhang et al. (2010)	Q	288, 290
[13472-08-7]	1.5×10^{1}		Zhang et al. (2010)	Q	288, 291
AVTLBBWTUPQRAY-UHFFFAOYSA-N	4.4×10^{-1}		Zhang et al. (2010)	Q	288, 292

A4.4 Amines, amides, amino acids (C, H, O, N)

Table A4.4: Amines, amides, amino acids (C, H, O, N)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
formamide CH_3NO [75-12-7] ZHNUHDYFZUAESO-UHFFFAOYSA-N	7.1×10^3 7.0×10^3 2.3×10^2		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
methyl nitrite CH_3ONO [624-91-9] BLLFVUPNHCTMSV-UHFFFAOYSA-N	1.5×10^{-1}		HSDB (2015)	Q	100
urea CH_4N_2O [57-13-6] XSQUKJJJFZCRTK-UHFFFAOYSA-N	5.7×10^6 5.7×10^6 1.0×10^7 1.0×10^7 1.1×10^5		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Mackay et al. (1995) Duchowicz et al. (2020)	V V V V Q	187
ethanolamine $HOC_2H_4NH_2$ [141-43-5] HZAXFHJVJLSVMW-UHFFFAOYSA-N	4.2×10^3 6.0×10^4 1.1×10^4 9.7×10^2	8300 5800	Kim et al. (2008) Bone et al. (1983) Modarresi et al. (2007) Nguyen (2013)	M M Q ?	552 12 68 567, 11
1,1'-azodiformamide $C_2H_4N_4O_2$ [123-77-3] XOZUGNYVDXMRKW-UHFFFAOYSA-N	1.2×10^7		HSDB (2015)	V	
ethyl nitrite C_2H_5ONO [109-95-5] QQZWEECEMNQSTG-UHFFFAOYSA-N	1.1×10^{-1}		HSDB (2015)	Q	100
carbamic acid, methyl ester $C_2H_5NO_2$ [598-55-0] GTCAXTIRRLKXRU-UHFFFAOYSA-N	2.5×10^2		HSDB (2015)	Q	100
acetaldoxime C_2H_5NO (acetaldehyde oxime) [107-29-9] FZENGILVLUJGJX-UHFFFAOYSA-N	1.7		HSDB (2015)	Q	449

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethanamide	5.3×10^3		Wolfenden (1976)	M	
C_2H_5NO	2.8×10^3		Mackay et al. (2006d)	V	
(acetamide)	2.8×10^3		Mackay et al. (1995)	V	
[60-35-5]	3.8×10^3		Yaws (2003)	X	238
DLFVBJFMPXGRIB-UHFFFAOYSA-N	9.0×10^2		HSDB (2015)	Q	100
	2.8×10^3		Gharagheizi et al. (2012)	Q	
	3.7×10^3		Gharagheizi et al. (2010)	Q	247
	4.2×10^3		Hilal et al. (2008)	Q	
	5.1×10^3		Modarresi et al. (2007)	Q	68
	2.2×10^3		Yaffe et al. (2003)	Q	249, 250
	2.2×10^2		Katritzky et al. (1998)	Q	
N-methylmethanamide	1.4×10^3	7200	Burkholder et al. (2019)	L	
C_2H_5NO	1.4×10^3	7200	Burkholder et al. (2015)	L	
(N-methylformamide)	1.4×10^3	7200	Brockbank (2013)	L	
[123-39-7]	1.5×10^3	7600	Bernauer and Dohnal (2008)	M	1
ATHHXGZTWNVVOU-UHFFFAOYSA-N	5.0×10^2		Duchowicz et al. (2020)	V	187
	4.9×10^2		HSDB (2015)	V	
	9.7×10^1		Duchowicz et al. (2020)	Q	
	5.6×10^2		Hilal et al. (2008)	Q	
	1.6×10^2		Modarresi et al. (2007)	Q	68
N-nitrosodimethylamine	3.9		Burkholder et al. (2019)	L	
$C_2H_6N_2O$	3.9		Burkholder et al. (2015)	L	
[62-75-9]	2.9×10^{-1}	13000	Thompson et al. (2018)	M	
UMFJAHHVKNCGLG-UHFFFAOYSA-N	4.1		Haruta et al. (2011)	M	12
	6.1	6400	Klein (1982)	M	
	5.2		Mirvish et al. (1976)	M	14
	3.0×10^{-1}		Mackay et al. (1995)	C	
	9.5		Hilal et al. (2008)	Q	
	3.6		Modarresi et al. (2007)	Q	68
	3.0×10^{-1}		Mackay et al. (2006d)	?	
methylnitrosourea $C_2H_5N_3O_2$ [684-93-5] ZRKWMRDKSOPRRS-UHFFFAOYSA-N	$>1.9\times10^2$		Mirvish et al. (1976)	M	14
ethanediamide	5.0×10^5		Duchowicz et al. (2020)	V	187
$C_2H_4N_2O_2$	2.2×10^6		Duchowicz et al. (2020)	Q	
[471-46-5] YIKSCQDJHCMVMK-UHFFFAOYSA-N					
nitrosoazetidine $C_3H_6N_2O$ [15216-10-1] SNKTZBNDUVWOAZ-UHFFFAOYSA-N	$>1.9\times10^2$		Mirvish et al. (1976)	M	14

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methylnitrosoacetamide $C_3H_6N_2O_2$ [7417-67-6] FFLFWNRFMZRFKU-UHFFFAOYSA-N	8.6×10^{-2}		Mirvish et al. (1976)	M	14
ethylnitrosocyanamide $C_3H_5N_3O$ [38434-77-4] LMIMSGCBKHFTDY-UHFFFAOYSA-N	2.6×10^{-1}		Mirvish et al. (1976)	M	14
2-propenamide	5.8×10^{3}		Duchowicz et al. (2020)	V	187
C_3H_5NO	5.5×10^{3}		HSDB (2015)	V	
(acrylamide)	6.9×10^{3}		Mackay et al. (2006d)	V	
[79-06-1]	3.1×10^{4}		Lide and Frederikse (1995)	V	
HRPVXLWXLXDGHG-UHFFFAOYSA-N	6.9×10^{3}		Mackay et al. (1995)	V	
	2.9×10^{4}		Yaws (2003)	X	238, 38
	4.1×10^{2}		Duchowicz et al. (2020)	Q	
	7.3×10^{2}		Gharagheizi et al. (2012)	Q	
	2.9×10^{4}		Gharagheizi et al. (2010)	Q	247
	4.1×10^{3}		Hilal et al. (2008)	Q	
	7.3×10^{3}		Modarresi et al. (2007)	Q	68
		8400	Kühne et al. (2005)	Q	
		7900	Kühne et al. (2005)	?	
methylvinylnitrosamine $C_3H_6N_2O$ (N-nitrosomethylvinylamine) [4549-40-0] AWZVYNHQGTZJIH-UHFFFAOYSA-N	2.7		HSDB (2015)	Q	100
urethane	1.5×10^{2}		Duchowicz et al. (2020)	V	187
$C_3H_7NO_2$	1.5×10^{2}		HSDB (2015)	V	
[51-79-6]	2.5×10^{1}		Duchowicz et al. (2020)	Q	
JOYRKODLDBILNP-UHFFFAOYSA-N	1.1×10^{1}		Hilal et al. (2008)	Q	
	6.4×10^{1}		Modarresi et al. (2007)	Q	68
	7.3×10^{1}		Katritzky et al. (1998)	Q	
propanamide C_3H_7NO (propionamide) [79-05-0] QLNJFJADRCOGBJ-UHFFFAOYSA-N	3.3×10^{3}	8800	Plyasunov et al. (2001)	T	

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N,N-dimethylmethanamide	1.3×10^2	6600	Burkholder et al. (2019)	L	
C_3H_7NO	1.3×10^2	6600	Burkholder et al. (2015)	L	
(N,N-dimethylformamide)	1.4×10^2	7700	Brockbank (2013)	L	1, 568
[68-12-2]	1.6×10^2	7500	Bernauer and Dohnal (2008)	M	1
ZMXDDKWLCZADIW-UHFFFAOYSA-N	2.2×10^2		Abraham et al. (1994a)	R	
	4.5×10^1		Hilal et al. (2008)	Q	
	5.8		Modarresi et al. (2007)	Q	68
	2.6×10^1		Katritzky et al. (1998)	Q	
	2.2×10^2		Nirmalakhandan et al. (1997)	Q	
	1.6×10^2		Taft et al. (1985)	Q	
N-methylacetamide	2.1×10^3	7600	Burkholder et al. (2019)	L	
C_3H_7NO	2.1×10^3	7600	Burkholder et al. (2015)	L	
[79-16-3]	3.2×10^3	8900	Bernauer and Dohnal (2008)	M	1
OHLUUHNLEMFGTQ-UHFFFAOYSA-N	2.3×10^2		Duchowicz et al. (2020)	V	187
	2.3×10^2		HSDB (2015)	V	
	3.8×10^1		Duchowicz et al. (2020)	Q	
	1.4×10^2		Modarresi et al. (2007)	Q	68
N-methyl-N-nitrosoethanamine $C_3H_8N_2O$ (N-nitrosomethylethylamine) [10595-95-6] RTDCJKARQCRONF-UHFFFAOYSA-N	6.9		HSDB (2015)	Q	449
2-methoxyethanamine C_3H_9NO (2-methoxyethylamine) [109-85-3] ASUDFOJKTJLAIK-UHFFFAOYSA-N	2.5×10^1	7600	Cabani et al. (1978)	T	
2-(methylamino)ethanol C_3H_9NO [109-83-1] OPKOKAMJFNKNAS-UHFFFAOYSA-N	9.0×10^1		HSDB (2015)	V	
1-amino-2-propanol C_3H_9NO [78-96-6] HXKKHQJGJAFBHI-UHFFFAOYSA-N	4.2×10^4		HSDB (2015)	Q	547
2-amino-1-propanol C_3H_9NO (alaninol) [6168-72-5] BKMMTJMQCTUHRP-UHFFFAOYSA-N	1.3×10^3	7700	Nguyen (2013)	M	11

Table A4.4: Amines, amides, amino acids (C, H, O, N) (... continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-nitroso-N-methylurethane	3.9×10^{-1}		Mirvish et al. (1976)	M	14
$C_4H_8N_2O_3$	1.8		Duchowicz et al. (2020)	V	187
(N-nitroso-N-methylurethane)	1.8		HSDB (2015)	V	
[615-53-2]	1.6×10^{1}		Duchowicz et al. (2020)	Q	
CAUBWLYZCDDYEF-UHFFFAOYSA-N	3.2×10^{1}		Modarresi et al. (2007)	Q	68
dinitrosopiperazine	$>1.9\times10^{2}$		Mirvish et al. (1976)	M	14
$C_4H_8N_4O_2$					
[140-79-4]					
WNSYEWGYAFFSSQ-UHFFFAOYSA-N					
2-amino-3(methylamino)propionic acid	2.9×10^{7}		HSDB (2015)	Q	100
$C_4H_{10}N_2O_2$					
(3-(methylamino)-(DL)-alanine)					
[16676-91-8]					
UJVHVMNGOZXSOZ-UHFFFAOYSA-N					
N-nitrosodiethanolamine	2.0×10^{6}		HSDB (2015)	Q	449
$C_4H_{10}N_2O_3$					
[1116-54-7]					
YFCDLVPYFMHRQZ-UHFFFAOYSA-N					
N-nitrosodiethylamine	1.2×10^{-2}	3800	Thompson et al. (2018)	M	
$C_4H_{10}N_2O$	5.6	6300	Klein (1982)	M	
[55-18-5]	1.4		Mirvish et al. (1976)	M	14
WBNQDOYYEUMPFS-UHFFFAOYSA-N	7.1×10^{-1}		Keshavarz et al. (2022)	Q	
	7.5		Duchowicz et al. (2020)	Q	185
	3.9		Hilal et al. (2008)	Q	
	2.6		Modarresi et al. (2007)	Q	68
	2.7		Duchowicz et al. (2020)	?	186, 21
diethanolamine	3.3×10^{3}	1300	Nguyen (2013)	M	11
$C_4H_{11}NO_2$	2.6×10^{5}		Duchowicz et al. (2020)	V	187
[111-42-2]	2.5×10^{5}		HSDB (2015)	V	
ZBCBWPMODOFKDW-UHFFFAOYSA-N	1.0×10^{4}		Duchowicz et al. (2020)	Q	
diglycolamine	6.1×10^{3}	3700	Nguyen (2013)	M	33, 11
$C_4H_{11}NO_2$					
[929-06-6]					
GIAFURWZWWWBQT-UHFFFAOYSA-N					
3-methoxy-1-propanamine	2.1×10^{1}		Du et al. (2017)	M	480
$C_4H_{11}NO$	4.8×10^{1}	8700	Cabani et al. (1978)	T	
(3-methoxypropylamine)	4.9×10^{1}		Du et al. (2017)	Q	551
[5332-73-0]	1.4×10^{1}		Du et al. (2017)	Q	
FAXDZWQIWUSWJH-UHFFFAOYSA-N					

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-amino-2-methyl-1-propanol $C_4H_{11}NO$ [124-68-5] CBTVGIZVANVGBH-UHFFFAOYSA-N	2.1×10^{2} 7.0×10^{2} 1.8×10^{2} 9.3×10^{1}	 8500 	Du et al. (2017) Nguyen (2013) Du et al. (2017) Du et al. (2017)	M M Q Q	480 11 551
N,N-dimethylaminoethanol $C_4H_{11}NO$ (dimethylethanolamine) [108-01-0] UEEJHVSXFDXPFK-UHFFFAOYSA-N	9.3×10^{1} 2.6×10^{1} 4.4×10^{2}	7900 	Nguyen (2013) Duchowicz et al. (2020) Duchowicz et al. (2020)	M V Q	11 187
2-[(2-aminoethyl)amino]ethanol $C_4H_{12}N_2O$ [111-41-1] LHIJANUOQQMGNT-UHFFFAOYSA-N	9.0×10^{7}		HSDB (2015)	Q	100
tetramethylammonium hydroxide $C_4H_{13}NO$ [75-59-2] WGTYBPLFGIVFAS-UHFFFAOYSA-M	2.3×10^{10}		HSDB (2015)	Q	100
methacrylamide C_4H_7NO [79-39-0] FQPSGWSUVKBHSU-UHFFFAOYSA-N	8.8×10^{3}		Ebert et al. (2023)	?	317
acetone cyanohydrin C_4H_7NO [75-86-5] MWFMGBPGAXYFAR-UHFFFAOYSA-N	8.0×10^{1}		HSDB (2015)	V	
carbamic acid, 1-methylethyl ester $C_4H_9NO_2$ [1746-77-6] OVPLZYJGTGDFNB-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	100
propylcarbamate $C_4H_9NO_2$ [627-12-3] YNTOKMNHRPSGFU-UHFFFAOYSA-N	1.0×10^{2}		HSDB (2015)	V	
butanamide C_4H_9NO [541-35-5] DNSISZSEWVHGLH-UHFFFAOYSA-N	3.6×10^{3}		Ebert et al. (2023)	?	317

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N,N-dimethylacetamide	6.1×10^{1}	7800	Burkholder et al. (2019)	L	
C_4H_9NO	6.1×10^{1}	7800	Burkholder et al. (2015)	L	
[127-19-5]	4.4×10^{2}	8000	Brockbank (2013)	L	
FXHOOIRPVKKKFG-UHFFFAOYSA-N	4.4×10^{2}	8600	Bernauer and Dohnal (2008)	M	1
	1.7×10^{2}		Hilal et al. (2008)	Q	
	1.3×10^{1}		Modarresi et al. (2007)	Q	68
	3.6×10^{2}		Taft et al. (1985)	Q	
2-butanone, oxime	8.1		HSDB (2015)	V	
C_4H_9NO					
[96-29-7]					
WHIVNJATOVLWBW-UHFFFAOYSA-N					
nitrosoethylurethane	5.2×10^{2}		HSDB (2015)	Q	100
$C_5H_{10}N_2O_3$					
(N-ethyl-N-nitrosourethane)					
[614-95-9]					
RAUQLNDTFONODT-UHFFFAOYSA-N					
N,N-diethylmethanamide	1.3×10^{2}		Yaffe et al. (2003)	Q	249, 250
$C_5H_{11}NO$					
(N,N-diethylformamide)					
[617-84-5]					
SUAKHGWARZSWIH-UHFFFAOYSA-N					
N-nitroso-N-butylurea	4.3×10^{4}		HSDB (2015)	Q	100
$C_5H_{11}N_3O_2$					
[869-01-2]					
LSWOCDLIYSKTRX-UHFFFAOYSA-N					
N-methyldiethanolamine	3.3×10^{3}		Du et al. (2017)	M	480
$C_5H_{13}NO_2$	3.9×10^{3}	3800	Nguyen (2013)	M	11
[105-59-9]	4.0×10^{5}	12000	Kim et al. (2008)	M	552
CRVGTESFCCXCTH-UHFFFAOYSA-N	3.1×10^{5}		Duchowicz et al. (2020)	V	187
	3.2×10^{5}		HSDB (2015)	V	
	1.3×10^{5}		Duchowicz et al. (2020)	Q	
	2.4×10^{3}		Du et al. (2017)	Q	551
	1.9×10^{3}		Du et al. (2017)	Q	
methylbutylnitrosamine	1.7		Mirvish et al. (1976)	M	14
$C_5H_{12}N_2O$					
[7068-83-9]					
PKTSCJXWLVREKX-UHFFFAOYSA-N					
2-(isopropylamino)ethanol	1.1×10^{2}		Du et al. (2017)	M	480
$C_5H_{13}NO$	1.4×10^{1}		Du et al. (2017)	Q	551
[109-56-8]	5.4×10^{1}		Du et al. (2017)	Q	
RILLZYSZSDGYGV-UHFFFAOYSA-N					

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-(dimethylamino)-1,2-propanediol	6.7×10^2		Du et al. (2017)	M	480
$C_5H_{13}NO_2$	6.1×10^3		Du et al. (2017)	Q	551
[623-57-4]	6.4×10^2		Du et al. (2017)	Q	
QCMHUGYTOGXZIW-UHFFFAOYSA-N					
2-amino-2-ethyl-1,3-propanediol	7.1×10^2		Du et al. (2017)	M	480
$C_5H_{13}NO_2$	4.0×10^4		Du et al. (2017)	Q	551
[115-70-8]	2.7×10^3		Du et al. (2017)	Q	
IOAOAKDONABGPZ-UHFFFAOYSA-N					
daminozide	2.3×10^4		Duchowicz et al. (2020)	V	187
$C_6H_{11}NO_3$	4.1×10^3		Duchowicz et al. (2020)	Q	
[1596-84-5]	7.0×10^1		Maniere et al. (2011)	?	166
NOQGZXFMHARMLW-UHFFFAOYSA-N					
methylpentylnitrosamine	2.0		Mirvish et al. (1976)	M	14
$C_6H_{14}N_2O$					
[13256-07-0]					
KSFCDINBDBFFSI-UHFFFAOYSA-N					
ethylbutylnitrosamine	9.9×10^{-1}		Mirvish et al. (1976)	M	14
$C_6H_{14}N_2O$					
[4549-44-4]					
ZGMCNGHHUQZNIH-UHFFFAOYSA-N					
nitrosohexamethyleneimine	4.3×10^1		Mirvish et al. (1976)	M	14
$C_6H_{12}N_2O$					
[932-83-2]					
UZMVSVHUTOAPTD-UHFFFAOYSA-N					
2,6-dimethylnitrosomorpholine	3.5×10^1		Mirvish et al. (1976)	M	14
$C_6H_{12}N_2O_2$					
[1456-28-6]					
DPYMAXOKJUBANR-UHFFFAOYSA-N					
2,6-dimethyldinitrosopiperazine	$>1.9\times10^2$		Mirvish et al. (1976)	M	14
$C_6H_{12}N_4O_2$					
[55380-34-2]					
JIWAGFGPBKDFQN-UHFFFAOYSA-N					
N-(1-methylethyl)-2-propenamide	4.3×10^2		HSDB (2015)	Q	100
$C_6H_{11}NO$					
(N-isopropylacrylamide)					
[2210-25-5]					
QNILTEGFHQSKFF-UHFFFAOYSA-N					
hexanamide	1.8×10^3		Ebert et al. (2023)	?	317
$C_6H_{13}NO$					
[628-02-4]					
ALBYIUDWACNRRB-UHFFFAOYSA-N					

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-butylacetamide $C_6H_{13}NO$ [1119-49-9] GYLDXXLJMRTVSS-UHFFFAOYSA-N	2.7×10^{3} 5.2×10^{2}		Gibbs et al. (1991) Hilal et al. (2008)	M Q	
N-(1-methylethyl)-N-nitroso-2-propanamine $C_6H_{14}N_2O$ (nitrosodiisopropylamine) [601-77-4] AUIKJTGFPFLMFP-UHFFFAOYSA-N	1.2 3.4×10^{-1} 1.1		Mirvish et al. (1976) Hilal et al. (2008) Modarresi et al. (2007)	M Q Q	14 68
N-nitrosodipropylamine $C_6H_{14}N_2O$ (N,N-dipropylnitrosamine) [621-64-7] YLKFDHTUAUWZPQ-UHFFFAOYSA-N	1.8 2.8 2.8 1.6 5.8 1.3		Mirvish et al. (1976) Mackay et al. (2006d) Mackay et al. (1995) Mackay et al. (1995) Hilal et al. (2008) Modarresi et al. (2007)	M V V C Q Q	14 68
N-(2-hydroxyethyl)piperazine $C_6H_{14}N_2O$ [103-76-4] WFCSWCVEJLETKA-UHFFFAOYSA-N	2.9×10^{3}	6400	Nguyen (2013)	M	33, 11
N-ethyldiethanolamine $C_6H_{15}NO_2$ [139-87-7] AKNUHUCEWALCOI-UHFFFAOYSA-N	9.0×10^{4}		HSDB (2015)	Q	100
triethanolamine $C_6H_{15}NO_3$ [102-71-6] GSEJCLTVZPLZKY-UHFFFAOYSA-N	1.4×10^{7} 1.4×10^{7} 3.3×10^{7}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
o-aminophenol C_6H_7NO (2-aminophenol) [95-55-6] CDAWCLOXVUBKRW-UHFFFAOYSA-N	4.9×10^{4}		HSDB (2015)	Q	100
4-aminophenol C_6H_7NO [123-30-8] PLIKAWJENQZMHA-UHFFFAOYSA-N	2.7×10^{4} 2.7×10^{4} 1.8×10^{4}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
3-aminophenol C_6H_7NO [591-27-5] CWLKGDAVCFYWJK-UHFFFAOYSA-N	3.7×10^{4}		HSDB (2015)	Q	100

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-(2-hydroxyethyl)morpholine	1.4×10^{3}		Du et al. (2017)	M	480
$C_6H_{13}NO_2$	6.0×10^{1}		Du et al. (2017)	Q	551
[622-40-2]	1.7×10^{3}		Du et al. (2017)	Q	
KKFDCBRMNNSAAW-UHFFFAOYSA-N					
4-hydroxy-N-methylpiperidine	1.3×10^{3}		Du et al. (2017)	M	480
$C_6H_{13}NO$	4.6×10^{3}		Du et al. (2017)	Q	551
[106-52-5]	1.1×10^{3}		Du et al. (2017)	Q	
BAUWRHPMUVYFOD-UHFFFAOYSA-N					
dimethylaminoethoxyethanol	8.3×10^{2}		Du et al. (2017)	M	480
$C_6H_{15}NO_2$	4.3×10^{3}	8500	Nguyen (2013)	M	11
[1704-62-7]	5.6×10^{2}		Du et al. (2017)	Q	551
YSAANLSYLSUVHB-UHFFFAOYSA-N	6.2×10^{2}		Du et al. (2017)	Q	
2-(diethylamino)ethanol	5.9		Du et al. (2017)	M	480
$C_6H_{15}NO$	3.2		Du et al. (2017)	Q	551
[100-37-8]	1.8×10^{1}		Du et al. (2017)	Q	
BFSVOASYOCHEOV-UHFFFAOYSA-N					
bis(2-methoxyethyl)amine	1.1×10^{2}		Du et al. (2017)	M	480
$C_6H_{15}NO_2$	2.3×10^{2}		Du et al. (2017)	Q	551
[111-95-5]	1.5×10^{2}		Du et al. (2017)	Q	
IBZKBSXREAQDTO-UHFFFAOYSA-N					
cyclohexanone oxime	4.3×10^{1}		Duchowicz et al. (2020)	V	187
$C_6H_{11}NO$	1.4×10^{1}		Duchowicz et al. (2020)	Q	
[100-64-1]					
VEZUQRBDRNJBJY-UHFFFAOYSA-N					
p-diaminoanisole	2.5×10^{5}		HSDB (2015)	Q	100
$C_7H_{10}N_2O$					
(2-methoxy-1,4-benzenediamine)					
[5307-02-8]					
HGUYBLVGLMAUFF-UHFFFAOYSA-N					
4-methoxy-1,3-benzenediamine	1.4×10^{4}		HSDB (2015)	Q	100
$C_7H_{10}N_2O$					
[615-05-4]					
BAHPQISAXRFLCL-UHFFFAOYSA-N					

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-cyano-N-[(ethylamino)carbonyl]-2-(methoxyimino)acetamide	3.0×10^{4}		Duchowicz et al. (2020)	V	187
$C_7H_{10}N_4O_3$	3.0×10^{4}		HSDB (2015)	V	
(cymoxanil)	6.2×10^{2}		Barcelo and Hennion (1997)	X	569
[57966-95-7]	9.9×10^{8}		Duchowicz et al. (2020)	Q	
XERJKGMBORTKEO-UHFFFAOYSA-N	3.2×10^{1}		Goodarzi et al. (2010)	Q	570, 571
	2.6×10^{4}		Maniere et al. (2011)	?	242, 495, 166
	3.0×10^{4}		Maniere et al. (2011)	?	242, 572, 166
isocyanatocyclohexane	5.8×10^{-3}		HSDB (2015)	Q	100
$C_7H_{11}NO$					
[3173-53-3]					
KQWGXHWJMSMDJJ-UHFFFAOYSA-N					
L-theanine	1.1×10^{10}		HSDB (2015)	Q	449
$C_7H_{14}N_2O_3$					
[3081-61-6]					
DATAGRPVKZEWHA-YFKPBYRVSA-N					
tetryl	3.7×10^{3}		HSDB (2015)	Q	100
$C_7H_5N_5O_8$					
[479-45-8]					
AGUIVNYEYSCPNI-UHFFFAOYSA-N					
anthranilic acid	2.6×10^{5}		HSDB (2015)	Q	100
$C_7H_7NO_2$					
[118-92-3]					
RWZYAGGXGHYGMB-UHFFFAOYSA-N					
3-aminobenzoic acid	3.7×10^{6}		Ebert et al. (2023)	?	317
$C_7H_7NO_2$					
[99-05-8]					
XFDUHJPVQKIXHO-UHFFFAOYSA-N					
4-aminobenzoic acid	6.6×10^{4}		HSDB (2015)	V	
$C_7H_7NO_2$					
[150-13-0]					
ALYNCZNDIQEVRV-UHFFFAOYSA-N					
salicylamide	2.0×10^{4}		Abraham et al. (2019)	Q	
$C_7H_7NO_2$	3.4×10^{4}		HSDB (2015)	Q	100
[65-45-2]					
SKZKKFZAGNVIMN-UHFFFAOYSA-N					

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
mesalamine $C_7H_7NO_3$ [89-57-6] KBOPZPXVLCULAV-UHFFFAOYSA-N	2.0×10^{6}		HSDB (2015)	Q	100
N-phenylformamide C_7H_7NO [103-70-8] DYDNPESBYVVLBO-UHFFFAOYSA-N	1.2×10^{3}		HSDB (2015)	Q	100
benzamide			Mackay et al. (2006d)	V	560
C_7H_7NO	2.2×10^{4}		Mackay et al. (1995)	V	
[55-21-0]	4.7×10^{4}		Abraham et al. (1994a)	R	
KXDAEFPNCMNJSK-UHFFFAOYSA-N	5.2×10^{3}		Keshavarz et al. (2022)	Q	
	9.0×10^{2}		Duchowicz et al. (2020)	Q	300
	3.8×10^{3}		Hilal et al. (2008)	Q	
	2.7×10^{4}		Modarresi et al. (2007)	Q	68
	8.2×10^{3}		Nirmalakhandan et al. (1997)	Q	
	4.0×10^{4}		Duchowicz et al. (2020)	?	186, 21
	4.0×10^{4}		HSDB (2015)	?	421
anthranilamide $C_7H_8N_2O$ (2-aminobenzamide) [88-68-6] PXBFMLJZNCDSMP-UHFFFAOYSA-N	1.3×10^{7}		HSDB (2015)	Q	100
N-methyl-N-nitrosobenzenamine $C_7H_8N_2O$ [614-00-6] MAXCWSIJKVASQC-UHFFFAOYSA-N	2.0		HSDB (2015)	Q	100
2-methoxy-benzenamine	1.1×10^{1}		Duchowicz et al. (2020)	V	187
C_7H_9NO	1.2×10^{1}		Abraham et al. (1994a)	R	
(2-methoxyaniline)	6.7×10^{1}		Duchowicz et al. (2020)	Q	
[90-04-0]	1.1×10^{1}		HSDB (2015)	Q	100
VMPITZXILSNTON-UHFFFAOYSA-N	2.8×10^{1}		Hilal et al. (2008)	Q	
	5.6		Modarresi et al. (2007)	Q	68
	1.5×10^{1}		Nirmalakhandan et al. (1997)	Q	
3-methoxy-benzenamine	9.0×10^{1}		Abraham et al. (1994a)	R	
C_7H_9NO	9.0×10^{1}		HSDB (2015)	Q	100
(3-methoxyaniline)	1.8×10^{2}		Hilal et al. (2008)	Q	
[536-90-3]	2.8×10^{1}		Modarresi et al. (2007)	Q	68
NCBZRJODKRCREW-UHFFFAOYSA-N	6.4×10^{1}		English and Carroll (2001)	Q	231, 232
	1.5×10^{1}		Nirmalakhandan et al. (1997)	Q	

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methoxy-benzenamine	1.5×10^{2}		Altschuh et al. (1999)	M	
C_7H_9NO	1.2×10^{2}		Abraham et al. (1994a)	R	
(4-methoxyaniline)	1.8×10^{2}		Keshavarz et al. (2022)	Q	
[104-94-9]	5.8×10^{1}		Duchowicz et al. (2020)	Q	
BHAAPTBBJKJZER-UHFFFAOYSA-N	1.4×10^{2}		Hilal et al. (2008)	Q	
	2.8×10^{1}		Modarresi et al. (2007)	Q	68
	9.9×10^{1}		English and Carroll (2001)	Q	231, 232
	1.5×10^{1}		Nirmalakhandan et al. (1997)	Q	
	1.5×10^{2}		Duchowicz et al. (2020)	?	186, 21
4-(methylamino)phenol	2.2×10^{4}		HSDB (2015)	Q	100
C_7H_9NO					
(N-methyl-4-aminophenol)					
[150-75-4]					
ZFIQGRISGKSVAG-UHFFFAOYSA-N					
3-(diethylamino)-1,2-propanediol	5.4×10^{2}		Du et al. (2017)	M	480
$C_7H_{17}NO_2$	7.0×10^{2}		Du et al. (2017)	Q	551
[621-56-7]	2.6×10^{2}		Du et al. (2017)	Q	
LTACQVCHVAUOKN-UHFFFAOYSA-N					
1-(2-hydroxyethyl)piperidine	5.1×10^{1}		Du et al. (2017)	M	480
$C_7H_{15}NO$	6.1×10^{-1}		Du et al. (2017)	Q	551
(2-piperidinoethanol)	4.9×10^{1}		Du et al. (2017)	Q	
[3040-44-6]					
KZTWONRVIPPDKH-UHFFFAOYSA-N					
2-piperidineethanol	3.9×10^{2}		Du et al. (2017)	M	480
$C_7H_{15}NO$	1.2×10^{2}		Du et al. (2017)	Q	551
[1484-84-0]	2.3×10^{2}		Du et al. (2017)	Q	
PTHDBHDZSMGHKF-UHFFFAOYSA-N					
emylcamate	3.0×10^{-1}		Duchowicz et al. (2020)	V	187
$C_7H_{15}NO_2$	8.7		Duchowicz et al. (2020)	Q	
[78-28-4]					
SLWGJZPKHAXZQL-UHFFFAOYSA-N					
defenuron	8.5×10^{5}		MacBean (2012a)	?	12
$C_8H_{10}N_2O$					
[1007-36-9]					
SQBHGDSDVWCPHN-UHFFFAOYSA-N					
N-methyl-N-nitrosobenzenemethanamine	7.9×10^{-1}		Mirvish et al. (1976)	M	14
$C_8H_{10}N_2O$	1.2×10^{2}		Hilal et al. (2008)	Q	
[937-40-6]	3.8×10^{1}		Modarresi et al. (2007)	Q	68
NGXUJKBJBFLCAR-UHFFFAOYSA-N					

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
norepinephrine $C_8H_{11}NO_3$ [51-41-2] SFLSHLFXELFNJZ-QMMMGPOBSA-N	3.1×10^{13}		HSDB (2015)	Q	100
2,4-dimethoxyaniline $C_8H_{11}NO_2$ [2735-04-8] GEQNZVKIDIPGCO-UHFFFAOYSA-N	1.6×10^{1}		Ebert et al. (2023)	?	319
4-methoxy-2-methylbenzenamine $C_8H_{11}NO$ (*m*-cresidine) [102-50-1] CDGNLUSBENXDGG-UHFFFAOYSA-N	8.2×10^{1}		HSDB (2015)	Q	100
p-cresidine $C_8H_{11}NO$ [120-71-8] WXWCDTXEKCVRRO-UHFFFAOYSA-N	8.0×10^{1}		HSDB (2015)	Q	100
N-nitrosodi-N-butylamine $C_8H_{18}N_2O$ [924-16-3] YGJHZCLPZAZIHH-UHFFFAOYSA-N	7.2×10^{-1} 7.5×10^{-1} 1.1		Mirvish et al. (1976) Hilal et al. (2008) Modarresi et al. (2007)	M Q Q	14 68
(diisopropylamino)-ethanol $C_8H_{19}NO$ [96-80-0] ZYWUVGFIXPNBDL-UHFFFAOYSA-N	2.2 2.3 2.4 1.9×10^{2} 8.2×10^{1}		Du et al. (2017) Du et al. (2017) Du et al. (2017) Hilal et al. (2008) Modarresi et al. (2007)	M Q Q Q Q	480 551 68
phthalamide $C_8H_8N_2O_2$ [88-96-0] NAYYNDKKHOIIOD-UHFFFAOYSA-N	7.0×10^{6}		HSDB (2015)	Q	100
acetaminophen $C_8H_9NO_2$ [103-90-2] RZVAJINKPMORJF-UHFFFAOYSA-N	1.5×10^{7}		HSDB (2015)	Q	100
methyl anthranilate $C_8H_9NO_2$ [134-20-3] VAMXMNNIEUEQDV-UHFFFAOYSA-N	5.2 5.2 3.6 2.6×10^{2}		Duchowicz et al. (2020) HSDB (2015) Dupeux et al. (2022) Duchowicz et al. (2020)	V V Q Q	187 260

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4'-aminoacetophenone C_8H_9NO (4-acetylaniline) [99-92-3] GPRYKVSEZCQIHD-UHFFFAOYSA-N	2.2×10^3		HSDB (2015)	Q	100
N-phenylacetamide C_8H_9NO (acetanilide) [103-84-4] FZERHIULMFGESH-UHFFFAOYSA-N	4.7×10^2 1.5×10^3 1.6×10^3		Yaws (2003) Dupeux et al. (2022) HSDB (2015)	X Q Q	259 260 100
tropine $C_8H_{15}NO$ [120-29-6] CYHOMWAPJJPNMW-UHFFFAOYSA-N	1.3×10^3 2.6×10^3 5.6×10^2		Du et al. (2017) Du et al. (2017) Du et al. (2017)	M Q Q	480 551
bis[2-(N,N-dimethylamino)ethyl] ether $C_8H_{20}N_2O$ [3033-62-3] GTEXIOINCJRBIO-UHFFFAOYSA-N	7.9×10^1 2.4×10^2 7.9×10^1		Du et al. (2017) Du et al. (2017) Du et al. (2017)	M Q Q	480 551
methylcarbamic acid, 3-methylphenyl ester $C_9H_{11}NO_2$ (metolcarb) [1129-41-5] VOEYXMAFNDNNED-UHFFFAOYSA-N	1.2×10^4		HSDB (2015)	V	
phenylcarbamic acid, ethyl ester $C_9H_{11}NO_2$ [101-99-5] LBKPGNUOUPTQKA-UHFFFAOYSA-N	3.4×10^2		HSDB (2015)	Q	100
ethyl anthranilate $C_9H_{11}NO_2$ [87-25-2] TWLLPUMZVVGILS-UHFFFAOYSA-N	6.2×10^2		HSDB (2015)	Q	100
benzocaine $C_9H_{11}NO_2$ [94-09-7] BLFLLBZGZJTVJG-UHFFFAOYSA-N	6.2×10^2		HSDB (2015)	Q	100
1-(4-aminophenyl)-1-propanone $C_9H_{11}NO$ (4-aminopropiophenone) [70-69-9] FSWXOANXOQPCFF-UHFFFAOYSA-N	2.1×10^3		HSDB (2015)	Q	100

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(4-ethoxyphenyl)urea $C_9H_{12}N_2O_2$ (dulcin) [150-69-6] GGLIEWRLXDLBBF-UHFFFAOYSA-N	6.2×10^5		HSDB (2015)	Q	449
fenuron $C_9H_{12}N_2O$ [101-42-8] XXOYNJXVWVNOOJ-UHFFFAOYSA-N	4.9×10^3		Duchowicz et al. (2020)	V	187
	8.7×10^2		Mackay et al. (2006d)	V	
	3.7×10^3		Suntio et al. (1988)	V	12
	3.6×10^1		Barcelo and Hennion (1997)	X	569
	9.6		Duchowicz et al. (2020)	Q	
	1.0×10^4		HSDB (2015)	Q	100
	4.4		Goodarzi et al. (2010)	Q	570, 573
epinephrine $C_9H_{13}NO_3$ [51-43-4] UCTWMZQNUQWSLP-UHFFFAOYSA-N	1.4×10^{13}		HSDB (2015)	Q	100
meprobamate $C_9H_{18}N_2O_4$ [57-53-4] NPPQSCRMBWNHMW-UHFFFAOYSA-N	5.5×10^4		HSDB (2015)	Q	100
propamocarb $C_9H_{20}N_2O_2$ [24579-73-5] WZZLDXDUQPOXNW-UHFFFAOYSA-N	2.1×10^3		Keshavarz et al. (2022)	Q	
	1.6×10^3		Duchowicz et al. (2020)	Q	185
	1.6×10^3		Hilal et al. (2008)	Q	
	3.3×10^2		Modarresi et al. (2007)	Q	68
	6.7×10^3		Duchowicz et al. (2020)	?	186, 21
	1.2×10^8		Maniere et al. (2011)	?	242, 166
proximpham $C_{10}H_{12}N_2O_2$ [2828-42-4] LATYTXGNKNKTDS-UHFFFAOYSA-N	3.9×10^3		MacBean (2012a)	?	12
dioxacarb $C_{10}H_{13}NO_4$ [6988-21-2] SDKQRNRRDYRQKY-UHFFFAOYSA-N	6.7×10^5		Duchowicz et al. (2020)	V	187
	2.2×10^4		Duchowicz et al. (2020)	Q	
	6.7×10^5		MacBean (2012a)	?	
phenol, 3,5-dimethyl-, methylcarbamate $C_{10}H_{13}NO_2$ (3,5-xylyl methylcarbamate) [2655-14-3] CVQODEWAPZVVBU-UHFFFAOYSA-N	5.5×10^1		Duchowicz et al. (2020)	V	187
	9.1		Duchowicz et al. (2020)	Q	
	2.5×10^2		HSDB (2015)	Q	100
	4.3×10^2		MacBean (2012a)	?	

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
phenylcarbamic acid, 1-methylethyl ester $C_{10}H_{13}NO_2$ [122-42-9] VXPLXMJHHKHSOA-UHFFFAOYSA-N	5.4×10^{1} 5.5×10^{1} 3.2×10^{-2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
xylylcarb $C_{10}H_{13}NO_2$ [2425-10-7] WCJYTPVNMWIZCG-UHFFFAOYSA-N	9.1×10^{1} 9.4×10^{1} 9.1		Watanabe (1993) Duchowicz et al. (2020) Duchowicz et al. (2020)	M V Q	187
phenacetin $C_{10}H_{13}NO_2$ [62-44-2] CPJSUEIXXCENMM-UHFFFAOYSA-N	4.6×10^{4} 4.7×10^{4} 2.7		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
ephedrine $C_{10}H_{15}NO$ [299-42-3] KWGRBVOPPLSCSI-PSASIEDQSA-N	1.1×10^{5}		HSDB (2015)	Q	449
m-cumenyl methylcarbamate $C_{11}H_{15}NO_2$ (3-isopropylphenyl methyl carbamate) [64-00-6] GYKXQTKSWLAUIT-UHFFFAOYSA-N	1.6×10^{2}		HSDB (2015)	Q	100
propoxur $C_{11}H_{15}NO_3$ [114-26-1] ISRUGXGCCGIOQO-UHFFFAOYSA-N	2.9×10^{3} 5.1×10^{5} 7.1×10^{3} 7.7 7.6×10^{-2} 1.4		HSDB (2015) Mackay et al. (2006d) Siebers et al. (1994) Suntio et al. (1988) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V V V X Q	 12 569 570
methocarbamol $C_{11}H_{15}NO_5$ [532-03-6] GNXFOGHNGIVQEH-UHFFFAOYSA-N	1.5×10^{10}		HSDB (2015)	Q	100
aminocarb $C_{11}H_{16}N_2O_2$ [2032-59-9] IMIDOCRTMDIQIJ-UHFFFAOYSA-N	1.9×10^{3} 1.8×10^{4}		Mackay et al. (2006d) HSDB (2015)	V Q	 100
monodesmethylisoproturon $C_{11}H_{16}N_2O$ [34123-57-4] DOULWWSSZVEPIN-UHFFFAOYSA-N	2.8×10^{5}		Otto et al. (1997)	V	

Table A4.4: Amines, amides, amino acids (C, H, O, N) (... continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cycluron $C_{11}H_{22}N_2O$ [2163-69-1] DQZCVNGCTZLGAQ-UHFFFAOYSA-N	8.2×10^{2}		HSDB (2015)	Q	100
methylneodecanamide $C_{11}H_{23}NO$ [105726-67-8] GELCOLZWXWHMIB-UHFFFAOYSA-N	4.1×10^{1}		HSDB (2015)	Q	100
isoprocarb $C_{11}H_{15}NO_2$ [2631-40-5] QBSJMKIUCUGGNG-UHFFFAOYSA-N	7.4×10^{2} 7.6		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
4-(phenylazo)phenol $C_{12}H_{10}N_2O$ (4-hydroxyazobenzene) [1689-82-3] BEYOBVMPDRKTNR-UHFFFAOYSA-N	1.5×10^{4} 1.5×10^{4} 1.0×10^{4}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
1-naphthaleneacetamide $C_{12}H_{11}NO$ [86-86-2] XFNJVKMNNVCYEK-UHFFFAOYSA-N	9.8×10^{7}		Maniere et al. (2011)	?	12, 166
carbetamide $C_{12}H_{16}N_2O_3$ [16118-49-3] AMRQXHFXNZFDCH-UHFFFAOYSA-N	1.1 3.7 5.2×10^{7}		Barcelo and Hennion (1997) Goodarzi et al. (2010) Maniere et al. (2011)	X Q ?	569 570 12, 166
N-nitrosodiphenylamine $C_{12}H_{10}N_2O$ (N,N-Diphenylnitrosamine) [86-30-6] UBUCNCOMADRQHX-UHFFFAOYSA-N	8.7×10^{-3} 8.7×10^{-3} 1.5×10^{-2} 8.2		Mackay et al. (2006d) Mackay et al. (1995) Mackay et al. (1995) HSDB (2015)	V V C Q	100
carbaryl $C_{12}H_{11}NO_2$ [63-25-2] CVXBEEMKQHEXEN-UHFFFAOYSA-N	$>9.9\times10^{1}$ 3.6×10^{3} 3.0×10^{3} 2.2×10^{4} 2.3×10^{3} 7.7×10^{2} 7.6×10^{1} 2.3×10^{3} 3.5×10^{3} 1.2×10^{2} 8.1 1.4×10^{3} 3.1×10^{3}		Mabury and Crosby (1996) Watanabe (1993) Duchowicz et al. (2020) Mackay et al. (2006d) Meylan and Howard (1991) Suntio et al. (1988) Barcelo and Hennion (1997) Howard and Meylan (1997) Armbrust (2000) Duchowicz et al. (2020) Goodarzi et al. (2010) Hilal et al. (2008) Meylan and Howard (1991)	M M V V V V X X C Q Q Q Q	187 12 569 448 570, 573

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,4'-oxybisbenzenamine $C_{12}H_{12}N_2O$ (bis(4-aminophenyl) ether) [101-80-4] HLBLWEWZXPIGSM-UHFFFAOYSA-N	6.6×10^5		HSDB (2015)	Q	100
carbofuran $C_{12}H_{15}NO_3$ [1563-66-2] DUEPRVBVGDRKAG-UHFFFAOYSA-N	2.4×10^1		Chao et al. (2017)	M	
	$>9.9\times10^1$		Mabury and Crosby (1996)	M	
	2.2×10^4		HSDB (2015)	V	
	2.0×10^4		Mackay et al. (2006d)	V	
	2.0×10^3		Suntio et al. (1988)	V	12
	1.9×10^1		Barcelo and Hennion (1997)	X	569
	4.6×10^1		Goodarzi et al. (2010)	Q	570
phenol, 3-methyl-5-(1-methylethyl)-, methylcarbamate	1.1×10^2		Duchowicz et al. (2020)	V	187
$C_{12}H_{16}NO_2$ (promecarb) [2631-37-0] DTAPQAJKAFRNJB-UHFFFAOYSA-N	1.1×10^2		HSDB (2015)	V	
	4.1		Duchowicz et al. (2020)	Q	
	3.1×10^2		MacBean (2012a)	?	
fenobucarb $C_{12}H_{17}NO_2$ [3766-81-2] DIRFUJHNVNOBMY-UHFFFAOYSA-N	1.5×10^2		Watanabe (1993)	M	
	1.7×10^2		Duchowicz et al. (2020)	V	187
	8.2		Duchowicz et al. (2020)	Q	
diethyltoluamide $C_{12}H_{17}NO$ (DEET) [134-62-3] MMOXZBCLCQITDF-UHFFFAOYSA-N	4.7×10^2		HSDB (2015)	Q	100
N,N-dimethyl-N'-[4-(1-methylethyl)phenyl]-urea $C_{12}H_{18}N_2O$ (isoproturon) [34123-59-6] PUIYMUZLKQOUOZ-UHFFFAOYSA-N	8.8×10^4		Duchowicz et al. (2020)	V	187
	8.1×10^4		Mackay et al. (2006d)	V	
	9.5×10^4		Otto et al. (1997)	V	
	1.1×10^5		Siebers et al. (1994)	V	
	2.3		Duchowicz et al. (2020)	Q	
dimorpholinodiethyl ether $C_{12}H_{24}N_2O_3$ [6425-39-4] ZMSQJSMSLXVTKN-UHFFFAOYSA-N	1.8×10^3	2600	Nguyen (2013)	M	11
carisoprodol $C_{12}H_{24}N_2O_4$ [78-44-4] OFZCIYFFPZCNJE-UHFFFAOYSA-N	1.4×10^4		HSDB (2015)	Q	100

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-hydroxy-4'-nitroazobenzene $C_{12}H_9N_3O_3$ [1435-60-5] NRJPVIOTANUINF-YPKPFQOOSA-N	4.0×10^{5} 1.4×10^{6}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
2,4-dinitro-N-phenyl-benzenamine $C_{12}H_9N_3O_4$ [961-68-2] RHTVQEPJVKUMPI-UHFFFAOYSA-N	1.3×10^{4} 6.6×10^{5}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
N-(2,4-dinitrophenyl)-N-(4-hydroxyphenyl)amine $C_{12}H_9N_3O_5$ [119-15-3] BCPQALWAROJVLE-UHFFFAOYSA-N	6.8×10^{6} 1.4×10^{9}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
disperse orange 3 $C_{12}H_{10}N_4O_2$ [730-40-5] UNBOSJFEZZJZLR-UHFFFAOYSA-N	3.5×10^{4} 1.9×10^{5}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
diethylpropion $C_{13}H_{19}NO$ [90-84-6] XXEPPPIWZFICOJ-UHFFFAOYSA-N	4.3×10^{1}		HSDB (2015)	Q	100
salbutamol $C_{13}H_{21}NO_3$ (albuterol) [18559-94-9] NDAUXUAQIAJITI-UHFFFAOYSA-N	1.5×10^{10}		HSDB (2015)	Q	100
disperse blue 1 $C_{14}H_{12}N_4O_2$ [2475-45-8] JSFUMBWFPQSADC-UHFFFAOYSA-N	4.7×10^{1}		HSDB (2015)	V	
3,3'-dimethoxybenzidine $C_{14}H_{16}N_2O_2$ [119-90-4] JRBJSXQPQWSCCF-UHFFFAOYSA-N	2.1×10^{5}		HSDB (2015)	Q	100
aspartame $C_{14}H_{18}N_2O_5$ [22839-47-0] IAOZJIPTCAWIRG-QWRGUYRKSA-N	3.9×10^{12}		HSDB (2015)	Q	100

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dinobuton $C_{14}H_{18}N_2O_7$ (dessin) [973-21-7] HDWLUGYOLUHEMN-UHFFFAOYSA-N	6.2×10^{2}		HSDB (2015)	Q	100
N-(2-methylcyclohexyl)-N'-phenylurea $C_{14}H_{20}N_2O$ (siduron) [1982-49-6] JXVIIQLNUPXOII-UHFFFAOYSA-N	1.5×10^{5}		HSDB (2015)	V	
butralin $C_{14}H_{21}N_3O_4$ [33629-47-9] SPNQRCTZKIBOAX-UHFFFAOYSA-N	2.0 2.0		HSDB (2015) Mackay et al. (2006d)	V V	
lauramine oxide $C_{14}H_{31}NO$ [1643-20-5] SYELZBGXAIXKHU-UHFFFAOYSA-N	1.5×10^{5}		HSDB (2015)	Q	100
2-aminoanthraquinone $C_{14}H_9NO_2$ [117-79-3] XOGPDSATLSAZEK-UHFFFAOYSA-N	1.1×10^{5} 1.1×10^{5} 3.1×10^{5}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
1-amino-9,10-anthracenedione $C_{14}H_9NO_2$ [82-45-1] KHUFHLFHOQVFGB-UHFFFAOYSA-N	2.0×10^{3} 9.8×10^{4}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
1-amino-4-hydroxy-9,10-anthracenedione $C_{14}H_9NO_3$ [116-85-8] AQXYVFBSOOBBQV-UHFFFAOYSA-N	3.8×10^{5} 4.2×10^{5}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
1,4-diamino-9,10-anthracenedione $C_{14}H_{10}N_2O_2$ [128-95-0] FBMQNRKSAWNXBT-UHFFFAOYSA-N	2.1×10^{4} 1.3×10^{7}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
N,N-dimethyl-4-[(4-nitrophenyl)azo]-benzenamine $C_{14}H_{14}N_4O_2$ [2491-74-9] LSFRFLVWCKLQTO-UHFFFAOYSA-N	1.5×10^{2} 1.0×10^{4}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
karbutilate $C_{14}H_{21}N_3O_3$ [4849-32-5] OWNAXTAAAQTBSP-UHFFFAOYSA-N	1.8×10^{8}		Ebert et al. (2023)	?	319
diethofencarb $C_{14}H_{21}NO_4$ [87130-20-9] LNJNFVJKDJYTEU-UHFFFAOYSA-N	1.2×10^{1} 1.3×10^{-1}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
1-amino-2-methyl-9,10-anthracenedione $C_{15}H_{11}NO_2$ (1-amino-2-methylanthraquinone) [82-28-0] ZLCUIOWQYBYEBG-UHFFFAOYSA-N	8.2×10^{6}		HSDB (2015)	Q	100
N-2-fluorenylacetamide $C_{15}H_{13}NO$ (2-acetylaminofluorene) [53-96-3] CZIHNRWJTSTCEX-UHFFFAOYSA-N	5.2×10^{4}		HSDB (2015)	Q	100
tebutam $C_{15}H_{23}NO$ [35256-85-0] RJKCKKDSSSRYCB-UHFFFAOYSA-N	3.8×10^{1} 1.5×10^{-1} 6.7×10^{1}		Duchowicz et al. (2020) Duchowicz et al. (2020) MacBean (2012a)	V Q ?	187
isopropalin $C_{15}H_{23}N_3O_4$ [33820-53-0] NEKOXWSIMFDGMA-UHFFFAOYSA-N	1.9×10^{-1}		Mackay et al. (2006d)	V	
dodine $C_{15}H_{33}N_3O_2$ (doguadine) [2439-10-3] YIKWKLYQRFRGPM-UHFFFAOYSA-N	1.1×10^{5} 9.9×10^{5} 1.1×10^{5}		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	187 242, 166
metalaxyl $C_{15}H_{21}NO_4$ [57837-19-1] ZQEIXNIJLIKNTD-UHFFFAOYSA-N	3.3×10^{3} 4.0×10^{4} 8.5×10^{4}		HSDB (2015) Mackay et al. (2006d) Burkhard and Guth (1981)	V V V	
metalaxyl-m $C_{15}H_{21}NO_4$ [70630-17-0] ZQEIXNIJLIKNTD-GFCCVEGCSA-N	2.8×10^{4} 2.1×10^{2} 2.9×10^{4}		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	187 166

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
metoprolol $C_{15}H_{25}NO_3$ [37350-58-6] IUBSYMUCCVWXPE-UHFFFAOYSA-N	4.7×10^{5}		HSDB (2015)	Q	100
1-(methylamino)anthraquinone $C_{15}H_{11}NO_2$ [82-38-2] SVTDYSXXLJYUTM-UHFFFAOYSA-N	3.3×10^{2} 7.1×10^{4}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
4'-[(2-hydroxy-5-methylphenyl)azo]acetanilide $C_{15}H_{15}N_3O_2$ [2832-40-8] PXOZAFXVEWKXED-UHFFFAOYSA-N	6.6×10^{5} 3.2×10^{5}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
desmedipham $C_{16}H_{16}N_2O_4$ [13684-56-5] WZJZMXBKUWKXTQ-UHFFFAOYSA-N	2.3×10^{6}		Ebert et al. (2023)	?	367
phenmedipham $C_{16}H_{16}N_2O_4$ (betanal) [13684-63-4] IDOWTHOLJBTAFI-UHFFFAOYSA-N	1.2×10^{7} 1.2×10^{7} 1.2×10^{5} 4.5 5.3×10^{2} 2.0×10^{7}		Duchowicz et al. (2020) HSDB (2015) Barcelo and Hennion (1997) Duchowicz et al. (2020) Goodarzi et al. (2010) Maniere et al. (2011)	V V X Q Q ?	187 569 570, 571 12, 166
fenam $C_{16}H_{17}NO$ [957-51-7] QAHFOPIILNICLA-UHFFFAOYSA-N	2.7×10^{5} 4.1×10^{5} 2.7×10^{5} 4.9×10^{1}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Duchowicz et al. (2020)	V V V Q	187
difenoxuron $C_{16}H_{18}N_2O_3$ [14214-32-5] AMVYOVYGIJXTQB-UHFFFAOYSA-N	5.6×10^{7}		MacBean (2012a)	?	
butacarb $C_{16}H_{25}NO_2$ [2655-19-8] SLZWBCGZQRRUNG-UHFFFAOYSA-N	2.2×10^{2}		HSDB (2015)	V	
oseltamivir $C_{16}H_{28}N_2O_4$ [196618-13-0] VSZGPKBBMSAYNT-RRFJBIMHSA-N	3.4×10^{10}		HSDB (2015)	Q	100

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N,N-bis(2-hydroxyethyl)dodecanamide $C_{16}H_{33}NO_3$ [120-40-1] AOMUHOFOVNGZAN-UHFFFAOYSA-N	4.6×10^{6}		HSDB (2015)	Q	100
1,4-bis(methylamino)-9,10-anthracenedione $C_{16}H_{14}N_2O_2$ [2475-44-7] QOSTVEDABRQTSU-UHFFFAOYSA-N	5.2×10^{4}		Duchowicz et al. (2020)	V	187
	7.5×10^{6}		Duchowicz et al. (2020)	Q	
metominostrobin $C_{16}H_{16}N_2O_3$ [133408-50-1] HIIRDDUVRXCDBN-SDXDJHTJSA-N	2.5×10^{4}		Duchowicz et al. (2020)	V	187
	8.6×10^{6}		Duchowicz et al. (2020)	Q	
1-[(2-methoxyphenyl)azo]-2-naphthol $C_{17}H_{14}N_2O_2$ [1229-55-6] ALLOLPOYFRLCCX-VHEBQXMUSA-N	9.0×10^{4}		HSDB (2015)	Q	100
furalaxyl $C_{17}H_{19}NO_4$ [57646-30-7] CIEXPHRYOLIQQD-UHFFFAOYSA-N	1.1×10^{4}		MacBean (2012a)	?	
fenoxycarb $C_{17}H_{19}NO_4$ [72490-01-8] HJUFTIJOISQSKQ-UHFFFAOYSA-N	2.3×10^{4}		Duchowicz et al. (2020)	V	187
	2.5×10^{4}		Duchowicz et al. (2020)	V	187
	2.3×10^{7}		HSDB (2015)	V	
	1.2×10^{4}		Mackay et al. (2006d)	V	
	8.4×10^{2}		Duchowicz et al. (2020)	Q	
	8.4×10^{2}		Duchowicz et al. (2020)	Q	
	3.0×10^{4}		Maniere et al. (2011)	?	242, 166
bifenazate $C_{17}H_{20}N_2O_3$ [149877-41-8] VHLKTXFWDRXILV-UHFFFAOYSA-N	1.0×10^{3}		MacBean (2012b)	X	352
	$>9.9\times10^{2}$		Maniere et al. (2011)	?	12, 166
napropamide $C_{17}H_{21}NO_2$ [15299-99-7] WXZVAROIGSFCFJ-UHFFFAOYSA-N	1.2×10^{4}		HSDB (2015)	V	
	1.2×10^{4}		Maniere et al. (2011)	?	242, 166
napropamide-M $C_{17}H_{21}NO_2$ [41643-35-0] WXZVAROIGSFCFJ-CYBMUJFWSA-N	3.8×10^{4}		Ebert et al. (2023)	?	319

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
padimate O $C_{17}H_{27}NO_2$ [21245-02-3] WYWZRNAHINYAEF-UHFFFAOYSA-N	2.5		HSDB (2015)	Q	449
nadolol $C_{17}H_{27}NO_4$ [42200-33-9] VWPOSFSPZNDTMJ-UHFFFAOYSA-N	7.0×10^{8}		HSDB (2015)	Q	100
2,6-di-*tert*-butyl-4-(dimethylaminomethyl)phenol $C_{17}H_{29}NO$ [88-27-7] VMZVBRIIHDRYGK-UHFFFAOYSA-N	4.8×10^{3} 2.4×10^{2} 1.3 4.8×10^{1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
mepronil $C_{17}H_{19}NO_2$ [55814-41-0] BCTQJXQXJVLSIG-UHFFFAOYSA-N	8.4×10^{2} 4.7		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
daimuron $C_{17}H_{20}N_2O$ [42609-52-9] NNYRZQHKCHEXSD-UHFFFAOYSA-N	9.9×10^{3} 2.6×10^{1}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
naptalam $C_{18}H_{13}NO_3$ [132-66-1] JXTHEWSKYLZVJC-UHFFFAOYSA-N	$>2.3\times10^{10}$		MacBean (2012a)	?	
citrus red 2 $C_{18}H_{16}N_2O_3$ [6358-53-8] ULLJIFAIUSUJBP-ZZEZOPTASA-N	1.9×10^{7}		HSDB (2015)	Q	100
kresoxim-methyl $C_{18}H_{19}NO_4$ [143390-89-0] ZOTBXTZVPHCKPN-UHFFFAOYSA-N	2.7×10^{3} 2.8×10^{3}		HSDB (2015) Maniere et al. (2011)	V ?	 242, 166
dinocap $C_{18}H_{24}N_2O_6$ [39300-45-3] RNDNTTTUTQAXII-GORDUTHDSA-N	2.1×10^{3}		HSDB (2015)	V	
orysastrobin $C_{18}H_{25}N_5O_5$ [248593-16-0] JHIPUJPTQJYEQK-ZLHHXESBSA-N	2.9×10^{5}		Ebert et al. (2023)	?	319

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
spiroxamine	4.0×10^{2}		Maniere et al. (2011)	?	12, 166
$C_{18}H_{35}NO_2$	2.0×10^{2}		Maniere et al. (2011)	?	12, 166
[118134-30-8]					
PUYXTUJWRLOUCW-UHFFFAOYSA-N					
capsaicin	9.9×10^{7}		HSDB (2015)	Q	100
$C_{18}H_{27}NO_3$					
[404-86-4]					
YKPUWZUDDOIDPM-SOFGYWHQSA-N					
mandestrobin	1.5×10^{6}		Maniere et al. (2011)	?	12, 166
$C_{19}H_{23}NO_3$					
[173662-97-0]					
PDPWCKVFIFAQIQ-UHFFFAOYSA-N					
dimoxystrobin	2.2×10^{7}		Maniere et al. (2011)	?	242, 166
$C_{19}H_{22}N_2O_3$					
[149961-52-4]					
WXUZAHCNPWONDH-DYTRJAOYSA-N					
(*RS*)-α-2-naphthoxypropionanilide	1.6×10^{5}		Hilal et al. (2008)	Q	
$C_{19}H_{17}NO_2$	7.5×10^{4}		Modarresi et al. (2007)	Q	68
(naproanilide)					
[52570-16-8]					
LVKTWOXHRYGDMM-UHFFFAOYSA-N					
phenylbutazone	1.5×10^{3}		HSDB (2015)	Q	100
$C_{19}H_{20}N_2O_2$					
[50-33-9]					
VYMDGNCVAMGZFE-UHFFFAOYSA-N					
phenisopham	1.3×10^{4}		MacBean (2012a)	?	
$C_{19}H_{22}N_2O_4$					
[57375-63-0]					
PWEOEHNGYFXZLI-UHFFFAOYSA-N					
formoterol	1.1×10^{17}		HSDB (2015)	Q	100
$C_{19}H_{24}N_2O_4$					
[73573-87-2]					
BPZSYCZIITTYBL-ORAYPTAESA-N					
benalaxyl-m	4.3×10^{3}		Maniere et al. (2011)	?	12, 166
$C_{20}H_{23}NO_3$					
[98243-83-5]					
CJPQIRJHIZUAQP-MRXNPFEDSA-N					
benalaxyl	8.5×10^{1}		Duchowicz et al. (2020)	V	187
$C_{20}H_{23}NO_3$	8.3×10^{1}		Mackay et al. (2006d)	V	
[71626-11-4]	5.1×10^{1}		Duchowicz et al. (2020)	Q	
CJPQIRJHIZUAQP-UHFFFAOYSA-N	1.5×10^{2}		Maniere et al. (2011)	?	12, 166

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tralkoxydim $C_{20}H_{27}NO_3$ [87820-88-0] SOTLWPHEAQOHHC-UHFFFAOYSA-N	4.1×10^{4}		HSDB (2015)	V	
neotame $C_{20}H_{30}N_2O_5$ [165450-17-9] HLIAVLHNDJUHFG-HOTGVXAUSA-N	4.3×10^{3}		HSDB (2015)	Q	100
colchicine $C_{22}H_{25}NO_6$ [64-86-8] IAKHMKGGTNLKSZ-MRXNPFEDSA-N	5.5×10^{11}		HSDB (2015)	Q	100
tebufenozide $C_{22}H_{28}N_2O_2$ [112410-23-8] QYPNKSZPJQQLRK-UHFFFAOYSA-N	7.6×10^{2} $>1.5\times10^{4}$		HSDB (2015) Maniere et al. (2011)	V ?	 166
methoxyfenozide $C_{22}H_{28}N_2O_3$ [161050-58-4] QCAWEPFNJXQPAN-UHFFFAOYSA-N	2.6×10^{6} $>6.1\times10^{3}$		HSDB (2015) Maniere et al. (2011)	Q ?	100 12, 166
propoxyphene $C_{22}H_{29}NO_2$ [469-62-5] XLMALTXPSGQGBX-PGRDOPGGSA-N	4.3×10^{3}		HSDB (2015)	Q	100
(*Z*)-13-docosenamide $C_{22}H_{43}NO$ (erucamide) [112-84-5] UAUDZVJPLUQNMU-KTKRTIGZSA-N	3.5		HSDB (2015)	Q	547
butroxydim $C_{24}H_{33}NO_4$ [138164-12-2] ZOGDSYNXUXQGHF-XIEYBQDHSA-N	1.7×10^{4}		MacBean (2012a)	?	
2,2-bis[4-(4-aminophenoxy)phenyl]propane $C_{27}H_{26}N_2O_2$ [13080-86-9] KMKWGXGSGPYISJ-UHFFFAOYSA-N	2.0×10^{8} 2.8×10^{8} 1.0×10^{8} 3.1×10^{10}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,4-bis[(4-methylphenyl)amino]-9,10-anthracenedione $C_{28}H_{22}N_2O_2$ (D&C Green No. 6) [128-80-3] TVRGPOFMYCMNRB-UHFFFAOYSA-N	6.6×10^{10}		HSDB (2015)	Q	100
mifepristone $C_{29}H_{35}NO_2$ [84371-65-3] VKHAHZOOUSRJNA-GCNJZUOMSA-N	2.0×10^{-1}		HSDB (2015)	Q	100
2'-anilino-6'-[ethyl(3-methylbutyl)amino]-3'-methylspiro[isobenzofuran-1(3H),9'-[9H]xanthene]-3-one	8.4×10^{7}		Zhang et al. (2010)	Q	288, 289
$C_{34}H_{34}N_2O_3$	2.0×10^{8}		Zhang et al. (2010)	Q	288, 290
[70516-41-5]	3.5×10^{8}		Zhang et al. (2010)	Q	288, 291
HUSIBQLZEMMTCQ-UHFFFAOYSA-N	8.0×10^{8}		Zhang et al. (2010)	Q	288, 292
spinetoram	1.0×10^{2}		Maniere et al. (2011)	?	242, 572, 166
$C_{42}H_{69}NO_{10}$	1.1×10^{4}		Maniere et al. (2011)	?	242, 572, 166
[935545-74-7]	1.6×10^{2}		Maniere et al. (2011)	?	242, 574, 166
GOENIMGKWNZVDA-OAMCMWGQSA-N	2.0×10^{3}		Maniere et al. (2011)	?	242, 166
	2.9×10^{2}		Maniere et al. (2011)	?	242, 495, 166
	2.9×10^{3}		Maniere et al. (2011)	?	242, 495, 166
	4.3×10^{1}		Maniere et al. (2011)	?	242, 574, 166
	2.5×10^{2}		Maniere et al. (2011)	?	242, 166
spinosad	5.3×10^{6}		Maniere et al. (2011)	?	242, 166
$C_{42}H_{71}NO_9$	4.3×10^{4}		Maniere et al. (2011)	?	242, 166
[168316-95-8]					
RQOIAWYOVOXMST-UHFFFAOYSA-N					
emamectin benzoate	5.8×10^{3}		HSDB (2015)	V	
$C_{56}H_{81}NO_{15}$	2.5×10^{1}		Maniere et al. (2011)	?	242, 575, 166
[155569-91-8]	5.9×10^{3}		Maniere et al. (2011)	?	242, 495, 166
GCKZANITAMOIAR-UHFFFAOYSA-N	7.7×10^{4}		Maniere et al. (2011)	?	242, 572, 166

Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
glutamic acid	9.0×10^{7}		Yaws (2003)	X	238
$C_5H_9NO_4$	1.8×10^{10}		Gharagheizi et al. (2012)	Q	
[617-65-2]	9.6×10^{7}		Gharagheizi et al. (2010)	Q	247
WHUUTDBJXJRKMK-UHFFFAOYSA-N	9.9×10^{10}		Saxena and Hildemann (1996)	E	403
asparagine	9.9×10^{10}		Saxena and Hildemann (1996)	E	403
$C_4H_8N_2O_3$					
[70-47-3]					
DCXYFEDJOCDNAF-UWTATZPHSA-N					
serine	3.9×10^{10}		Saxena and Hildemann (1996)	E	403
$C_3H_7NO_3$					
[302-84-1]					
MTCFGRXMJLQNBG-UHFFFAOYSA-N					
glutamine	3.3×10^{10}		HSDB (2015)	Q	449
$C_5H_{10}N_2O_3$	9.9×10^{10}		Saxena and Hildemann (1996)	E	403
[56-85-9]					
ZDXPYRJPNDTMRX-GSVOUGTGSA-N					
glycine	1.2×10^{11}	16000	Brimblecombe et al. (1992)	V	
$C_2H_5NO_2$	8.9×10^{5}		Saxena and Hildemann (1996)	E	403
[56-40-6]					
DHMQDGOQFOQNFH-UHFFFAOYSA-N					
arginine	9.9×10^{14}		Saxena and Hildemann (1996)	E	403
$C_6H_{14}N_4O_2$					
[74-79-3]					
ODKSFYDXXFIFQN-SCSAIBSYSA-N					
alanine	3.5×10^{10}	16000	Brimblecombe et al. (1992)	V	
$C_3H_7NO_2$	5.9×10^{5}		Saxena and Hildemann (1996)	E	403
[302-72-7]					
QNAYBMKLOCPYGJ-UHFFFAOYSA-N					
leucine	2.0×10^{5}		Saxena and Hildemann (1996)	E	403
$C_6H_{13}NO_2$					
[328-39-2]					
ROHFNLRQFUQHCH-UHFFFAOYSA-N					

A4.5 Heterocycles with oxygen and nitrogen (C, H, O, N)

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyanuric acid	1.1×10^{9}		HSDB (2015)	Q	100
$C_3H_3N_3O_3$	1.1×10^{9}		Zhang et al. (2010)	Q	288, 289
[108-80-5]	3.4×10^{5}		Zhang et al. (2010)	Q	288, 290
ZFSLODLOARCGLH-UHFFFAOYSA-N	4.2×10^{10}		Zhang et al. (2010)	Q	288, 291
	4.0×10^{7}		Zhang et al. (2010)	Q	288, 292
isoxazole	4.0×10^{-1}		Duchowicz et al. (2020)	V	187
C_3H_3NO	5.4×10^{-1}		Duchowicz et al. (2020)	Q	
[288-14-2]	2.4×10^{-1}		Hilal et al. (2008)	Q	
CTAPFRYPJLPFDF-UHFFFAOYSA-N	2.1×10^{-1}		Modarresi et al. (2007)	Q	68
glycidamide $C_3H_5NO_2$ [5694-00-8] FMAZQSYXRGRESX-UHFFFAOYSA-N	7.7×10^{4}		HSDB (2015)	Q	100
cyclonite $C_3H_6N_6O_6$ [121-82-4] XTFIVUDBNACUBN-UHFFFAOYSA-N	4.9×10^{5}		HSDB (2015)	V	
5-methyl-3-(2H)-isoxazolone	4.7×10^{3}		Duchowicz et al. (2020)	V	187
$C_4H_5NO_2$	4.7×10^{2}		Duchowicz et al. (2020)	Q	
(hymexazol)	5.0×10^{3}		Hilal et al. (2008)	Q	
[10004-44-1]	1.6×10^{2}		Modarresi et al. (2007)	Q	68
KGVPNLBXJKTABS-UHFFFAOYSA-N	7.1×10^{3}		Maniere et al. (2011)	?	242, 166
3-amino-1H-pyridazin-6-one $C_4H_5N_3O$ (maleic hydrazide) [10071-13-3] MMZLICVOTDAZOX-UHFFFAOYSA-N	1.2×10^{7}		Ebert et al. (2023)	?	319
maleic hydrazide $C_4H_4N_2O_2$ [123-33-1] BGRDGMRNKXEXQD-UHFFFAOYSA-N	2.5×10^{7}		Maniere et al. (2011)	?	12, 166
allantoin $C_4H_6N_4O_3$ [97-59-6] POJWUDADGALRAB-UHFFFAOYSA-N	2.9×10^{12}		HSDB (2015)	Q	100
2-pyrrolidinone	9.3×10^{3}		Duchowicz et al. (2020)	V	187
C_4H_7NO	9.3×10^{3}		HSDB (2015)	V	
[616-45-5]	1.2×10^{3}		Duchowicz et al. (2020)	Q	
HNJBEVLQSNELDL-UHFFFAOYSA-N					

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-nitrosomorpholine	3.9×10^{2}		Mirvish et al. (1976)	M	14
$C_4H_8N_2O_2$	9.0×10^{2}		Hilal et al. (2008)	Q	
[59-89-2]	1.5×10^{2}		Modarresi et al. (2007)	Q	68
ZKXDGKXYMTYWTB-UHFFFAOYSA-N					
N-nitrosopyrrolidine	1.5×10^{2}	8500	Klein (1982)	M	
$C_4H_8N_2O$	1.9×10^{2}		Mirvish et al. (1976)	M	14
[930-55-2]	3.4×10^{1}		Hilal et al. (2008)	Q	
WNYADZVDBIBLJJ-UHFFFAOYSA-N					
cyclotetramethylenetetranitramine	1.1×10^{4}		HSDB (2015)	Q	100
$C_4H_8N_8O_8$					
[2691-41-0]					
UZGLIIJVICEWHF-UHFFFAOYSA-N					
1-oxa-4-azacyclohexane	1.9×10^{2}	7800	Nguyen (2013)	M	11
C_4H_9NO	8.5		Duchowicz et al. (2020)	V	187
(morpholine)	8.2		HSDB (2015)	V	
[110-91-8]	7.3×10^{1}	8400	Cabani et al. (1975a)	T	
YNAVUWVOSKDBBP-UHFFFAOYSA-N	2.2×10^{1}		Duchowicz et al. (2020)	Q	
	1.6×10^{2}		Hilal et al. (2008)	Q	
	8.1×10^{1}		Modarresi et al. (2007)	Q	68
	9.5×10^{1}		English and Carroll (2001)	Q	231, 275
	1.0×10^{1}		Nirmalakhandan et al. (1997)	Q	
	4.2×10^{1}		Yaws (1999)	?	21, 12
1-aziridineethanol	1.3×10^{4}		HSDB (2015)	Q	100
C_4H_9NO					
[1072-52-2]					
VYONOYYDEFODAJ-UHFFFAOYSA-N					
2-ethyl-3-methoxypyrazine	6.7×10^{-1}		Buttery et al. (1971)	M	
$C_4N_2H_3(C_2H_5)OCH_3$	2.5×10^{1}		Hilal et al. (2008)	Q	
[25680-58-4]	2.6		Modarresi et al. (2007)	Q	68
DPCILIMHENXHQX-UHFFFAOYSA-N					
2-isobutyl-3-methoxypyrazine	1.7×10^{-1}		Karl et al. (2003)	M	
$C_4N_2H_3(C_4H_9)OCH_3$	2.0×10^{-1}		Buttery et al. (1971)	M	
[24683-00-9]	1.3		Modarresi et al. (2007)	Q	68
UXFSPRAGHGMRSQ-UHFFFAOYSA-N					
N-nitrosopiperidine	1.1×10^{1}		Mirvish et al. (1976)	M	14
$C_5H_{10}N_2O$	2.9×10^{1}		Hilal et al. (2008)	Q	
[100-75-4]	9.6		Modarresi et al. (2007)	Q	68
UWSDONTXWQOZFN-UHFFFAOYSA-N	3.4		Katritzky et al. (1998)	Q	
butyl carbamate	1.1×10^{2}		HSDB (2015)	Q	100
$C_5H_{11}NO_2$					
[592-35-8]					
SKKTUOZKZKCGTB-UHFFFAOYSA-N					

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methyl-1-oxa-4-azacyclohexane	5.0		Du et al. (2017)	M	480
$C_5H_{11}NO$	1.2×10^1	10000	Leng et al. (2015a)	M	
(N-methylmorpholine;	1.8×10^1	8300	Cabani et al. (1975a)	T	
4-methylmorpholine)					
[109-02-4]	9.6		Du et al. (2017)	Q	551
SJRJJKPEHAURKC-UHFFFAOYSA-N	3.6		Du et al. (2017)	Q	
	5.7		Hilal et al. (2008)	Q	
	6.4		Modarresi et al. (2007)	Q	68
	1.4×10^1		English and Carroll (2001)	Q	231, 232
	1.7×10^1		Nirmalakhandan et al. (1997)	Q	
allopurinol	4.9×10^8		HSDB (2015)	Q	100
$C_5H_4N_4O$					
[315-30-0]					
OFCNXPDARWKPPY-UHFFFAOYSA-N					
4-methoxypyridine		7100	Arnett and Chawla (1979)	?	561
$C_5H_4NOCH_3$					
[620-08-6]					
XQABVLBGNWBWIV-UHFFFAOYSA-N					
N-methyl-2-pyrrolidone	3.1×10^3	11000	Brockbank (2013)	L	1
C_5H_9NO	2.1×10^3	9100	Bernauer and Dohnal (2009)	M	
[872-50-4]	3.1×10^3		Kim et al. (2000)	M	
SECXISVLQFMRJM-UHFFFAOYSA-N	2.8×10^3		Keshavarz et al. (2022)	Q	
	1.0×10^1		Duchowicz et al. (2020)	Q	185
	3.7×10^1		Modarresi et al. (2007)	Q	68
	3.1×10^3		Duchowicz et al. (2020)	?	186, 21
5,5-dimethyl-2,4-	3.5×10^3		HSDB (2015)	Q	100
imidazolidinedione					
$C_5H_8N_2O_2$	3.6×10^3		Zhang et al. (2010)	Q	288, 289
[77-71-4]	1.6×10^5		Zhang et al. (2010)	Q	288, 290
YIROYDNZEPTFOL-UHFFFAOYSA-N	5.1×10^6		Zhang et al. (2010)	Q	288, 291
	1.6×10^5		Zhang et al. (2010)	Q	288, 292
1-methyluracil	2.3×10^3		Duchowicz et al. (2020)	V	187
$C_5H_6N_2O_2$	2.1×10^5		Duchowicz et al. (2020)	Q	
[615-77-0]					
XBCXJKGHPABGSD-UHFFFAOYSA-N					
2-azacycloheptanone	1.8×10^5		HSDB (2015)	V	
$C_6H_{11}NO$	2.0×10^3		Hwang et al. (1992)	V	
(caprolactam)	3.9×10^4		Abraham et al. (2019)	Q	
[105-60-2]					
JBKVHLHDHHXQEQ-UHFFFAOYSA-N					

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-acetylpyrrolidine $C_6H_{11}NO$ [4030-18-6] LNWWQYYLZVZXKS-UHFFFAOYSA-N	6.2×10^{3}		Gibbs et al. (1991)	M	
glucosamine $C_6H_{13}NO_5$ [3416-24-8] MSWZFWKMSRAUBD-IVMDWMLBSA-N	1.3×10^{10}		HSDB (2015)	Q	100
N-ethylmorpholine $C_6H_{13}NO$ [100-74-3] HVCNXQOWACZAFN-UHFFFAOYSA-N	4.0×10^{2}		HSDB (2015)	Q	100
3-formylpyridine C_6H_5NO [500-22-1] QJZUKDFHGGYHMC-UHFFFAOYSA-N	6.5×10^{1}		Abraham et al. (1994a)	R	
	6.5×10^{1}		Keshavarz et al. (2022)	Q	
	1.5×10^{1}		Duchowicz et al. (2020)	Q	
	1.0×10^{2}		Hilal et al. (2008)	Q	
	2.7×10^{1}		Modarresi et al. (2007)	Q	68
	6.5×10^{1}		Yaffe et al. (2003)	Q	249, 250
	1.2×10^{2}		English and Carroll (2001)	Q	231, 275
	3.8×10^{1}		Nirmalakhandan et al. (1997)	Q	
	6.6×10^{1}		Duchowicz et al. (2020)	?	186, 21
4-formylpyridine C_6H_5NO [872-85-5] BGUWFUQJCDRPTL-UHFFFAOYSA-N	5.6×10^{1}		Abraham et al. (1994a)	R	
	6.5×10^{1}		Keshavarz et al. (2022)	Q	
	1.5×10^{1}		Duchowicz et al. (2020)	Q	300
	1.0×10^{2}		Hilal et al. (2008)	Q	
	2.2×10^{1}		Modarresi et al. (2007)	Q	68
	6.5×10^{1}		Yaffe et al. (2003)	Q	249, 273
	6.4×10^{1}		English and Carroll (2001)	Q	231, 232
	3.8×10^{1}		Nirmalakhandan et al. (1997)	Q	
	5.6×10^{1}		Duchowicz et al. (2020)	?	186, 21
niacinamide $C_6H_6N_2O$ [98-92-0] DFPAKSUCGFBDDF-UHFFFAOYSA-N	3.4×10^{6}		HSDB (2015)	Q	100
metronidazole $C_6H_9N_3O_3$ [443-48-1] VAOCPAMSLUNLGC-UHFFFAOYSA-N	5.8×10^{5}		HSDB (2015)	Q	100
nicotinic acid $C_6H_5NO_2$ [59-67-6] PVNIIMVLHYAWGP-UHFFFAOYSA-N	2.5×10^{4}		Abraham et al. (2019)	Q	

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
isonicotinic acid $C_6H_5NO_2$ [55-22-1] TWBYWOBDOCUKOW-UHFFFAOYSA-N	1.6×10^{4}		Abraham et al. (2019)	Q	
1-methylthymine $C_6H_8N_2O_2$ [4160-72-9] GKMIDMKPBOUSBQ-UHFFFAOYSA-N	1.7×10^{4}		Ebert et al. (2023)	?	367
glydant $C_7H_{12}N_2O_4$ (1,3-dimethylol-5,5-dimethylhydantoin) [6440-58-0] WSDISUOETYTPRL-UHFFFAOYSA-N	1.4×10^{6}		HSDB (2015)	Q	100
3-quinuclidinol $C_7H_{13}NO$ [1619-34-7] IVLICPVPXWEGCA-UHFFFAOYSA-N	1.7×10^{3} 1.8×10^{4} 5.1×10^{3} 1.2×10^{4}		Du et al. (2017) Du et al. (2017) Du et al. (2017) HSDB (2015)	M Q Q Q	480 551 100
dinotefuran $C_7H_{14}N_4O_3$ [165252-70-0] YKBZOVFACRVRJN-UHFFFAOYSA-N	1.5×10^{8}		HSDB (2015)	V	
1,2,3-benzotriazin-4(1H)-one $C_7H_5N_3O$ [90-16-4] DMSSTTLDFWKBSX-UHFFFAOYSA-N	3.1×10^{4}		HSDB (2015)	Q	100
4-acetylpyridine C_7H_7NO [1122-54-9] WMQUKDQWMMOHSA-UHFFFAOYSA-N	1.6×10^{2} 8.8×10^{1} 5.0 1.9×10^{2} 4.1×10^{1} 8.0×10^{1} 2.7×10^{1} 1.6×10^{2}		Abraham et al. (1994a) Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) English and Carroll (2001) Nirmalakhandan et al. (1997) Duchowicz et al. (2020)	R Q Q Q Q Q Q ?	 300 68 231, 232 186, 21
3-acetylpyridine C_7H_7NO [350-03-8] WEGYGNROSJDEIW-UHFFFAOYSA-N	4.6×10^{2} 8.8×10^{1} 5.0 1.9×10^{2} 5.2×10^{1} 2.7×10^{1} 4.6×10^{2}		Abraham et al. (1994a) Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Nirmalakhandan et al. (1997) Duchowicz et al. (2020)	R Q Q Q Q Q ?	 300 68 186, 21

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
theophylline $C_7H_8N_4O_2$ [58-55-9] ZFXYFBGIUFBOJW-UHFFFAOYSA-N	5.5×10^{8}		HSDB (2015)	Q	100
theobromine $C_7H_8N_4O_2$ [83-67-0] YAPQBXQYLJRXSA-UHFFFAOYSA-N	6.2×10^{5}		HSDB (2015)	Q	100
2-pyridineethanol C_7H_9NO [103-74-2] BXGYBSJAZFGIPX-UHFFFAOYSA-N	6.6×10^{4}		HSDB (2015)	Q	100
caffeine $C_8H_{10}N_4O_2$ [58-08-2] RYYVLZVUVIJVGH-UHFFFAOYSA-N	9.0×10^{5}		HSDB (2015)	V	
acyclovir $C_8H_{11}N_5O_3$ [59277-89-3] MKUXAQIIEYXACX-UHFFFAOYSA-N	3.1×10^{16}		HSDB (2015)	Q	100
2-methoxy-3-(1-methylethyl)-pyrazine $C_8H_{12}N_2O$ [25773-40-4] NTOPKICPEQUPPH-UHFFFAOYSA-N	2.1×10^{1} 1.5×10^{1}		Wu et al. (2022a) Hilal et al. (2008)	Q Q	415
simeton $C_8H_{15}N_5O$ [673-04-1] HKAMKLBXTLTVCN-UHFFFAOYSA-N	1.5×10^{4} 2.5×10^{4}		Hilal et al. (2008) Abraham et al. (2007)	Q Q	
N-isobutylmorpholine $C_8H_{17}NO$ [10315-98-7] QKVSMSABRNCNRS-UHFFFAOYSA-N		8100 6000	Kühne et al. (2005) Kühne et al. (2005)	Q ?	
phthalimide $C_8H_5NO_2$ [85-41-6] XKJCHHZQLQNZHY-UHFFFAOYSA-N	9.9×10^{2}		HSDB (2015)	Q	100
furazolidone $C_8H_7N_3O_5$ [67-45-8] PLHJDBGFXBMTGZ-UHFFFAOYSA-N	3.0×10^{5}		HSDB (2015)	Q	100

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,6-tetrahydrophthalimide $C_8H_9NO_2$ [85-40-5] CIFFBTOJCKSRJY-UHFFFAOYSA-N	3.3×10^{2}		HSDB (2015)	Q	100
N-nitrosonornicotine $C_9H_{11}N_3O$ [16543-55-8] XKABJYQDMJTNGQ-UHFFFAOYSA-N	5.8×10^{4}		HSDB (2015)	Q	449
9-[(1,3-dihydroxy-2-propoxy)methyl]guanine $C_9H_{13}N_5O_4$ (ganciclovir) [82410-32-0] IRSCQMHQWWYFCW-UHFFFAOYSA-N	6.6×10^{17}		HSDB (2015)	Q	100
2-*sec*-butyl-3-methoxypyrazine $C_9H_{14}N_2O$ [24168-70-5] QMQDJVIJVPEQHE-UHFFFAOYSA-N	2.0×10^{-1}		Ebert et al. (2023)	?	367
atraton $C_9H_{17}N_5O$ [1610-17-9] PXWUKZGIHQRDHL-UHFFFAOYSA-N	6.4×10^{3} 1.1×10^{4} 2.2×10^{3}		Hilal et al. (2008) Abraham et al. (2007) MacBean (2012a)	Q Q ?	
4-hydroxy-2,2,6,6-tetramethyl-1-piperidinyloxy $C_9H_{18}NO_2$ [2226-96-2] UZFMOKQJFYMBGY-UHFFFAOYSA-N	3.3×10^{9}		HSDB (2015)	Q	100
8-hydroxyquinoline C_9H_7NO [148-24-3] MCJGNVYPOGVAJF-UHFFFAOYSA-N	1.7×10^{1} 1.7×10^{1} 8.9×10^{1} 5.5×10^{2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Maniere et al. (2011)	V V Q ?	187 242, 166
carbendazim $C_9H_9N_3O_2$ [10605-21-7] TWFZGCMQGLPBSX-UHFFFAOYSA-N	4.7×10^{5} 6.5×10^{5}		HSDB (2015) Mackay et al. (2006d)	V V	
metamitron $C_{10}H_{10}N_4O$ [41394-05-2] VHCNQEUWZYOAEV-UHFFFAOYSA-N	1.0×10^{6} 2.2×10^{6} 4.5×10^{3} 2.8×10^{7} 1.6×10^{7} 1.1×10^{7}		Barcelo and Hennion (1997) Delgado and Alderete (2003) Goodarzi et al. (2010) Delgado and Alderete (2003) Delgado and Alderete (2003) Maniere et al. (2011)	X C Q Q Q ?	569 570 242, 166

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pymetrozin $C_{10}H_{11}N_5O$ [123312-89-0] QHMTXANCGGJZRX-UHFFFAOYSA-N	3.3×10^{5}		HSDB (2015)	V	
3-oxo-N-phenylbutanamide $C_{10}H_{11}NO_2$ (acetoacetanilide) [102-01-2] DYRDKSSFIWVSNM-UHFFFAOYSA-N	2.3×10^{6}		HSDB (2015)	Q	100
2,3'-didehydro-3'-deoxythymidine (stavudine) $C_{10}H_{12}N_2O_4$ (stavudine) [3056-17-5] XNKLLVCARDGLGL-JGVFFNPUSA-N	4.3×10^{9}		HSDB (2015)	Q	100
cotinine $C_{10}H_{12}N_2O$ [486-56-6] UIKROCXWUNQSPJ-UHFFFAOYSA-N	3.0×10^{6}		HSDB (2015)	Q	100
4-(N-nitroso-N-methylamino)-1-(3-pyridyl)-1-butanone $C_{10}H_{13}N_3O_2$ [64091-91-4] FLAQQSHRLBFIEZ-UHFFFAOYSA-N	1.2×10^{8}		HSDB (2015)	Q	100
9-(4-hydroxy-3-hydroxymethylbut-1-yl)guanine $C_{10}H_{15}N_5O_3$ (penciclovir) [39809-25-1] JNTOCHDNEULJHD-UHFFFAOYSA-N	1.0×10^{26}		HSDB (2015)	Q	100
anatoxin A $C_{10}H_{15}NO$ [64285-06-9] SGNXVBOIDPPRJJ-UHFFFAOYSA-N	1.5×10^{3}		HSDB (2015)	Q	100
dimetilan $C_{10}H_{16}N_4O_3$ [644-64-4] RDBIYWSVMRVKSG-UHFFFAOYSA-N	2.4×10^{5}		HSDB (2015)	Q	100
isolan $C_{10}H_{17}N_3O_2$ [119-38-0] RNNBHZYEKNHLKT-UHFFFAOYSA-N	4.9×10^{3}		HSDB (2015)	Q	100

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
amicarbazone $C_{10}H_{19}N_5O_2$ [129909-90-6] ORFPWVRKFLOQHK-UHFFFAOYSA-N	1.5×10^{7}		MacBean (2012b)	X	352
prometone	1.1×10^{4}		HSDB (2015)	V	
$C_{10}H_{19}N_5O$	1.1×10^{4}		Mackay et al. (2006d)	V	
(prometon)	1.1×10^{4}		Suntio et al. (1988)	V	12
[1610-18-0]	1.1×10^{2}		Barcelo and Hennion (1997)	X	569
ISEUFVQQFVOBCY-UHFFFAOYSA-N	6.9×10^{1}		Goodarzi et al. (2010)	Q	570
	2.7×10^{3}		Hilal et al. (2008)	Q	
	5.1×10^{3}		Abraham et al. (2007)	Q	
secbumeton	2.8×10^{3}		Mackay et al. (2006d)	V	
$C_{10}H_{19}N_5O$	2.9×10^{3}		Suntio et al. (1988)	V	12
[26259-45-0]	5.0×10^{3}		Hilal et al. (2008)	Q	
ZJMZZNVGNSWOOM-UHFFFAOYSA-N	7.2×10^{3}		Abraham et al. (2007)	Q	
	2.7×10^{3}		MacBean (2012a)	?	
terbumeton	2.1×10^{3}		Mackay et al. (2006d)	V	
$C_{10}H_{19}N_5O$	2.4×10^{3}		Hilal et al. (2008)	Q	
[33693-04-8]	1.6×10^{3}		Abraham et al. (2007)	Q	
BCQMBFHBDZVHKU-UHFFFAOYSA-N					
kinetin $C_{10}H_9N_5O$ [525-79-1] QANMHLXAZMSUEX-UHFFFAOYSA-N	8.2×10^{8}		HSDB (2015)	Q	100
isouron	7.3×10^{4}		Duchowicz et al. (2020)	V	187
$C_{10}H_{17}N_3O_2$	3.3×10^{1}		Duchowicz et al. (2020)	Q	
[55861-78-4]					
JLLJHQLUZAKJFH-UHFFFAOYSA-N					
fuberidazole $C_{11}H_8N_2O$ [3878-19-1] UYJUZNLFJAWNEZ-UHFFFAOYSA-N	1.9×10^{5}		Ebert et al. (2023)	?	319
carbadox $C_{11}H_{10}N_4O_4$ [6804-07-5] OVGGLBAWFMIPPY-WUXMJOGZSA-N	2.2×10^{17}		HSDB (2015)	Q	100
bendiocarb	2.5×10^{2}		Duchowicz et al. (2020)	V	187
$C_{11}H_{13}NO_4$	2.5×10^{2}		HSDB (2015)	V	
[22781-23-3]	2.7×10^{2}		Mackay et al. (2006d)	V	
XEGGRYVFLWGFHI-UHFFFAOYSA-N	2.0×10^{2}		Duchowicz et al. (2020)	Q	

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,5-trimethylphenol, methylcarbamate $C_{11}H_{15}NO_2$ (2,3,5-trimethacarb) [2655-15-4] NYOKZHDTNBDPOB-UHFFFAOYSA-N	4.5×10^{1}		HSDB (2015)	V	
butalbital $C_{11}H_{16}N_2O_3$ [77-26-9] UZVHFVZFNXBMQJ-UHFFFAOYSA-N	1.6×10^{7}		HSDB (2015)	Q	100
dexrazoxane $C_{11}H_{16}N_4O_4$ [24584-09-6] BMKDZUISNHGIBY-ZETCQYMHSA-N	4.7×10^{13}		HSDB (2015)	Q	100
pentobarbital $C_{11}H_{18}N_2O_3$ [76-74-4] WEXRUCMBJFQVBZ-UHFFFAOYSA-N	1.2×10^{7}		HSDB (2015)	Q	100
pirimor $C_{11}H_{18}N_4O_2$ (pirimicarb) [23103-98-2] YFGYUFNIOHWBOB-UHFFFAOYSA-N	1.2×10^{4} 3.1×10^{3} 5.0×10^{3} 5.9×10^{3} 3.1×10^{3} 3.4×10^{4} 3.0×10^{4} 3.0×10^{4} 2.8×10^{4}		HSDB (2015) Mackay et al. (2006d) Siebers and Mattusch (1996) Siebers et al. (1994) Suntio et al. (1988) Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011)	V V V V V ? ? ? ?	 12 12 12, 576, 166 12, 577, 166 12, 578, 166 12, 166
ethirimol $C_{11}H_{19}N_3O$ [23947-60-6] BBXXLROWFHWFQY-UHFFFAOYSA-N	3.6×10^{3}		Mackay et al. (2006d)	V	
pyroquilon $C_{11}H_{11}NO$ [57369-32-1] XRJLAOUDSILTFT-UHFFFAOYSA-N	5.1×10^{3}		Ebert et al. (2023)	?	319
fenfuram $C_{12}H_{11}NO_2$ [24691-80-3] JFSPBVWPKOEZCB-UHFFFAOYSA-N	2.5×10^{4}		Mackay et al. (2006d)	V	

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
oxabetrinil $C_{12}H_{12}N_2O_3$ [74782-23-3] WFVUIONFJOAYPK-UHFFFAOYSA-N	8.6×10^{1}		Ebert et al. (2023)	?	319
phenobarbital $C_{12}H_{12}N_2O_3$ [50-06-6] DDBREPKUVSBGFI-UHFFFAOYSA-N	5.8×10^{8}		HSDB (2015)	Q	100
triaziquone $C_{12}H_{13}N_3O_2$ [68-76-8] PXSOHRWMIRDKMP-UHFFFAOYSA-N	1.1×10^{10}		HSDB (2015)	Q	100
triallyl cyanurate $C_{12}H_{15}N_3O_3$ [101-37-1] BJELTSYBAHKXRW-UHFFFAOYSA-N	2.3×10^{1} 1.8×10^{3} 1.9×10^{2} 4.1×10^{4}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
entecavir $C_{12}H_{15}N_5O_3$ [142217-69-4] QDGZDCVAUDNJFG-FXQIFTODSA-N	6.2×10^{15}		HSDB (2015)	Q	100
metaxalone $C_{12}H_{15}NO_3$ [1665-48-1] IMWZZHHPURKASS-UHFFFAOYSA-N	3.7×10^{4}		HSDB (2015)	Q	100
phendimetrazine $C_{12}H_{17}NO$ [634-03-7] MFOCDFTXLCYLKU-UHFFFAOYSA-N	3.7×10^{2}		HSDB (2015)	Q	100
hexazinone $C_{12}H_{20}N_4O_2$ [51235-04-2] CAWXEEYDBZRFPE-UHFFFAOYSA-N	$>9.9\times10^{1}$ 4.4×10^{6}		Mabury and Crosby (1996) HSDB (2015)	M V	
picaridin $C_{12}H_{23}NO_3$ [119515-38-7] QLHULAHOXSSASE-UHFFFAOYSA-N	3.3×10^{5}		HSDB (2015)	Q	100
lenacil $C_{13}H_{18}N_2O_2$ [2164-08-1] ZTMKADLOSYKWCA-UHFFFAOYSA-N	1.3×10^{5} 3.8×10^{4} 7.7×10^{6}		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	187 242, 166

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pyrinuron $C_{13}H_{12}N_4O_3$ (pyriminil) [53558-25-1] CLKZWXHKFXZIMA-UHFFFAOYSA-N	5.4×10^{10}		HSDB (2015)	Q	100
melatonin $C_{13}H_{16}N_2O_2$ [73-31-4] DRLFMBDRBRZALE-UHFFFAOYSA-N	3.8×10^{8}		HSDB (2015)	Q	449
dibenz[b, f]][1,4]oxazepine $C_{13}H_9NO$ [257-07-8] NPUACKRELIJTFM-UHFFFAOYSA-N	2.4×10^{-3}		HSDB (2015)	Q	100
oxadixyl $C_{14}H_{18}N_2O_4$ [77732-09-3] UWVQIROCRJWDKL-UHFFFAOYSA-N	2.0×10^{6}		Ebert et al. (2023)	?	319
benomyl $C_{14}H_{18}N_4O_3$ [17804-35-2] RIOXQFHNBCKOKP-UHFFFAOYSA-N	5.2×10^{5} 3.1×10^{5} 1.8×10^{5} 2.0×10^{6}		Mackay et al. (2006d) Keshavarz et al. (2022) Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q Q ?	 186, 21
trimethoprim $C_{14}H_{18}N_4O_3$ [738-70-5] IEDVJHCEMCRBQM-UHFFFAOYSA-N	4.1×10^{8}		HSDB (2015)	Q	100
ethoxyquin $C_{14}H_{19}NO$ [91-53-2] DECIPOUIJURFOJ-UHFFFAOYSA-N	8.0		Ebert et al. (2023)	?	319
famciclovir $C_{14}H_{19}N_5O_4$ [104227-87-4] GGXKWVWZWMLJEH-UHFFFAOYSA-N	1.0×10^{8}		HSDB (2015)	Q	100
furmecyclox $C_{14}H_{21}NO_3$ [60568-05-0] QTDRLOKFLJJHTG-UHFFFAOYSA-N	1.4×10^{2}		MacBean (2012a)	?	
oxcarbazepine $C_{15}H_{12}N_2O_2$ [28721-07-5] CTRLABGOLIVAIY-UHFFFAOYSA-N	1.4×10^{7}		HSDB (2015)	Q	100

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
phenytoin $C_{15}H_{12}N_2O_2$ [57-41-0] CXOFVDLJLONNDW-UHFFFAOYSA-N	9.7×10^{5}		HSDB (2015)	Q	100
carbamazepine $C_{15}H_{12}N_2O$ [298-46-4] FFGPTBGBLSHEPO-UHFFFAOYSA-N	9.0×10^{4}		HSDB (2015)	Q	100
propylthiouracil $C_{15}H_{12}N_2O$ [51-52-5] KNAHARQHSZJURB-UHFFFAOYSA-N	9.0×10^{3}		HSDB (2015)	Q	100
ancymidol $C_{15}H_{16}N_2O_2$ [12771-68-5] HUTDUHSNJYTCAR-UHFFFAOYSA-N	9.1×10^{5} 1.5×10^{6} 4.7×10^{6} 6.3×10^{5}		Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Duchowicz et al. (2020)	Q Q Q ?	 186, 21
imazethapyr $C_{15}H_{19}N_3O_3$ [81335-77-5] XVOKUMIPKHGGTN-UHFFFAOYSA-N	9.9×10^{10}		HSDB (2015)	Q	100
imazamox $C_{15}H_{19}N_3O_4$ [114311-32-9] NUPJIGQFXCQJBK-UHFFFAOYSA-N	1.1×10^{13} 2.0×10^{11}		HSDB (2015) Maniere et al. (2011)	Q ?	100 242, 166
cycloheximide $C_{15}H_{23}NO_4$ [66-81-9] YPHMISFOHDHNIV-FSZOTQKASA-N	2.8×10^{9}		HSDB (2015)	Q	100
oxymatrine $C_{15}H_{24}N_2O_2$ [16837-52-8] XVPBINOPNYFXID-LHDUFFHYSA-N	9.9×10^{12}		HSDB (2015)	Q	100
triapenthenol $C_{15}H_{25}N_3O$ [76608-88-3] CNFMJLVJDNGPHR-UKTHLTGXSA-N	4.0×10^{4}		Ebert et al. (2023)	?	319
mebendazole $C_{16}H_{13}N_3O_3$ [31431-39-7] OPXLLQIJSORQAM-UHFFFAOYSA-N	1.8×10^{10}		HSDB (2015)	Q	100

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
imazamethabenz-methyl $C_{16}H_{20}N_2O_3$ [81405-85-8] FFCCBBNQPIMUJI-UHFFFAOYSA-N	2.6×10^{6}		HSDB (2015)	V	
nifedipine $C_{17}H_{18}N_2O_6$ [21829-25-4] HYIMSNHJOBLJNT-UHFFFAOYSA-N	1.4×10^{8}		HSDB (2015)	Q	100
oxymorphone $C_{17}H_{19}NO_4$ [76-41-5] UQCNKQCJZOAFTQ-UHFFFAOYSA-N	2.4×10^{13}		HSDB (2015)	Q	100
desomorphine $C_{17}H_{21}NO_2$ [427-00-9] LNNWVNGFPYWNQE-UHFFFAOYSA-N	2.4×10^{6}		HSDB (2015)	Q	100
cocaine $C_{17}H_{21}NO_4$ [50-36-2] ZPUCINDJVBIVPJ-PFSRBDOWSA-N	2.3×10^{5} 2.3×10^{5} 7.9×10^{4}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
N-(2-ethylhexyl)-5-norbornene-2,3-dicarboximide $C_{17}H_{25}NO_2$ [113-48-4] WLLGXSLBOPFWQV-UHFFFAOYSA-N	3.5×10^{1}		HSDB (2015)	Q	100
imazaquin $C_{17}H_{17}N_3O_3$ [81335-37-7] CABMTIJINOIHOD-UHFFFAOYSA-N	2.7×10^{11}		Maniere et al. (2011)	?	12, 166
(*E*)-pyriminobac-methyl $C_{17}H_{19}N_3O_6$ [147411-69-6] USSIUIGPBLPCDF-KEBDBYFISA-N	7.3×10^{2}		Ebert et al. (2023)	?	319
(*Z*)-pyriminobac-methyl $C_{17}H_{19}N_3O_6$ [147411-70-9] USSIUIGPBLPCDF-JMIUGGIZSA-N	1.9×10^{4}		Ebert et al. (2023)	?	319
imiprothrin $C_{17}H_{22}N_2O_4$ [72963-72-5] VPRAQYXPZIFIOH-UHFFFAOYSA-N	1.6×10^{5} 6.9×10^{3}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
iprovalicarb $C_{18}H_{28}N_2O_3$ [140923-17-7] NWUWYYSKZYIQAE-LBAUFKAWSA-N	7.1×10^{5}		Maniere et al. (2011)	?	12, 166
quinophthalone $C_{18}H_{11}NO_2$ [8003-22-3] IZMJMCDDWKSTTK-UHFFFAOYSA-N	1.6×10^{8}		HSDB (2015)	Q	100
pefurazoate $C_{18}H_{23}N_3O_4$ [101903-30-4] WBTYBAGIHOISOQ-UHFFFAOYSA-N	1.8×10^{3}		Ebert et al. (2023)	?	319
tetramethrin $C_{19}H_{25}NO_4$ [7696-12-0] CXBMCYHAMVGWJQ-UHFFFAOYSA-N	5.8		HSDB (2015)	V	
isoxaben $C_{19}H_{25}NO_4$ [82558-50-7] PMHURSZHKKJGBM-UHFFFAOYSA-N	7.8×10^{3} 7.8×10^{3} 5.3×10^{3} 5.1×10^{3}		Duchowicz et al. (2020) MacBean (2012b) Duchowicz et al. (2020) Maniere et al. (2011)	V X Q ?	187 352 12, 166
alfuzosin $C_{19}H_{27}N_5O_4$ [81403-80-7] WNMJYKCGWZFFKR-UHFFFAOYSA-N	1.0×10^{14}		HSDB (2015)	Q	100
2,6-dimethyl-4-tridecylmorpholine $C_{19}H_{39}NO$ (tridemorph) [24602-86-6] YTOPFCCWCSOHFV-UHFFFAOYSA-N	5.8×10^{-2}		Ebert et al. (2023)	?	319
pyriproxyfen $C_{20}H_{19}NO_3$ [95737-68-1] NHDHVHZZCFYRSB-UHFFFAOYSA-N	1.6×10^{4} $>1.4\times10^{1}$		HSDB (2015) Maniere et al. (2011)	Q ?	100 73, 166
papaverine $C_{20}H_{21}NO_4$ [58-74-2] XQYZDYMELSJDRZ-UHFFFAOYSA-N	1.3×10^{7}		HSDB (2015)	Q	100
fenazaquin $C_{20}H_{22}N_2O$ [120928-09-8] DMYHGDXADUDKCQ-UHFFFAOYSA-N	2.1×10^{2} 9.9×10^{1} 4.7×10^{1} 1.8×10^{1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Maniere et al. (2011)	V V Q ?	187 242, 166

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bitertanol $C_{20}H_{23}N_3O_2$ [55179-31-2] VGPIBGGRCVEHQZ-UHFFFAOYSA-N	1.2×10^{4}		Mackay et al. (2006d)	V	
bitertanol diastereoisomer a $C_{20}H_{23}N_3O_2$ [70585-36-3] VGPIBGGRCVEHQZ-OALUTQOASA-N	3.1×10^{6}		Mackay et al. (2006d)	V	
bitertanol diastereoisomer b $C_{20}H_{23}N_3O_2$ [70585-38-5] VGPIBGGRCVEHQZ-RBUKOAKNSA-N	1.5×10^{6}		Mackay et al. (2006d)	V	
naltrexone $C_{20}H_{23}NO_4$ [16590-41-3] DQCKKXVULJGBQN-UHFFFAOYSA-N	2.3×10^{13}		HSDB (2015)	Q	100
D-lysergic acid N,N-diethylamide $C_{20}H_{25}N_3O$ (LSD) [50-37-3] VAYOSLLFUXYJDT-UHFFFAOYSA-N	6.6×10^{10}		HSDB (2015)	Q	100
ibogaine $C_{20}H_{26}N_2O$ [83-74-9] HSIBGVUMFOSJPD-UHFFFAOYSA-N	8.2×10^{5}		HSDB (2015)	Q	100
fenpropimorph $C_{20}H_{33}NO$ [67564-91-4] RYAUSSKQMZRMAI-ALOPSCKCSA-N	6.2 6.2×10^{-2} 7.9×10^{-2} 3.6×10^{-1}		Mackay et al. (2006d) Barcelo and Hennion (1997) Goodarzi et al. (2010) Maniere et al. (2011)	V X Q ?	 569 570 242, 166
strychnine $C_{21}H_{22}N_2O_2$ [57-24-9] QMGVPVSNSZLJIA-UHFFFAOYSA-N	1.6×10^{8}		HSDB (2015)	Q	100
nalmefene $C_{21}H_{25}NO_3$ [55096-26-9] WJBLNOPPDWQMCH-UHFFFAOYSA-N	5.5×10^{10}		HSDB (2015)	Q	100
benztropine $C_{21}H_{25}NO$ [86-13-5] GIJXKZJWITVLHI-UHFFFAOYSA-N	4.5×10^{3}		HSDB (2015)	Q	100

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
stanozolol $C_{21}H_{32}N_2O$ [10418-03-8] LKAJKIOFIWVMDJ-KIWJEFSTSA-N	9.0×10^{2}		HSDB (2015)	Q	100
spirotetramat	1.4×10^{7}		Maniere et al. (2011)	?	242, 495, 166
$C_{21}H_{27}NO_5$	1.6×10^{7}		Maniere et al. (2011)	?	242, 579, 166
[203313-25-1]	9.2×10^{6}		Maniere et al. (2011)	?	242, 575, 166
CLSVJBIHYWPGQY-GGYDESQDSA-N					
diacetylmorphine	1.6×10^{7}		Duchowicz et al. (2020)	V	187
$C_{21}H_{23}NO_5$	2.7×10^{5}		Duchowicz et al. (2020)	Q	
(heroin) [561-27-3] GVGLGOZIDCSQPN-PVHGPHFFSA-N					
pyrametostrobin $C_{21}H_{23}N_3O_4$ [915410-70-7] DWTVBEZBWMDXIY-UHFFFAOYSA-N	2.2×10^{4}		Ebert et al. (2023)	?	319
azoxystrobin	1.4×10^{8}		HSDB (2015)	V	
$C_{22}H_{17}N_3O_5$	1.4×10^{8}		Maniere et al. (2011)	?	242, 166
[131860-33-8] WFDXOXNFNRHQEC-GHRIWEEISA-N					
famoxadone	2.1×10^{2}		HSDB (2015)	V	
$C_{22}H_{18}N_2O_4$	2.2×10^{2}		Maniere et al. (2011)	?	242, 166
[131807-57-3] PCCSBWNGDMYFCW-UHFFFAOYSA-N					
tadalafil $C_{22}H_{19}N_3O_4$ [171596-29-5] WOXKDUGGOYFFRN-IIBYNOLFSA-N	2.0×10^{12}		HSDB (2015)	Q	100
bisacodyl $C_{22}H_{19}NO_4$ [603-50-9] KHOITXIGCFIULA-UHFFFAOYSA-N	1.4×10^{6}		HSDB (2015)	Q	100
fentanyl $C_{22}H_{28}N_2O$ [437-38-7] PJMPHNIQZUBGLI-UHFFFAOYSA-N	1.1×10^{6}		HSDB (2015)	Q	100

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-(triphenylmethyl)morpholine $C_{23}H_{23}NO$ (trifenmorph) [1420-06-0] ZJMLMBICUVVJDX-UHFFFAOYSA-N	7.6×10^{4} 3.2		HSDB (2015) MacBean (2012a)	Q ?	100
brucine $C_{23}H_{26}N_2O_4$ [357-57-3] RRKTZKIUPZVBMF-UHFFFAOYSA-N	4.7×10^{10}		HSDB (2015)	Q	100
mycophenolate mofetil $C_{23}H_{31}NO_7$ [128794-94-5] RTGDFNSFWBGLEC-SYZQJQIISA-N	1.8×10^{9}		HSDB (2015)	Q	100
pinoxaden $C_{23}H_{32}N_2O_4$ [243973-20-8] MGOHCFMYLBAPRN-UHFFFAOYSA-N	1.1×10^{6} 1.1×10^{6}		HSDB (2015) Maniere et al. (2011)	V ?	 166
fenpyroximate $C_{24}H_{27}N_3O_4$ [134098-61-6] YYJNOYZRYGDPNH-MFKUBSTISA-N	4.6 7.6 5.8×10^{4}		Duchowicz et al. (2020) MacBean (2012b) Duchowicz et al. (2020)	V X Q	187 352
valsartan $C_{24}H_{29}N_5O_3$ [137862-53-4] ACWBQPMHZXGDFX-QFIPXVFZSA-N	3.2×10^{12}		HSDB (2015)	Q	100
donepezil $C_{24}H_{29}NO_3$ [120014-06-4] ADEBPBSSDYVVLD-UHFFFAOYSA-N	8.2×10^{6}		HSDB (2015)	Q	100
chromafenozide $C_{24}H_{30}N_2O_3$ [143807-66-3] HPNSNYBUADCFDR-UHFFFAOYSA-N	5.1×10^{5} 6.2×10^{5} 5.6×10^{5}		Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011)	? ? ?	12, 495, 166 12, 579, 166 12, 575, 166
cyenopyrafen $C_{24}H_{31}N_3O_2$ [560121-52-0] APJLTUBHYCOZJI-VZCXRCSSSA-N	1.6×10^{3}		Ebert et al. (2023)	?	319

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-[4-[4-(2-benzoxazolyl)styryl]phenyl]-5-methylbenzoxazole	7.5×10^{8}		Zhang et al. (2010)	Q	288, 289
$C_{29}H_{20}N_2O_2$	6.2×10^{6}		Zhang et al. (2010)	Q	288, 290
[5242-49-9]	1.2×10^{5}		Zhang et al. (2010)	Q	288, 291
SOTPOQQKAUOHRO-BQYQJAHWSA-N	9.5×10^{7}		Zhang et al. (2010)	Q	288, 292
2-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol	7.2×10^{9}		Zhang et al. (2010)	Q	288, 289
$C_{30}H_{29}N_3O$	5.8×10^{5}		Zhang et al. (2010)	Q	288, 290
[70321-86-7]	1.4×10^{7}		Zhang et al. (2010)	Q	288, 291
OLFNXLXEGXRUOI-UHFFFAOYSA-N	8.8×10^{6}		Zhang et al. (2010)	Q	288, 292
fenpicoxamid $C_{31}H_{38}N_2O_{11}$ [517875-34-2] QGTOTYJSCYHYFK-RBODFLQRSA-N	4.2×10^{2}		Maniere et al. (2011)	?	166
norbormide $C_{33}H_{25}N_3O_3$ [991-42-4] DNTHHIVFNQZZRD-UHFFFAOYSA-N	3.7×10^{17}		HSDB (2015)	Q	100
reserpine $C_{33}H_{40}N_2O_9$ [50-55-5] QEVHRUUCFGRFIF-UHFFFAOYSA-N	1.8×10^{17}		HSDB (2015)	Q	100
telmisartan $C_{33}H_{30}N_4O_2$ [144701-48-4] RMMXLENWKUUMAY-UHFFFAOYSA-N	1.9×10^{14}		Abraham et al. (2019)	Q	
telaprevir $C_{36}H_{53}N_7O_6$ [402957-28-2] BBAWEDCPNXPBQM-GDEBMMAJSA-N	1.3×10^{25}		HSDB (2015)	Q	100
lopinavir $C_{37}H_{48}N_4O_5$ [192725-17-0] KJHKTHWMRKYKJE-WRHCQWCJSA-N	2.3×10^{22}		HSDB (2015)	Q	100
atazanavir $C_{38}H_{52}N_6O_7$ [198904-31-3] AXRYRYVKAWYZBR-GASGPIRDSA-N	2.7×10^{26}		HSDB (2015)	Q	100

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tylosin $C_{46}H_{77}NO_{17}$ [1401-69-0] WBPYTXDJUQJLPQ-SNQVITFCSA-N	1.7×10^{32}		HSDB (2015)	Q	100
nystatin $C_{47}H_{75}NO_{17}$ [1400-61-9] VQOXZBDYSJBXMA-QFHUWGMOSA-N	4.9×10^{4}		HSDB (2015)	Q	100
1,3,5-tris(3,5-di-*tert*-butyl-4-hydroxybenzyl)-1,3,5-triazinane-2,4,6-trione	6.1×10^{20}		Zhang et al. (2010)	Q	288, 289
$C_{48}H_{69}N_3O_6$	1.3×10^{12}		Zhang et al. (2010)	Q	288, 290
[27676-62-6]	3.4×10^{10}		Zhang et al. (2010)	Q	288, 291
VNQNXQYZMPJLQX-UHFFFAOYSA-N	8.2×10^{14}		Zhang et al. (2010)	Q	288, 292

A4.6 Nitrates ($RONO_2$)

Table A4.6: Nitrates ($RONO_2$)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
urea nitrate $CH_5N_3O_4$ [124-47-0] AYTGUZPQPXGYFS-UHFFFAOYSA-N	5.8×10^{11}		HSDB (2015)	Q	100
methyl nitrate CH_3ONO_2 [598-58-3] LRMHVVPPGGOAJQ-UHFFFAOYSA-N	2.0×10^{-2}	4700	Burkholder et al. (2019)	L	
	2.0×10^{-2}	4700	Burkholder et al. (2015)	L	
	2.0×10^{-2}	4700	Sander et al. (2011)	L	
	2.0×10^{-2}	4700	Sander et al. (2006)	L	
	2.0×10^{-2}	4700	Kames and Schurath (1992)	M	
	2.6×10^{-2}		Schwartz (1986)	C	88
	1.6×10^{-2}		Wang et al. (2017)	Q	81, 239
	1.3×10^{-1}		Wang et al. (2017)	Q	81, 240
	1.0×10^{-3}		Wang et al. (2017)	Q	81, 241
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	6.2×10^{-2}		Hilal et al. (2008)	Q	
		4900	Kühne et al. (2005)	Q	
		4800	Kühne et al. (2005)	?	
ethyl nitrate $C_2H_5ONO_2$ [625-58-1] IDNUEBSJWINEMI-UHFFFAOYSA-N	1.6×10^{-2}	5400	Burkholder et al. (2019)	L	
	1.6×10^{-2}	5400	Burkholder et al. (2015)	L	
	1.6×10^{-2}	5400	Sander et al. (2011)	L	
	1.6×10^{-2}	5400	Sander et al. (2006)	L	
	1.6×10^{-2}	5400	Kames and Schurath (1992)	M	
	1.2×10^{-2}		Wang et al. (2017)	Q	81, 239
	6.5×10^{-2}		Wang et al. (2017)	Q	81, 240
	9.1×10^{-4}		Wang et al. (2017)	Q	81, 241
	3.3×10^{-2}		HSDB (2015)	Q	100
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	3.9×10^{-2}		Hilal et al. (2008)	Q	
1-propyl nitrate $C_3H_7ONO_2$ [627-13-4] JNTOKFNBDFMTIV-UHFFFAOYSA-N	1.1×10^{-2}	5500	Burkholder et al. (2019)	L	
	1.1×10^{-2}	5500	Burkholder et al. (2015)	L	
	1.1×10^{-2}	5500	Sander et al. (2011)	L	
	1.1×10^{-2}	5500	Sander et al. (2006)	L	
	9.0×10^{-3}	5600	Staudinger and Roberts (2001)	L	
	7.4×10^{-3}	4600	Hauff et al. (1998)	M	
	1.1×10^{-2}	5500	Kames and Schurath (1992)	M	
	1.1×10^{-2}		Hauff et al. (1998)	V	
	3.6×10^{-3}		Keshavarz et al. (2022)	Q	
	6.9×10^{-3}		Duchowicz et al. (2020)	Q	185

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	1.0×10^{-2}		Wang et al. (2017)	Q	81, 239
	3.1×10^{-2}		Wang et al. (2017)	Q	81, 240
	6.2×10^{-4}		Wang et al. (2017)	Q	81, 241
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.5×10^{-2}		Hilal et al. (2008)	Q	
	5.3×10^{-2}		Modarresi et al. (2007)	Q	68
		5600	Kühne et al. (2005)	Q	
	7.8×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4600	Kühne et al. (2005)	?	
2-propyl nitrate	7.8×10^{-3}	5400	Burkholder et al. (2019)	L	
$C_3H_7ONO_2$	7.8×10^{-3}	5400	Burkholder et al. (2015)	L	
(isopropyl nitrate)	7.8×10^{-3}	5400	Sander et al. (2011)	L	
[1712-64-7]	7.8×10^{-3}	5400	Sander et al. (2006)	L	
GAPFWGOSHOCNBM-UHFFFAOYSA-N	6.6×10^{-3}	5400	Staudinger and Roberts (2001)	L	
	5.5×10^{-3}	4300	Hauff et al. (1998)	M	
	7.8×10^{-3}	5400	Kames and Schurath (1992)	M	
	8.1×10^{-3}		Hauff et al. (1998)	V	
	3.6×10^{-3}		Keshavarz et al. (2022)	Q	
	2.7×10^{-3}		Duchowicz et al. (2020)	Q	185
	1.1×10^{-2}		Wang et al. (2017)	Q	81, 239
	2.4×10^{-2}		Wang et al. (2017)	Q	81, 240
	7.1×10^{-4}		Wang et al. (2017)	Q	81, 241
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.9		Raventos-Duran et al. (2010)	Q	246
	1.7×10^{-2}		Hilal et al. (2008)	Q	
	4.9×10^{-2}		Modarresi et al. (2007)	Q	68
		4600	Kühne et al. (2005)	Q	
	6.1×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4300	Kühne et al. (2005)	?	
1-butyl nitrate	1.0×10^{-2}	5800	Burkholder et al. (2019)	L	
$C_4H_9ONO_2$	1.0×10^{-2}	5800	Burkholder et al. (2015)	L	
[928-45-0]	1.0×10^{-2}	5800	Sander et al. (2011)	L	
QQHZPQUHCAKSOL-UHFFFAOYSA-N	1.0×10^{-2}	5800	Sander et al. (2006)	L	
	8.8×10^{-3}	6000	Staudinger and Roberts (2001)	L	
	6.3×10^{-3}	5200	Hauff et al. (1998)	M	
	1.0×10^{-2}	5800	Kames and Schurath (1992)	M	
	1.0×10^{-2}	6000	Luke et al. (1989)	M	
	8.5×10^{-3}		Hauff et al. (1998)	V	
	4.8×10^{-3}		Keshavarz et al. (2022)	Q	
	1.0×10^{-2}		Duchowicz et al. (2020)	Q	
	8.9×10^{-3}		Wang et al. (2017)	Q	81, 239
	2.0×10^{-2}		Wang et al. (2017)	Q	81, 240

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	3.0×10^{-4}		Wang et al. (2017)	Q	81, 241
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.7×10^{-2}		Hilal et al. (2008)	Q	
	4.2×10^{-2}		Modarresi et al. (2007)	Q	68
		5900	Kühne et al. (2005)	Q	
	6.4×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		5800	Kühne et al. (2005)	?	
2-butyl nitrate	6.4×10^{-3}	5400	Burkholder et al. (2019)	L	
$C_4H_9ONO_2$	6.4×10^{-3}	5400	Burkholder et al. (2015)	L	
[924-52-7]	6.4×10^{-3}	5400	Sander et al. (2011)	L	
DYONNFFVDNILGI-UHFFFAOYSA-N	6.4×10^{-3}	5400	Sander et al. (2006)	L	
	6.4×10^{-3}	6100	Staudinger and Roberts (2001)	L	
	4.4×10^{-3}		Hauff et al. (1998)	M	
	6.4×10^{-3}	5400	Kames and Schurath (1992)	M	
	6.3×10^{-3}	5600	Luke et al. (1989)	M	
	6.4×10^{-3}		Hauff et al. (1998)	V	
	8.9×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.5×10^{-2}		Wang et al. (2017)	Q	81, 240
	5.5×10^{-4}		Wang et al. (2017)	Q	81, 241
		4900	Kühne et al. (2005)	Q	
		5400	Kühne et al. (2005)	?	
isobutyl nitrate	7.0×10^{-3}	5200	Kames and Schurath (1992)	M	
$C_4H_9ONO_2$	4.8×10^{-3}		Keshavarz et al. (2022)	Q	
[543-29-3]	3.9×10^{-3}		Duchowicz et al. (2020)	Q	
LNNXFUZKZLXPOF-UHFFFAOYSA-N	8.9×10^{-3}		Wang et al. (2017)	Q	81, 239
	2.0×10^{-2}		Wang et al. (2017)	Q	81, 240
	4.6×10^{-4}		Wang et al. (2017)	Q	81, 241
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.6×10^{-2}		Hilal et al. (2008)	Q	
	4.4×10^{-2}		Modarresi et al. (2007)	Q	68
	4.4×10^{-3}		Duchowicz et al. (2020)	?	186, 21
1-pentyl nitrate	6.6×10^{-3}	6300	Hauff et al. (1998)	M	
$C_5H_{11}ONO_2$	1.2×10^{-2}		Kames and Schurath (1992)	M	12
(amyl nitrate)	4.0×10^{-3}		Hauff et al. (1998)	V	
[1002-16-0]	6.5×10^{-3}		Keshavarz et al. (2022)	Q	
HSNWZBCBUUSSQD-UHFFFAOYSA-N	1.3×10^{-2}		Duchowicz et al. (2020)	Q	
	6.9×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.4×10^{-2}		Wang et al. (2017)	Q	81, 240
	4.8×10^{-4}		Wang et al. (2017)	Q	81, 241
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.3×10^{-2}		Hilal et al. (2008)	Q	
	3.8×10^{-2}		Modarresi et al. (2007)	Q	68
		6300	Kühne et al. (2005)	Q	
	5.9×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		6300	Kühne et al. (2005)	?	
2-pentyl nitrate	3.7×10^{-3}	6400	Staudinger and Roberts (2001)	L	
$C_5H_{11}ONO_2$	3.7×10^{-3}	5100	Hauff et al. (1998)	M	
(MCM:PEBNO3)	3.6×10^{-3}	6300	Kames and Schurath (1992)	M	
[21981-48-6]	4.8×10^{-3}		Hauff et al. (1998)	V	
RWRBSYOTDDOXKC-UHFFFAOYSA-N	3.4×10^{-3}	6000	Wieser et al. (2023)	Q	439
	6.5×10^{-3}		Keshavarz et al. (2022)	Q	
	5.0×10^{-3}		Duchowicz et al. (2020)	Q	300
	8.3×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.0×10^{-2}		Wang et al. (2017)	Q	81, 240
	4.8×10^{-4}		Wang et al. (2017)	Q	81, 241
	9.5×10^{-3}		Hilal et al. (2008)	Q	
	3.6×10^{-2}		Modarresi et al. (2007)	Q	68
		5300	Kühne et al. (2005)	Q	
	3.3×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		5100	Kühne et al. (2005)	?	
3-pentyl nitrate	3.8×10^{-3}	5300	Hauff et al. (1998)	M	
$C_5H_{13}ONO_2$	4.9×10^{-3}		Hauff et al. (1998)	V	
[82944-59-0]	6.5×10^{-3}		Keshavarz et al. (2022)	Q	
WQZKKVJFBZPJSU-UHFFFAOYSA-N	5.0×10^{-3}		Duchowicz et al. (2020)	Q	300
	8.3×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.0×10^{-2}		Wang et al. (2017)	Q	81, 240
	3.7×10^{-4}		Wang et al. (2017)	Q	81, 241
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	9.2×10^{-3}		Hilal et al. (2008)	Q	
	4.0×10^{-2}		Modarresi et al. (2007)	Q	68
		5300	Kühne et al. (2005)	Q	
	3.6×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		5300	Kühne et al. (2005)	?	
3-methyl-1-butanol nitrate	5.0×10^{-3}	5900	Hauff et al. (1998)	M	
$C_5H_{11}ONO_2$	6.5×10^{-3}		Keshavarz et al. (2022)	Q	
(isoamyl nitrate)	5.0×10^{-3}		Duchowicz et al. (2020)	Q	185
[543-87-3]	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
NTHGIYFSMNNHSC-UHFFFAOYSA-N	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-2}		Hilal et al. (2008)	Q	

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	3.8×10^{-2}		Modarresi et al. (2007)	Q	68
		6300	Kühne et al. (2005)	Q	
	4.5×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		5900	Kühne et al. (2005)	?	
pentaerythritol tetranitrate	7.6×10^{3}		HSDB (2015)	V	
$C_5H_8N_4O_{12}$	1.2		Yaws (2003)	X	238
[78-11-5]	8.2×10^{5}		Zhang et al. (2010)	Q	288, 289
TZRXHJWUDPFEEY-UHFFFAOYSA-N	1.1×10^{4}		Zhang et al. (2010)	Q	288, 290
	7.9×10^{4}		Zhang et al. (2010)	Q	288, 291
	3.6×10^{3}		Zhang et al. (2010)	Q	288, 292
	1.2		Gharagheizi et al. (2010)	Q	247
1-hexyl nitrate	7.6×10^{-3}	6700	Hauff et al. (1998)	M	
$C_6H_{13}ONO_2$	3.6×10^{-3}		Hauff et al. (1998)	V	
[20633-11-8]	8.8×10^{-3}		Keshavarz et al. (2022)	Q	
AGDYNDJUZRMYRG-UHFFFAOYSA-N	1.5×10^{-2}		Duchowicz et al. (2020)	Q	185
	5.8×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.0×10^{-2}		Wang et al. (2017)	Q	81, 240
	2.4×10^{-4}		Wang et al. (2017)	Q	81, 241
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	9.5×10^{-3}		Hilal et al. (2008)	Q	
	3.1×10^{-2}		Modarresi et al. (2007)	Q	68
		6600	Kühne et al. (2005)	Q	
	6.6×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		6700	Kühne et al. (2005)	?	
2-nitrooxyethanol	3.9×10^{2}		Burkholder et al. (2019)	L	
$HOC_2H_4ONO_2$	3.9×10^{2}		Burkholder et al. (2015)	L	
[16051-48-2]	3.9×10^{2}		Sander et al. (2011)	L	
HTKIMWYSDZQQBP-UHFFFAOYSA-N	3.9×10^{2}		Sander et al. (2006)	L	
	3.8×10^{2}	8600	Shepson et al. (1996)	M	
	3.9×10^{2}		Kames and Schurath (1992)	M	12
	5.7×10^{1}		Keshavarz et al. (2022)	Q	
	9.0×10^{-1}		Duchowicz et al. (2020)	Q	300
	4.2×10^{1}		Wang et al. (2017)	Q	81, 239
	5.5×10^{2}		Wang et al. (2017)	Q	81, 240
	7.6		Wang et al. (2017)	Q	81, 241
	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{2}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{2}		Raventos-Duran et al. (2010)	Q	246
	1.7×10^{2}		Hilal et al. (2008)	Q	
	8.5×10^{1}		Modarresi et al. (2007)	Q	68
		9200	Kühne et al. (2005)	Q	
	3.8×10^{2}		Duchowicz et al. (2020)	?	186, 21
		8700	Kühne et al. (2005)	?	

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-nitrooxy-2-propanol	6.6×10^{1}		Burkholder et al. (2019)	L	
$C_3H_7O_4N$	6.6×10^{1}		Burkholder et al. (2015)	L	
[20266-65-3]	6.6×10^{1}		Sander et al. (2011)	L	
OMDFJTSKBNDDRM-UHFFFAOYSA-N	6.6×10^{1}		Sander et al. (2006)	L	
	1.1×10^{2}	10000	Shepson et al. (1996)	M	
	6.6×10^{1}		Kames and Schurath (1992)	M	580, 12
	7.2×10^{1}		Kames and Schurath (1992)	M	580, 12
	7.7×10^{1}		Keshavarz et al. (2022)	Q	
	9.3×10^{-1}		Duchowicz et al. (2020)	Q	
	3.9×10^{1}		Wang et al. (2017)	Q	81, 239
	3.6×10^{2}		Wang et al. (2017)	Q	81, 240
	1.7		Wang et al. (2017)	Q	81, 241
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{2}		Raventos-Duran et al. (2010)	Q	246
	9.5×10^{1}		Hilal et al. (2008)	Q	
	5.5×10^{1}		Modarresi et al. (2007)	Q	68
	1.1×10^{2}		Duchowicz et al. (2020)	?	186, 21
2-nitrooxy-1-propanol	7.2×10^{1}		Burkholder et al. (2019)	L	
$C_3H_7O_4N$	7.2×10^{1}		Burkholder et al. (2015)	L	
[20266-74-4]	7.2×10^{1}		Sander et al. (2011)	L	
HGCMMKIIGJXXMW-UHFFFAOYSA-N	7.2×10^{1}		Sander et al. (2006)	L	
	4.4×10^{1}	8800	Shepson et al. (1996)	M	
	6.6×10^{1}		Kames and Schurath (1992)	M	580, 12
	7.2×10^{1}		Kames and Schurath (1992)	M	580, 12
	7.7×10^{1}		Keshavarz et al. (2022)	Q	
	9.3×10^{-1}		Duchowicz et al. (2020)	Q	185
	3.9×10^{1}		Wang et al. (2017)	Q	81, 239
	2.7×10^{2}		Wang et al. (2017)	Q	81, 240
	1.6		Wang et al. (2017)	Q	81, 241
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{2}		Raventos-Duran et al. (2010)	Q	246
	8.6×10^{1}		Hilal et al. (2008)	Q	
	6.9×10^{1}		Modarresi et al. (2007)	Q	68
	4.4×10^{1}		Duchowicz et al. (2020)	?	186, 21
1-nitrooxy-2-butanol	8.9×10^{1}		Treves et al. (2000)	M	28
$C_4H_9O_4N$	5.7×10^{1}	9200	Shepson et al. (1996)	M	
[147794-11-4]	1.0×10^{2}		Keshavarz et al. (2022)	Q	
KNUQGVIXAYDSOX-UHFFFAOYSA-N	1.7		Duchowicz et al. (2020)	Q	300
	3.2×10^{1}		Wang et al. (2017)	Q	81, 239
	1.9×10^{2}		Wang et al. (2017)	Q	81, 240
	1.1		Wang et al. (2017)	Q	81, 241
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	246
	6.1×10^{1}		Hilal et al. (2008)	Q	
	5.4×10^{1}		Modarresi et al. (2007)	Q	68
	5.7×10^{1}		Duchowicz et al. (2020)	?	186, 21
2-nitrooxy-1-butanol	8.8×10^{1}		Treves et al. (2000)	M	28
$C_4H_9O_4N$	5.9×10^{1}	9600	Shepson et al. (1996)	M	
[147794-12-5]	1.0×10^{2}		Keshavarz et al. (2022)	Q	
YXMNEYKMHSBVTD-UHFFFAOYSA-N	1.7		Duchowicz et al. (2020)	Q	300
	3.2×10^{1}		Wang et al. (2017)	Q	81, 239
	1.6×10^{2}		Wang et al. (2017)	Q	81, 240
	1.6		Wang et al. (2017)	Q	81, 241
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{1}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	246
	6.0×10^{1}		Hilal et al. (2008)	Q	
	5.4×10^{1}		Modarresi et al. (2007)	Q	68
	5.9×10^{1}		Duchowicz et al. (2020)	?	186, 21
2-nitrooxy-3-butanol	1.0×10^{2}	9500	Shepson et al. (1996)	M	
$C_4H_9O_4N$	1.0×10^{2}		Keshavarz et al. (2022)	Q	
[147794-10-3]	6.8×10^{-1}		Duchowicz et al. (2020)	Q	300
CGFCSKMZZXPWEY-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	81, 239
	2.0×10^{2}		Wang et al. (2017)	Q	81, 240
	9.3×10^{-1}		Wang et al. (2017)	Q	81, 241
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	272, 244
	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	246
	5.4×10^{1}		Hilal et al. (2008)	Q	
	7.4×10^{1}		Modarresi et al. (2007)	Q	68
	1.0×10^{2}		Duchowicz et al. (2020)	?	186, 21
3-nitrooxy-1-butanol	1.4×10^{2}		Treves et al. (2000)	M	28
$C_4H_9O_4N$	2.6×10^{1}		Wang et al. (2017)	Q	81, 239
FOHXKGXDMSQVTH-UHFFFAOYSA-N	5.1×10^{2}		Wang et al. (2017)	Q	81, 240
	5.0		Wang et al. (2017)	Q	81, 241
4-nitrooxy-1-butanol	2.9×10^{2}		Treves et al. (2000)	M	28
$C_4H_9O_4N$	2.2×10^{1}		Wang et al. (2017)	Q	81, 239
[22911-39-3]	7.4×10^{2}		Wang et al. (2017)	Q	81, 240
FBOGSWRRYABFKU-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
4-nitrooxy-2-butanol	1.3×10^{2}		Treves et al. (2000)	M	28
$C_4H_9O_4N$	2.6×10^{1}		Wang et al. (2017)	Q	81, 239
(3-hydroxy-1-nitrooxy-butane)	6.5×10^{2}		Wang et al. (2017)	Q	81, 240
[141299-18-5]	3.4		Wang et al. (2017)	Q	81, 241
WUKDMTQXKGFHBU-UHFFFAOYSA-N					

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
4-nitrooxy-1-pentanol	2.0×10^2		Treves et al. (2000)	M	28
$C_5H_{11}O_4N$	2.0×10^1		Wang et al. (2017)	Q	81, 239
SVIFKHUNGQLAEN-UHFFFAOYSA-N	3.4×10^2		Wang et al. (2017)	Q	81, 240
	1.3×10^1		Wang et al. (2017)	Q	81, 241
5-nitrooxy-1-pentanol	2.0×10^2		Ebert et al. (2023)	?	581
$C_5H_{11}O_4N$					
DVOSRLSVEOCANS-UHFFFAOYSA-N					
5-nitrooxy-2-pentanol	3.6×10^2		Treves et al. (2000)	M	28
$C_5H_{11}O_4N$	2.1×10^1	9900	Wieser et al. (2023)	Q	439
(MCM:HO2C5NO3)	2.0×10^1		Wang et al. (2017)	Q	81, 239
RIQPKERROQFFJK-UHFFFAOYSA-N	4.4×10^2		Wang et al. (2017)	Q	81, 240
	6.5		Wang et al. (2017)	Q	81, 241
1-nitrooxy-2-propanone	1.0×10^1		Burkholder et al. (2019)	L	
$CH_3COCH_2ONO_2$	1.0×10^1		Burkholder et al. (2015)	L	
(nitrooxyacetone)	1.0×10^1		Sander et al. (2011)	L	
[6745-71-7]	1.0×10^1		Sander et al. (2006)	L	
ISWXYJQANHQYSR-UHFFFAOYSA-N	1.0×10^1		Kames and Schurath (1992)	M	12
	7.6		Wang et al. (2017)	Q	81, 239
	1.4×10^2		Wang et al. (2017)	Q	81, 240
	5.0×10^{-1}		Wang et al. (2017)	Q	81, 241
	2.5×10^1		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^1		Raventos-Duran et al. (2010)	Q	245
	7.8×10^1		Raventos-Duran et al. (2010)	Q	246
	1.2×10^2		Hilal et al. (2008)	Q	
ISOP1N6CO	2.1×10^5	14000	Wieser et al. (2023)	Q	439
$C_5H_7NO_5$					
XXORYENTKCFFSM-UHFFFAOYSA-N					
C52COCONO2	6.7×10^1	11000	Wieser et al. (2023)	Q	439
$C_5H_7NO_5$					
QJXLMYNMVOSKND-UHFFFAOYSA-N					
ISOP1N23O4CO	1.5×10^3	12000	Wieser et al. (2023)	Q	439
$C_5H_7NO_5$					
WBVYILWVTRBTDJ-UHFFFAOYSA-N					
ROO6R7ONO2	7.5×10^4	13000	Wieser et al. (2023)	Q	439
$C_6H_{11}NO_5$					
COKJDYWOSQONMU-UHFFFAOYSA-N					
2-heptyl nitrate	2.3×10^{-3}	6600	Wieser et al. (2023)	Q	439
$C_7H_{15}NO_3$					
(C7H15ONO2)					
HHXLSUKHLTZWKR-UHFFFAOYSA-N					

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
C7OHONO2 $C_7H_{15}NO_4$ MZJHMUSTUUJGSJ-UHFFFAOYSA-N	1.2×10^{1}	11000	Wieser et al. (2023)	Q	439
C622CONO2 $C_7H_{11}NO_5$ DJCVHBPUJHAWIU-UHFFFAOYSA-N	9.9×10^{2}	14000	Wieser et al. (2023)	Q	439
2-octyl nitrate $C_8H_{17}NO_3$ (C8H17ONO2) QCOKASLKYUXYJH-UHFFFAOYSA-N	6.8	7000	Wieser et al. (2023)	Q	439
C8OHONO2 $C_8H_{17}NO_4$ UEQWMROPIQKFIM-UHFFFAOYSA-N	9.0	11000	Wieser et al. (2023)	Q	439
C824ONO2 $C_8H_{13}NO_5$ YMYILPYDFNRVBZ-UHFFFAOYSA-N	9.5×10^{6}	14000	Wieser et al. (2023)	Q	439
C819ONO2 $C_8H_{13}NO_6$ XLUWXWLWQTYVOF-UHFFFAOYSA-N	3.9×10^{6}	16000	Wieser et al. (2023)	Q	439
C92ONO2 $C_9H_{15}NO_5$ PNFDSIMYWKOAKE-UHFFFAOYSA-N	4.7×10^{5}	15000	Wieser et al. (2023)	Q	439
NORLIMONO2 $C_9H_{15}NO_6$ MUTWZANDXPDWFF-UHFFFAOYSA-N	3.8×10^{8}	16000	Wieser et al. (2023)	Q	439
C822CONO2 $C_9H_{13}NO_5$ RVFLVBTUEWAABB-UHFFFAOYSA-N	6.2×10^{1}	13000	Wieser et al. (2023)	Q	439
C817CONO2 $C_9H_{13}NO_6$ LHFXXFGIVAQFTO-UHFFFAOYSA-N	1.2×10^{5}	15000	Wieser et al. (2023)	Q	439
C9CONO2 $C_{10}H_{15}NO_5$ FNVMVXZLPDKVAS-UHFFFAOYSA-N	8.0×10^{1}	20000	Wieser et al. (2023)	Q	439
LIMONO2 $C_{10}H_{15}NO_5$ DEKWHDOXDJNWRD-UHFFFAOYSA-N	3.8×10^{4}	14000	Wieser et al. (2023)	Q	439

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1,2-ethanediol dinitrate	6.3		Burkholder et al. (2019)	L	
$O_3NCH_2CH_2ONO_2$	6.3		Burkholder et al. (2015)	L	
(1,2-ethane dinitrate)	6.3		Sander et al. (2011)	L	
[628-96-6]	6.3		Sander et al. (2006)	L	
UQXKXGWGFRWILX-UHFFFAOYSA-N	7.8×10^{-1}		Fischer and Ballschmiter (1998b)	M	582
	6.3		Kames and Schurath (1992)	M	12
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	9.9		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	246
	8.2		Hilal et al. (2008)	Q	
	4.9×10^{-1}		Modarresi et al. (2007)	Q	68
1,2-propanediol dinitrate	1.7		Burkholder et al. (2019)	L	
$C_3H_6(ONO_2)_2$	1.7		Burkholder et al. (2015)	L	
(1,2-propane dinitrate)	1.7		Sander et al. (2011)	L	
[6423-43-4]	1.7		Sander et al. (2006)	L	
PSXCGTLGGVDWFU-UHFFFAOYSA-N	3.2×10^{-1}		Fischer and Ballschmiter (1998b)	M	582
	1.7		Kames and Schurath (1992)	M	12
	1.0×10^{1}		HSDB (2015)	Q	100
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	3.1		Raventos-Duran et al. (2010)	Q	245
	9.9		Raventos-Duran et al. (2010)	Q	246
	2.7		Hilal et al. (2008)	Q	
1,3-propanediol dinitrate	1.6		Burkholder et al. (2019)	L	583
$C_3H_6N_2O_6$	1.6		Burkholder et al. (2015)	L	584
[3457-90-7]	1.3		Fischer and Ballschmiter (1998b)	M	582
KOSAMXZBGUIISK-UHFFFAOYSA-N	1.2		Raventos-Duran et al. (2010)	Q	243, 244
	3.9		Raventos-Duran et al. (2010)	Q	245
	9.9		Raventos-Duran et al. (2010)	Q	246
	4.4		Hilal et al. (2008)	Q	
1,2,3-propanetriol trinitrate	2.3×10^{2}		HSDB (2015)	V	
$C_3H_5N_3O_9$	1.9×10^{2}		Yaws (2003)	X	238, 12
(nitroglycerin)	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
[55-63-0]	3.9×10^{2}		Raventos-Duran et al. (2010)	Q	245
SNIOPGDIGTZGOP-UHFFFAOYSA-N	3.9×10^{3}		Raventos-Duran et al. (2010)	Q	246
	1.9×10^{2}		Gharagheizi et al. (2010)	Q	247
	3.9×10^{1}		Hilal et al. (2008)	Q	
	1.0×10^{2}		Yaws (1999)	?	21, 12
1,2-butanediol dinitrate	2.1×10^{-1}		Fischer and Ballschmiter (1998b)	M	582
$C_4H_8N_2O_6$	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
[20820-41-1]	1.6		Raventos-Duran et al. (2010)	Q	245
CTISQZXTUUHJNC-UHFFFAOYSA-N	7.8		Raventos-Duran et al. (2010)	Q	246

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1,3-butanediol dinitrate	5.7×10^{-1}		Fischer and Ballschmiter (1998b)	M	582
$C_4H_8N_2O_6$	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
[6423-44-5]	1.6		Raventos-Duran et al. (2010)	Q	245
DGFBULNMARLFTH-UHFFFAOYSA-N	7.8		Raventos-Duran et al. (2010)	Q	246
1,4-butanediol dinitrate	1.6		Fischer and Ballschmiter (1998b)	M	582
$C_4H_8N_2O_6$	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
[3457-91-8]	3.1		Raventos-Duran et al. (2010)	Q	245
QELUAJBXJAWSRC-UHFFFAOYSA-N	7.8		Raventos-Duran et al. (2010)	Q	246
	2.7		Hilal et al. (2008)	Q	
2,3-butanediol dinitrate	1.2×10^{-1}		Fischer and Ballschmiter (1998b)	M	582
$C_4H_8N_2O_6$	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
[6423-45-6]	1.6		Raventos-Duran et al. (2010)	Q	245
RVDDYBGRQLZMSB-UHFFFAOYSA-N	7.8		Raventos-Duran et al. (2010)	Q	246
1,2-pentanediol dinitrate	1.3×10^{-1}		Fischer and Ballschmiter (1998b)	M	582
$C_5H_{10}N_2O_6$					
[89365-05-9]					
MZWHVGLDAWPHHW-UHFFFAOYSA-N					
1,4-pentanediol dinitrate	3.9×10^{-1}		Fischer and Ballschmiter (1998b)	M	582
$C_5H_{10}N_2O_6$					
[25385-63-1]					
IUTIKUKYGRINOD-UHFFFAOYSA-N					
1,5-pentanediol dinitrate	1.2		Fischer and Ballschmiter (1998b)	M	582
$C_5H_{10}N_2O_6$	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
[3457-92-9]	2.0		Raventos-Duran et al. (2010)	Q	245
MIYIEPHJPVBSEV-UHFFFAOYSA-N	6.2		Raventos-Duran et al. (2010)	Q	246
(2R,4S)-2,4-pentanediol dinitrate	2.2×10^{-1}		Fischer and Ballschmiter (1998b)	M	582
$C_5H_{10}N_2O_6$					
(*cis*-2,4-pentanediol dinitrate)					
[208252-05-5]					
(2R,4R)-2,4-pentanediol dinitrate	1.4×10^{-1}		Fischer and Ballschmiter (1998b)	M	582
$C_5H_{10}N_2O_6$					
(*trans*-2,4-pentanediol dinitrate)					
[208252-04-4]					
1,2-hexanediol dinitrate	9.6×10^{-2}		Fischer and Ballschmiter (1998b)	M	582
$C_6H_{12}N_2O_6$					
[110539-07-6]					
UJKJGCZXZPXTGS-UHFFFAOYSA-N					
1,5-hexanediol dinitrate	2.7×10^{-1}		Fischer and Ballschmiter (1998b)	M	582
$C_6H_{12}N_2O_6$					
[206443-83-6]					
PGDWEAOSOZNKFU-UHFFFAOYSA-N					

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1,6-hexanediol dinitrate $C_6H_{12}N_2O_6$ [3457-93-0] GCVAYIWGKFFWEU-UHFFFAOYSA-N	1.5		Fischer and Ballschmiter (1998b)	M	582
2,5-hexanediol dinitrate $C_6H_{12}N_2O_6$ [99115-63-6] ISSLCMSTXXUOEU-UHFFFAOYSA-N	3.1×10^{-1} 6.2×10^{-1} 6.2×10^{-1} 4.9		Fischer and Ballschmiter (1998b) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010)	M Q Q Q	582 272, 244 245 246
(1R,2S)-1,2-cyclohexanediol dinitrate $C_6H_{10}N_2O_6$ (*cis*-1,2-cyclohexanediol dinitrate) [32342-28-2]	1.3		Fischer and Ballschmiter (1998b)	M	582
(1R,2R)-1,2-cyclohexanediol dinitrate $C_6H_{10}N_2O_6$ (*trans*-1,2-cyclohexanediol dinitrate) [32342-29-3]	5.2×10^{-1}		Fischer and Ballschmiter (1998b)	M	582
(1R,3S)-1,3-cyclohexanediol dinitrate $C_6H_{10}N_2O_6$ (*cis*-1,3-cyclohexanediol dinitrate) [170994-36-2]	3.4		Fischer and Ballschmiter (1998b)	M	582
(1R,3R)-1,3-cyclohexanediol dinitrate $C_6H_{10}N_2O_6$ (*trans*-1,3-cyclohexanediol dinitrate) [170994-41-9]	6.8×10^{-1}		Fischer and Ballschmiter (1998b)	M	582
1,7-heptanediol dinitrate $C_7H_{14}N_2O_6$ [3457-94-1] KIERETFMVSIXIJ-UHFFFAOYSA-N	1.1		Fischer and Ballschmiter (1998b)	M	582
(1R,2R)-1,2-cycloheptanediol dinitrate $C_7H_{12}N_2O_6$ (*trans*-1,2-cycloheptanediol dinitrate) [208252-06-6]	8.8×10^{-1}		Fischer and Ballschmiter (1998b)	M	582

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1,2-octanediol dinitrate $C_8H_{16}N_2O_6$ [121222-48-8] RLNKMZWMCSTIEM-UHFFFAOYSA-N	5.2×10^{-2}		Fischer and Ballschmiter (1998b)	M	582
1,8-octanediol dinitrate $C_8H_{16}N_2O_6$ [3457-95-2] BVIHOKFRPSZJEI-UHFFFAOYSA-N	7.8×10^{-1}		Fischer and Ballschmiter (1998b)	M	582
1,2-decanediol dinitrate $C_{10}H_{20}N_2O_6$ [60123-40-2] KKNGVXOJDIUADE-UHFFFAOYSA-N	2.0×10^{-2}		Fischer and Ballschmiter (1998b)	M	582
1,10-decanediol dinitrate $C_{10}H_{20}N_2O_6$ [3457-97-4] RHUZOYMELURURD-UHFFFAOYSA-N	4.3×10^{-1}		Fischer and Ballschmiter (1998b)	M	582
diethylene glycol dinitrate $C_4H_8N_2O_7$ [693-21-0] LYAGTVMJGHTIDH-UHFFFAOYSA-N	2.5×10^{1} 4.9×10^{1} 1.2×10^{2} 9.9×10^{2} 1.1×10^{2} 3.8		HSDB (2015) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Hilal et al. (2008) Modarresi et al. (2007)	V Q Q Q Q Q	 243, 244 245 246 68
ISOP1N2ONO2 $C_5H_8N_2O_6$ FQSKJUXVWIFNKX-UHFFFAOYSA-N	1.6	9400	Wieser et al. (2023)	Q	439
EPXISOPNONO2 $C_5H_8N_2O_7$ UAFKAIYDADHRMX-UHFFFAOYSA-N	5.3×10^{1}	13000	Wieser et al. (2023)	Q	439
ISOP1N23O4ONO2 $C_5H_8N_2O_7$ FSZUIXLMCRZJMS-UHFFFAOYSA-N	4.5×10^{1}	13000	Wieser et al. (2023)	Q	439
ISOP1N5ONO2 $C_5H_8N_2O_7$ WRGRJJOKHABEJT-UHFFFAOYSA-N	5.8×10^{4}	13000	Wieser et al. (2023)	Q	439
LIMAB15ONO22 $C_{10}H_{18}N_2O_8$ UNHNJOVXNACOSQ-UHFFFAOYSA-N	3.1×10^{7}	18000	Wieser et al. (2023)	Q	439

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
peroxyacetyl nitrate	2.8×10^{-2}	5700	Burkholder et al. (2019)	L	
$CH_3COOONO_2$	2.8×10^{-2}	5700	Burkholder et al. (2015)	L	
(PAN)	2.9×10^{-2}	5700	Warneck and Williams (2012)	L	
[2278-22-0]	2.8×10^{-2}	5700	Sander et al. (2011)	L	
VGQXTTSVLMQFHM-UHFFFAOYSA-N	2.8×10^{-2}	5700	Sander et al. (2006)	L	
	2.9×10^{-2}	5800	Leu and Zhang (1999)	L	
	3.0×10^{-2}	5600	Easterbrook et al. (2023)	M	
	2.3×10^{-2}	4800	Frenzel et al. (2000)	M	
	4.0×10^{-2}		Kames and Schurath (1995)	M	12
	2.8×10^{-2}	6500	Kames et al. (1991)	M	
	4.9×10^{-2}		Holdren et al. (1984)	M	375
	3.6×10^{-2}		Gaffney and Senum (1984)	X	391
	2.9×10^{-2}	5900	Pandis and Seinfeld (1989)	C	
	3.6×10^{-2}		Schwartz (1986)	C	88
	6.8×10^{-2}		Keshavarz et al. (2022)	Q	
	6.1×10^{-1}		Duchowicz et al. (2020)	Q	185
	4.9		Wang et al. (2017)	Q	81, 239
	1.0×10^{1}		Wang et al. (2017)	Q	81, 240
	7.4×10^{-4}		Wang et al. (2017)	Q	81, 241
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	4.9		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.2		Hilal et al. (2008)	Q	
	3.2		Modarresi et al. (2007)	Q	68
		4800	Kühne et al. (2005)	Q	
	3.6×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		6300	Kühne et al. (2005)	?	
			Warneck et al. (1996)	?	585
			Schurath et al. (1996)	W	586
peroxypropionyl nitrate	1.6×10^{-2}	6000	Easterbrook et al. (2023)	M	
$C_2H_5COOONO_2$	2.9×10^{-2}		Kames and Schurath (1995)	M	12
(PPN)	3.9		Wang et al. (2017)	Q	81, 239
[5796-89-4]	4.1		Wang et al. (2017)	Q	81, 240
TXINBPKSWKFMNB-UHFFFAOYSA-N	3.6×10^{-4}		Wang et al. (2017)	Q	81, 241
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
			Warneck et al. (1996)	?	585
			Schurath et al. (1996)	W	587

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
nitro butaneperoxoate	2.3×10^{-2}		Kames and Schurath (1995)	M	12
$C_3H_7COOONO_2$	3.2		Wang et al. (2017)	Q	81, 239
(PnBN)	2.2		Wang et al. (2017)	Q	81, 240
[27746-48-1]	2.6×10^{-4}		Wang et al. (2017)	Q	81, 241
HZUMMZVMNQSPFF-UHFFFAOYSA-N	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
			Warneck et al. (1996)	?	585
			Schurath et al. (1996)	W	588
peroxy-2-propenoyl nitrate	1.7×10^{-2}		Kames and Schurath (1995)	M	12
$CH_2C(CH_3)COOONO_2$	7.4		Wang et al. (2017)	Q	81, 239
(peroxymethacryloyl nitrate; MPAN)	4.8		Wang et al. (2017)	Q	81, 240
[88181-75-3]	2.4×10^{-4}		Wang et al. (2017)	Q	81, 241
LLZWPQFQEBKRLX-UHFFFAOYSA-N			Warneck et al. (1996)	W	585
			Schurath et al. (1996)	W	589
peroxy-isobutyryl nitrate	9.9×10^{-3}		Kames and Schurath (1995)	M	12
$C_3H_7COOONO_2$	3.6		Wang et al. (2017)	Q	81, 239
(PiBN)	2.3		Wang et al. (2017)	Q	81, 240
[65424-60-4]	1.8×10^{-4}		Wang et al. (2017)	Q	81, 241
BDNFHGUXBRZLRQ-UHFFFAOYSA-N	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	246
			Warneck et al. (1996)	?	585
			Schurath et al. (1996)	W	590
furoyl peroxynitrate	9.3×10^{-2}	8800	Roberts et al. (2022)	M	
$C_5H_3NO_6$	1.6×10^{-1}		Roberts et al. (2022)	Q	591
(fur-PAN)					
NMNZVYLGOWCHOD-UHFFFAOYSA-N					
MCM:CH3O2NO2	4.1×10^{-1}		Wang et al. (2017)	Q	81, 239
CH_3NO_4	1.5×10^{-1}		Wang et al. (2017)	Q	81, 240
LCFGXMPUQSXLCQ-UHFFFAOYSA-N	1.7×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:ETHO2HNO3	9.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_5NO_5$	2.8×10^{3}		Wang et al. (2017)	Q	81, 240
IYCQDYYQELIXMU-UHFFFAOYSA-N	3.1		Wang et al. (2017)	Q	81, 241
MCM:NO3CH2CO3H	1.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_2H_3NO_6$	2.3×10^{3}		Wang et al. (2017)	Q	81, 240
VLCOOHYMNNDETJ-UHFFFAOYSA-N	4.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:NO3CH2PAN	5.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_2N_2O_8$	1.9×10^{3}		Wang et al. (2017)	Q	81, 240
CSNUPQYBRZIENU-UHFFFAOYSA-N	3.0×10^{-4}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:ACRPAN	1.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_3H_3NO_5$	7.4		Wang et al. (2017)	Q	81, 240
[157258-66-7]	4.6×10^{-4}		Wang et al. (2017)	Q	81, 241
SFKRQQJZRXQGLC-UHFFFAOYSA-N	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	3.1		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	246
MCM:PR1O2HNO3	8.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_3H_7NO_5$	1.0×10^{3}		Wang et al. (2017)	Q	81, 240
FROUFTMXOYPVCX-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	81, 241
MCM:PR2O2HNO3	8.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_3H_7NO_5$	1.1×10^{3}		Wang et al. (2017)	Q	81, 240
UHIVGIHVGRYUPL-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	81, 241
MCM:PRNO3CO3H	1.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_3H_5NO_6$	1.0×10^{3}		Wang et al. (2017)	Q	81, 240
FMRKJWQAPYMRJD-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	81, 241
MCM:PRNO3PAN	5.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_3H_4N_2O_8$	4.6×10^{2}		Wang et al. (2017)	Q	81, 240
ZLJYZUGEJFPONP-UHFFFAOYSA-N	1.6×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:BU1ENO3OOH	6.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_5$	5.5×10^{2}		Wang et al. (2017)	Q	81, 240
MFTWJXGCASCYHP-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	81, 241
MCM:C3DBPAN	1.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_5$	5.8		Wang et al. (2017)	Q	81, 240
YVSVRLGWMDVSPN-UHFFFAOYSA-N	1.2×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:C42NO33OOH	8.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_5$	5.1×10^{2}		Wang et al. (2017)	Q	81, 240
CGBCWMNQUOIZIB-UHFFFAOYSA-N	9.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C43NO34OOH	6.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_5$	5.5×10^{2}		Wang et al. (2017)	Q	81, 240
BQDGWSCZHPCGGT-UHFFFAOYSA-N	6.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C4PAN9	1.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_4N_2O_8$	2.3×10^{3}		Wang et al. (2017)	Q	81, 240
SHASFEZZYJNCIM-UHFFFAOYSA-N	5.4×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:MPRANO3OOH	4.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_5$	3.2×10^{2}		Wang et al. (2017)	Q	81, 240
DTPMQEMACNJTBJ-UHFFFAOYSA-N	9.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:MPRBNO3OOH	4.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_5$	3.5×10^{2}		Wang et al. (2017)	Q	81, 240
RCQWCNCMOFDCKD-UHFFFAOYSA-N	5.1		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MPRBNO3PAN	2.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_6N_2O_8$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
RAYRXKOIFAVDJK-UHFFFAOYSA-N	2.1×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:MPRNO3CO3H	6.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	2.2×10^{2}		Wang et al. (2017)	Q	81, 240
HDNCPEGDTKOFQI-UHFFFAOYSA-N	5.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:NBUTDAOOH	2.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_5$	1.2×10^{3}		Wang et al. (2017)	Q	81, 240
ZIAMBHNGSMXNCM-UHFFFAOYSA-N	6.3		Wang et al. (2017)	Q	81, 241
MCM:NBUTDBNO3	4.1		Wang et al. (2017)	Q	81, 239
$C_4H_6N_2O_6$	3.6×10^{1}		Wang et al. (2017)	Q	81, 240
GCQJZAFTGYZGDG-UHFFFAOYSA-N	1.4×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:NBUTDBOOH	2.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_5$	4.0×10^{3}		Wang et al. (2017)	Q	81, 240
SSNXKZNERJCDKO-UHFFFAOYSA-N	5.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NC3CO3H	3.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_6$	5.0×10^{3}		Wang et al. (2017)	Q	81, 240
ZXNVOGOFZJSFAE-UHFFFAOYSA-N	3.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:TC4H9NO3	6.2×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_3$	9.1×10^{-3}		Wang et al. (2017)	Q	81, 240
[926-05-6]	1.0×10^{-3}		Wang et al. (2017)	Q	81, 241
AZAKMLHUDVIDFN-UHFFFAOYSA-N	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	246
MCM:C3ME3PAN	2.8		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	1.7		Wang et al. (2017)	Q	81, 240
OLNWAQLSTCXURT-UHFFFAOYSA-N	1.6×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:C3MNO3CO3H	9.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	3.2×10^{2}		Wang et al. (2017)	Q	81, 240
UNTXQXBLSROXLI-UHFFFAOYSA-N	2.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C3MNO3PAN	3.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_8$	1.6×10^{2}		Wang et al. (2017)	Q	81, 240
ULZBZSVLLIBTGC-UHFFFAOYSA-N	1.0×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:C43NO3CO3H	5.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	1.3×10^{2}		Wang et al. (2017)	Q	81, 240
KYFRJEXZVMOAMN-UHFFFAOYSA-N	1.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C43NO3PAN	2.2×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_8$	6.6×10^{1}		Wang et al. (2017)	Q	81, 240
WPFKHDFVFPXDFZ-UHFFFAOYSA-N	1.3×10^{-4}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:C4M2NO3OOH	4.5×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_5$	1.6×10^{2}		Wang et al. (2017)	Q	81, 240
BOAAVKBCMOPNIQ-UHFFFAOYSA-N	5.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C4MNO31OOH	6.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_5$	3.2×10^{2}		Wang et al. (2017)	Q	81, 240
LRRBWUKXCGVENZ-UHFFFAOYSA-N	7.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C4MNO32OOH	6.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_5$	3.2×10^{2}		Wang et al. (2017)	Q	81, 240
HXNZNKRZULBVRO-UHFFFAOYSA-N	4.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C4NO32MOOH	3.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_5$	1.7×10^{2}		Wang et al. (2017)	Q	81, 240
HCKTYRRBEFAEAC-UHFFFAOYSA-N	5.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C4NO3CO3H	8.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	3.0×10^{2}		Wang et al. (2017)	Q	81, 240
JPUVYTOGMBAUBQ-UHFFFAOYSA-N	1.7×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C4NO3M1OOH	3.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_5$	1.8×10^{2}		Wang et al. (2017)	Q	81, 240
MWSZSODDMCBKIX-UHFFFAOYSA-N	3.4		Wang et al. (2017)	Q	81, 241
MCM:C4NO3M2OOH	4.5×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_5$	1.5×10^{2}		Wang et al. (2017)	Q	81, 240
QXHHHGYKLMZJBA-UHFFFAOYSA-N	4.2		Wang et al. (2017)	Q	81, 241
MCM:C4NO3PAN	3.2×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_8$	1.6×10^{2}		Wang et al. (2017)	Q	81, 240
GGZFCBHNGNBLNW-UHFFFAOYSA-N	1.2×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:C51NO32OOH	6.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_5$	3.2×10^{2}		Wang et al. (2017)	Q	81, 240
YPLQKABNDDXYJG-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
MCM:C52NO31OOH	6.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_5$	3.2×10^{2}		Wang et al. (2017)	Q	81, 240
DCAGTGOPLFTTTQ-UHFFFAOYSA-N	4.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C52NO33OOH	6.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_5$	2.4×10^{2}		Wang et al. (2017)	Q	81, 240
FQGADFCNSPWVJM-UHFFFAOYSA-N	4.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C53NO32OOH	6.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_5$	2.6×10^{2}		Wang et al. (2017)	Q	81, 240
STNFTACLRXEYDM-UHFFFAOYSA-N	2.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C5PAN18	1.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_6N_2O_8$	2.2×10^{3}		Wang et al. (2017)	Q	81, 240
JYUXMKSXMIBDSN-UHFFFAOYSA-N	2.0×10^{-3}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C5PAN4	2.8		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	1.5		Wang et al. (2017)	Q	81, 240
LGNOWHJLTKBAFC-UHFFFAOYSA-N	1.3×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:C5PAN6	2.0		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	1.4		Wang et al. (2017)	Q	81, 240
VQRIYOXAZWZCOV-UHFFFAOYSA-N	1.6×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:IPEANO3	8.3×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_3$	1.5×10^{-2}		Wang et al. (2017)	Q	81, 240
QSSWLPYLLKHHLB-UHFFFAOYSA-N	4.0×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:IPEBNO3	8.3×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_3$	1.4×10^{-2}		Wang et al. (2017)	Q	81, 240
OTVLXFGCWJFXJU-UHFFFAOYSA-N	4.2×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:IPECNO3	5.1×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_3$	6.6×10^{-3}		Wang et al. (2017)	Q	81, 240
UENFRVTUGZKXNH-UHFFFAOYSA-N	7.6×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:NC4CO3H	2.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_6$	4.6×10^{3}		Wang et al. (2017)	Q	81, 240
SLKHOLOIOGBFQB-UHFFFAOYSA-N	1.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:NEOPNO3	5.1×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_3$	1.2×10^{-2}		Wang et al. (2017)	Q	81, 240
YJGBGWFCCCQXIM-UHFFFAOYSA-N	4.1×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:NISOPNO3	2.6	9400	Wieser et al. (2023)	Q	439
$C_5H_8N_2O_6$	2.7		Wang et al. (2017)	Q	81, 239
JGJBVRGABXKDRR-UHFFFAOYSA-N	3.0×10^{1}		Wang et al. (2017)	Q	81, 240
	1.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:NISOPOOH	9.7×10^{2}	11000	Wieser et al. (2023)	Q	439
$C_5H_9NO_5$	1.8×10^{3}		Wang et al. (2017)	Q	81, 239
IRFXVIPRKCCSLU-UHFFFAOYSA-N	3.0×10^{3}		Wang et al. (2017)	Q	81, 240
	3.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PPEN	2.8		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	1.5		Wang et al. (2017)	Q	81, 240
UUYNBJNAIGBJAO-UHFFFAOYSA-N	2.2×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:C42MNO3OOH	2.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_5$	4.5×10^{1}		Wang et al. (2017)	Q	81, 240
KKTQLMUUOWWZBO-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	81, 241
MCM:C62NO33OOH	5.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_5$	1.5×10^{2}		Wang et al. (2017)	Q	81, 240
PJRWVMFJYMZPCW-UHFFFAOYSA-N	4.2×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:C63NO32OOH	5.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_5$	1.9×10^{2}		Wang et al. (2017)	Q	81, 240
RLIDOIUHNSZVBK-UHFFFAOYSA-N	1.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C65NO36OOH	4.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_5$	2.2×10^{2}		Wang et al. (2017)	Q	81, 240
ZVRSMGCQHDCSBC-UHFFFAOYSA-N	2.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C65NO3CO3H	6.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	2.2×10^{2}		Wang et al. (2017)	Q	81, 240
RASQUKWKKRVIQJ-UHFFFAOYSA-N	1.4×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C65NO3PAN	3.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{10}N_2O_8$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
PNNYZMYYAAWSJH-UHFFFAOYSA-N	6.5×10^{-5}		Wang et al. (2017)	Q	81, 241
MCM:C66NO35OOH	4.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_5$	2.3×10^{2}		Wang et al. (2017)	Q	81, 240
YPVNGNKLOFDKIF-UHFFFAOYSA-N	9.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN10	2.6		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	1.3		Wang et al. (2017)	Q	81, 240
INNSDEOCGQAUTR-UHFFFAOYSA-N	1.8×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN15	1.6		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	9.8×10^{-1}		Wang et al. (2017)	Q	81, 240
GWYKJYISUPTXQD-UHFFFAOYSA-N	1.4×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN17	1.6		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	1.1		Wang et al. (2017)	Q	81, 240
CUMLTNLXWSMQLS-UHFFFAOYSA-N	1.7×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN18	3.0		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	1.4		Wang et al. (2017)	Q	81, 240
FPWBUKNMBKRQCI-UHFFFAOYSA-N	1.4×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN3	2.6		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	1.1		Wang et al. (2017)	Q	81, 240
BRVOFEXYGAZHOW-UHFFFAOYSA-N	1.5×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:CHEXNO3	2.0×10^{-2}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_3$	6.5×10^{-2}		Wang et al. (2017)	Q	81, 240
HLYOOCIMLHNMOG-UHFFFAOYSA-N	3.7×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:HEXBNO3	3.1×10^{-4}	6300	Wieser et al. (2023)	Q	439
$C_6H_{13}NO_3$	6.5×10^{-3}		Wang et al. (2017)	Q	81, 239
JLGBOJJVQLNMGV-UHFFFAOYSA-N	7.4×10^{-3}		Wang et al. (2017)	Q	81, 240
	4.3×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:HEXCNO3	6.5×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_3$	8.1×10^{-3}		Wang et al. (2017)	Q	81, 240
OJOZCOXRANAOPV-UHFFFAOYSA-N	3.2×10^{-4}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:M22C43NO3	4.8×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_3$	9.3×10^{-3}		Wang et al. (2017)	Q	81, 240
YUZOHIKIQPTSGJ-UHFFFAOYSA-N	3.7×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:M22C4NO3	4.6×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_3$	1.0×10^{-2}		Wang et al. (2017)	Q	81, 240
JOWPFKXUGRKJFA-UHFFFAOYSA-N	5.5×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:M23C43NO3	4.8×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_3$	7.4×10^{-3}		Wang et al. (2017)	Q	81, 240
PMABLOPIFVACLQ-UHFFFAOYSA-N	7.4×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:M23C4NO3	7.8×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_3$	1.5×10^{-2}		Wang et al. (2017)	Q	81, 240
HHRFTVZVEUIWEO-UHFFFAOYSA-N	4.4×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:M2PEANO3	6.5×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_3$	1.1×10^{-2}		Wang et al. (2017)	Q	81, 240
CETUNBADQVCCRS-UHFFFAOYSA-N	3.4×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:M2PEBNO3	7.8×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_3$	7.8×10^{-3}		Wang et al. (2017)	Q	81, 240
AYWPQHSAUPNICG-UHFFFAOYSA-N	3.6×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:M2PECNO3	7.8×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_3$	9.6×10^{-3}		Wang et al. (2017)	Q	81, 240
ZLERWGPAWILHHJ-UHFFFAOYSA-N	3.2×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:M2PEDNO3	4.6×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_3$	5.1×10^{-3}		Wang et al. (2017)	Q	81, 240
LFIPHSRTIDHJFT-UHFFFAOYSA-N	6.5×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:M33C4NO3	4.6×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_3$	9.8×10^{-3}		Wang et al. (2017)	Q	81, 240
DENSRMRCUIZNMK-UHFFFAOYSA-N	3.6×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:M3PEANO3	6.5×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_3$	1.3×10^{-2}		Wang et al. (2017)	Q	81, 240
HRVRJIMBNILCGN-UHFFFAOYSA-N	4.7×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:M3PEBNO3	7.8×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_3$	1.1×10^{-2}		Wang et al. (2017)	Q	81, 240
IEHIEWLLOPOHIZ-UHFFFAOYSA-N	4.1×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:M3PECNO3	4.6×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_3$	5.3×10^{-3}		Wang et al. (2017)	Q	81, 240
GFKONLNVJRACGN-UHFFFAOYSA-N	6.2×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:PHXN	2.2		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	1.1		Wang et al. (2017)	Q	81, 240
ITHMZXMFOKWUTQ-UHFFFAOYSA-N	1.8×10^{-4}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:HEPTNO3	5.4×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_7H_{15}NO_3$	6.3×10^{-3}		Wang et al. (2017)	Q	81, 240
RFSNRWONUSBTJN-UHFFFAOYSA-N	3.0×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:M2HEXANO3	6.2×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_7H_{15}NO_3$	5.9×10^{-3}		Wang et al. (2017)	Q	81, 240
YZGBSAOHUZMZSL-UHFFFAOYSA-N	4.0×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:M2HEXBNO3	3.7×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_7H_{15}NO_3$	3.9×10^{-3}		Wang et al. (2017)	Q	81, 240
CORAYZMLWQTCOE-UHFFFAOYSA-N	5.8×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:M3HEXANO3	6.2×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_7H_{15}NO_3$	6.6×10^{-3}		Wang et al. (2017)	Q	81, 240
ZIINVFVZOGZDQJ-UHFFFAOYSA-N	3.4×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:M3HEXBNO3	3.7×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_7H_{15}NO_3$	4.4×10^{-3}		Wang et al. (2017)	Q	81, 240
ADYNXMRWYWNUDX-UHFFFAOYSA-N	6.5×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:PHPTN	1.8		Wang et al. (2017)	Q	81, 239
$C_7H_{13}NO_5$	8.9×10^{-1}		Wang et al. (2017)	Q	81, 240
XCJVDRQLXVBBEC-UHFFFAOYSA-N	2.0×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:C8BCNO3	4.0×10^{-2}		Wang et al. (2017)	Q	81, 239
$C_8H_{13}NO_3$	3.2×10^{-2}		Wang et al. (2017)	Q	81, 240
OSNOKXIMBITXOJ-UHFFFAOYSA-N	3.6×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:OCTNO3	4.8×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_8H_{17}NO_3$	5.0×10^{-3}		Wang et al. (2017)	Q	81, 240
KDICWCURMCOQTP-UHFFFAOYSA-N	2.6×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:NONNO3	3.9×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_9H_{19}NO_3$	3.8×10^{-3}		Wang et al. (2017)	Q	81, 240
YXUXBXICIGKFLH-UHFFFAOYSA-N	2.5×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:DECNO3	3.0×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{21}NO_3$	3.0×10^{-3}		Wang et al. (2017)	Q	81, 240
VRGDYCVXNCXQKR-UHFFFAOYSA-N	2.8×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:NAPINAOOH	1.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_5$	2.3×10^{2}		Wang et al. (2017)	Q	81, 240
IKGBGFRUISEOBM-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NAPINBOOH	1.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_5$	2.5×10^{2}		Wang et al. (2017)	Q	81, 240
RUHGEBIMHPPSGQ-UHFFFAOYSA-N	6.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NBPINAOOH	1.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_5$	4.4×10^{2}		Wang et al. (2017)	Q	81, 240
VJCKFKSOBAWLFB-UHFFFAOYSA-N	3.5		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:NBPINBOOH	1.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_5$	3.8×10^{2}		Wang et al. (2017)	Q	81, 240
AWECGRRBHMAEGP-UHFFFAOYSA-N	7.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NC91CO3H	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_6$	4.8×10^{2}		Wang et al. (2017)	Q	81, 240
TWWSFGIBZQJYPL-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	81, 241
MCM:NC91PAN	8.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{14}N_2O_8$	2.6×10^{2}		Wang et al. (2017)	Q	81, 240
LCMKIEFNSOTVJY-UHFFFAOYSA-N	9.8×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:NLIMOOH	1.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_5$	6.9×10^{2}		Wang et al. (2017)	Q	81, 240
HSXYRSLOXSIYGP-UHFFFAOYSA-N	5.3		Wang et al. (2017)	Q	81, 241
MCM:UDECNO3	2.8×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{23}NO_3$	2.4×10^{-3}		Wang et al. (2017)	Q	81, 240
KGEKWWIIMVPQKA-UHFFFAOYSA-N	2.0×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:DDECNO3	2.2×10^{-3}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{25}NO_3$	1.9×10^{-3}		Wang et al. (2017)	Q	81, 240
BVAQOKLOUKLOJD-UHFFFAOYSA-N	1.9×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:NBCOOH	1.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{25}NO_5$	8.7×10^{2}		Wang et al. (2017)	Q	81, 240
BEFFZATUSVKAHP-UHFFFAOYSA-N	3.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C6H5CH2NO3	4.3×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_7H_7NO_3$	7.1×10^{-1}		Wang et al. (2017)	Q	81, 240
WOIVNLSVAKYSKX-UHFFFAOYSA-N	3.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:PBZN	1.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_7H_5NO_5$	2.6×10^{1}		Wang et al. (2017)	Q	81, 240
ONDCXZPWEKXYJE-UHFFFAOYSA-N	4.4×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:C6H5C2NO3	3.6×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_3$	5.6×10^{-1}		Wang et al. (2017)	Q	81, 240
REJUUAZLLYKBCW-UHFFFAOYSA-N	4.2×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C6H5CH2PAN	1.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_7NO_5$	4.7×10^{1}		Wang et al. (2017)	Q	81, 240
KKRIGRPRRNIVGL-UHFFFAOYSA-N	1.2×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:MXYLNO3	2.5×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_3$	6.5×10^{-1}		Wang et al. (2017)	Q	81, 240
OIEIRDPNAPXLBC-UHFFFAOYSA-N	3.1×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:MXYLPAN	8.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_8H_7NO_5$	2.3×10^{1}		Wang et al. (2017)	Q	81, 240
HJGURQOGPAEQPE-UHFFFAOYSA-N	4.1×10^{-3}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NSTYRENOOH	3.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_5$	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
LKBHTMHNYICJQS-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:OXYLNO3	2.5×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_3$	7.1×10^{-1}		Wang et al. (2017)	Q	81, 240
WKRHODAGVPDBTG-UHFFFAOYSA-N	2.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:OXYLPAN	8.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_8H_7NO_5$	3.1×10^{1}		Wang et al. (2017)	Q	81, 240
TXXXSKKGTSQWKQ-UHFFFAOYSA-N	3.2×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:PXYLNO3	2.5×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_3$	7.8×10^{-1}		Wang et al. (2017)	Q	81, 240
SHZSDLPSACZYMH-UHFFFAOYSA-N	3.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:PXYLPAN	8.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_8H_7NO_5$	2.6×10^{1}		Wang et al. (2017)	Q	81, 240
ZGFUWGCXWYZODV-UHFFFAOYSA-N	6.5×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:ETOLNO3	2.3×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_3$	3.2×10^{-1}		Wang et al. (2017)	Q	81, 240
LYNFROWVHACAMO-UHFFFAOYSA-N	1.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:PHC3NO3	3.3×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_3$	2.2×10^{-1}		Wang et al. (2017)	Q	81, 240
IFDAHDBLKMQHMM-UHFFFAOYSA-N	1.8×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:PHIC3NO3	2.2×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_3$	1.5×10^{-1}		Wang et al. (2017)	Q	81, 240
YCCLKZYFPBVILU-UHFFFAOYSA-N	3.8×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:TM123BNO3	1.6×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_3$	9.8×10^{-1}		Wang et al. (2017)	Q	81, 240
GDXSVUXDQKEMHM-UHFFFAOYSA-N	3.0×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:TM123BPAN	5.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_9NO_5$	3.9×10^{1}		Wang et al. (2017)	Q	81, 240
VMALQUVLPIFIEM-UHFFFAOYSA-N	4.5×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:TM124BNO3	1.6×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_3$	9.3×10^{-1}		Wang et al. (2017)	Q	81, 240
VLXWVVSZKXVGNM-UHFFFAOYSA-N	3.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:TM124BPAN	5.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_9NO_5$	3.0×10^{1}		Wang et al. (2017)	Q	81, 240
SSMPYZHCWJGIJH-UHFFFAOYSA-N	7.4×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:TMBNO3	1.6×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_3$	5.5×10^{-1}		Wang et al. (2017)	Q	81, 240
CHDZRXQPKVNDRJ-UHFFFAOYSA-N	2.8×10^{-2}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:TMBPAN	5.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_9NO_5$	1.9×10^{1}		Wang et al. (2017)	Q	81, 240
QURBGWBLEPWFEF-UHFFFAOYSA-N	4.0×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:DM35EBNO3	1.4×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{13}NO_3$	2.4×10^{-1}		Wang et al. (2017)	Q	81, 240
CZPIEIXHJQQIGZ-UHFFFAOYSA-N	1.7×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:EMPHPAN	4.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{11}NO_5$	1.1×10^{1}		Wang et al. (2017)	Q	81, 240
DPRDWMVUHNTRQI-UHFFFAOYSA-N	3.2×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:DE35TNO3	1.1×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{15}NO_3$	1.5×10^{-1}		Wang et al. (2017)	Q	81, 240
XLLLSPDIGUQFTC-UHFFFAOYSA-N	1.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:PHAN	6.2×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_3NO_6$	9.6×10^{3}		Wang et al. (2017)	Q	81, 240
KMDWHTZYVJXWAH-UHFFFAOYSA-N	6.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:A2PAN	7.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_3H_5NO_7$	2.3×10^{6}		Wang et al. (2017)	Q	81, 240
RQFAVCUBLOXLKI-UHFFFAOYSA-N	2.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C3PAN1	1.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_3H_5NO_6$	3.2×10^{4}		Wang et al. (2017)	Q	81, 240
ZDHDBTZUUXEIQG-UHFFFAOYSA-N	6.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:HO1C3NO3	2.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_3H_7NO_4$	1.2×10^{3}		Wang et al. (2017)	Q	81, 240
[100502-66-7]	6.3		Wang et al. (2017)	Q	81, 241
PTMLFFXFTRSBJW-UHFFFAOYSA-N	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	272, 244
	3.9×10^{2}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{2}		Raventos-Duran et al. (2010)	Q	246
MCM:IPROPOLPAN	5.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_3H_5NO_6$	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
VGQGEUUGHUVAJJ-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:BUTDANO3	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_4$	2.3×10^{3}		Wang et al. (2017)	Q	81, 240
JVISETCEJQRRQM-UHFFFAOYSA-N	3.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:BUTDBNO3	9.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_4$	2.5×10^{2}		Wang et al. (2017)	Q	81, 240
MVWTUBMDIKBQOB-UHFFFAOYSA-N	3.0		Wang et al. (2017)	Q	81, 241
MCM:C4PAN1	8.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	5.5×10^{4}		Wang et al. (2017)	Q	81, 240
ZAYFYZJEFHQRME-UHFFFAOYSA-N	2.1		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C4PAN2	1.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_7$	1.7×10^{7}		Wang et al. (2017)	Q	81, 240
KFPIYXZEKUAVMP-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C4PAN3	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	3.6×10^{4}		Wang et al. (2017)	Q	81, 240
PIBQEVCOTXTKAE-UHFFFAOYSA-N	4.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C4PAN4	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	2.0×10^{4}		Wang et al. (2017)	Q	81, 240
NXHSYZWHYBOEBH-UHFFFAOYSA-N	4.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C4PAN5	3.2×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	4.1×10^{3}		Wang et al. (2017)	Q	81, 240
BZGCEXLIVXRKKX-UHFFFAOYSA-N	5.5×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C4PAN7	3.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_6$	1.2×10^{5}		Wang et al. (2017)	Q	81, 240
YKQOPDHVAHDODD-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C4PAN8	1.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_6$	7.1×10^{3}		Wang et al. (2017)	Q	81, 240
QZCDOTFCQHJUGH-UHFFFAOYSA-N	6.5×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C56NO3	8.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_5$	9.1×10^{5}		Wang et al. (2017)	Q	81, 240
XYUWBXDQANMXIL-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:HMPAN	2.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_6$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
XPXMBKPWAOWOBP-UHFFFAOYSA-N	6.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:HO13C4NO3	8.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_5$	1.0×10^{6}		Wang et al. (2017)	Q	81, 240
IOYLZWMTXYBAPI-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO3C3PAN	5.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	6.2×10^{3}		Wang et al. (2017)	Q	81, 240
JGMDPJZYJFPSOE-UHFFFAOYSA-N	9.1×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:IBUTOLBNO3	2.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_4$	1.0×10^{2}		Wang et al. (2017)	Q	81, 240
ILMPSGIQBJFTRG-UHFFFAOYSA-N	6.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:IBUTOLCNO3	2.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_4$	6.9×10^{2}		Wang et al. (2017)	Q	81, 240
OARBGYKXUANYLR-UHFFFAOYSA-N	3.5		Wang et al. (2017)	Q	81, 241
MCM:MACRNBPAN	5.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_6N_2O_9$	7.6×10^{5}		Wang et al. (2017)	Q	81, 240
HHPQSZXZUAZGAQ-UHFFFAOYSA-N	1.8×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MACRNCO3H	2.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_7$	2.3×10^{6}		Wang et al. (2017)	Q	81, 240
VCAMMMQHKHRNFT-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MACRNPAN	9.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_6N_2O_9$	2.8×10^{5}		Wang et al. (2017)	Q	81, 240
YVNHVFURNFQJQM-UHFFFAOYSA-N	1.2×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:NBUTDAOH	9.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_4$	2.9×10^{2}		Wang et al. (2017)	Q	81, 240
ZANUSWCYRLKDAN-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	81, 241
MCM:TBUTOLNO3	2.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_4$	1.4×10^{2}		Wang et al. (2017)	Q	81, 240
SPXXYWSDFUWLEP-UHFFFAOYSA-N	9.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C3M3OH2PAN	4.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	4.9×10^{3}		Wang et al. (2017)	Q	81, 240
NSGPYXAFGPXNMV-UHFFFAOYSA-N	2.8×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C46PAN	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_6$	7.4×10^{4}		Wang et al. (2017)	Q	81, 240
WDMYRNZGJSFESH-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	81, 241
MCM:C4OH2CPAN	3.7×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_7$	3.5×10^{6}		Wang et al. (2017)	Q	81, 240
INCMEOVDRBCULR-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
MCM:C4OHPAN	4.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	3.7×10^{3}		Wang et al. (2017)	Q	81, 240
GAAOIPAQIRGTBI-UHFFFAOYSA-N	5.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C524NO3	1.7×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	2.6×10^{6}		Wang et al. (2017)	Q	81, 240
IRMGDWDXIVCKPE-UHFFFAOYSA-N	2.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C52NO3	2.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	5.0×10^{2}		Wang et al. (2017)	Q	81, 240
NBCYUKLMSBOGIC-UHFFFAOYSA-N	6.5		Wang et al. (2017)	Q	81, 241
MCM:C54NO3	4.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_5$	3.8×10^{5}		Wang et al. (2017)	Q	81, 240
OXSZOTYJVSIXIT-UHFFFAOYSA-N	9.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C57NO3CO3H	2.4×10^{10}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_8$	1.4×10^{9}		Wang et al. (2017)	Q	81, 240
BPRAPKBGVRGZEK-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C57NO3PAN	9.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_{10}$	2.7×10^{8}		Wang et al. (2017)	Q	81, 240
QHZGCLHPLOENFL-UHFFFAOYSA-N	2.5×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C58NO3CO3H	3.5×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_8$	5.8×10^{7}		Wang et al. (2017)	Q	81, 240
NFQMHUFQLLKQQS-UHFFFAOYSA-N	5.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C58NO3PAN	1.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_{10}$	4.2×10^{8}		Wang et al. (2017)	Q	81, 240
VIMTZSSJOGPGII-UHFFFAOYSA-N	8.5×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C5PAN10	1.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_7$	2.5×10^{7}		Wang et al. (2017)	Q	81, 240
YRCMXGZRWLAVBH-UHFFFAOYSA-N	9.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C5PAN11	5.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	2.4×10^{4}		Wang et al. (2017)	Q	81, 240
ISSHIIFFUOEHLT-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C5PAN12	7.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_7$	1.0×10^{7}		Wang et al. (2017)	Q	81, 240
VRGURBHINCFLEI-UHFFFAOYSA-N	9.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C5PAN13	1.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_7$	2.0×10^{7}		Wang et al. (2017)	Q	81, 240
GDYHQRWKNLRCBR-UHFFFAOYSA-N	5.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C5PAN14	9.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	2.2×10^{4}		Wang et al. (2017)	Q	81, 240
KAYGTWBSLGDXRV-UHFFFAOYSA-N	5.8×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C5PAN15	5.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	9.3×10^{3}		Wang et al. (2017)	Q	81, 240
DDVUSZKFLFMJLG-UHFFFAOYSA-N	5.0×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C5PAN17	2.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_6$	1.3×10^{5}		Wang et al. (2017)	Q	81, 240
WOHMTHRFBCBPEN-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C5PAN19	2.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_6$	1.0×10^{5}		Wang et al. (2017)	Q	81, 240
SXXBKHKGTQGHOF-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C5PAN1	8.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	4.0×10^{4}		Wang et al. (2017)	Q	81, 240
BXAPPDLQCWAVAO-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	81, 241
MCM:C5PAN3	8.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	3.3×10^{4}		Wang et al. (2017)	Q	81, 240
GANOVMQBFKDCJS-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	81, 241
MCM:C5PAN5	8.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	3.0×10^{4}		Wang et al. (2017)	Q	81, 240
SNADUXVVPGYKTN-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:C5PAN8	8.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	1.9×10^{4}		Wang et al. (2017)	Q	81, 240
AVADEHRLOLZNNT-UHFFFAOYSA-N	7.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:H2M3C4NO3	2.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	5.0×10^{2}		Wang et al. (2017)	Q	81, 240
KRCHLCXLZXFPMO-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	81, 241
MCM:HM22C3NO3	1.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	3.2×10^{2}		Wang et al. (2017)	Q	81, 240
GJZIQWDDCYOUOR-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
MCM:HM2C43NO3	2.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	4.1×10^{2}		Wang et al. (2017)	Q	81, 240
OLLXHFMQLUGEEM-UHFFFAOYSA-N	2.5		Wang et al. (2017)	Q	81, 241
MCM:HM33C3NO3	1.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	2.0×10^{2}		Wang et al. (2017)	Q	81, 240
LCUGTHWCLWAZIN-UHFFFAOYSA-N	5.3		Wang et al. (2017)	Q	81, 241
MCM:HO13C5NO3	8.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_5$	5.4×10^{5}		Wang et al. (2017)	Q	81, 240
HRXGEJHIRPMYKD-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO24C5NO3	8.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_5$	5.8×10^{5}		Wang et al. (2017)	Q	81, 240
GDKLMXJUXHUPHP-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO2C54NO3	2.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	2.8×10^{2}		Wang et al. (2017)	Q	81, 240
BDOVYOMPHMUDCA-UHFFFAOYSA-N	1.8		Wang et al. (2017)	Q	81, 241
MCM:HO2M2C4NO3	1.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	3.6×10^{2}		Wang et al. (2017)	Q	81, 240
JLEBTGVTEJACMC-UHFFFAOYSA-N	1.6		Wang et al. (2017)	Q	81, 241
MCM:HO3C5NO3	2.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	3.8×10^{2}		Wang et al. (2017)	Q	81, 240
VSJMKXXNGJNYTF-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	81, 241
MCM:INAHCO3H	1.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_8$	4.9×10^{7}		Wang et al. (2017)	Q	81, 240
NANYPKIUOGNJFQ-UHFFFAOYSA-N	5.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:INAHPAN	5.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_{10}$	6.8×10^{8}		Wang et al. (2017)	Q	81, 240
ISRNXRSYOJKFEQ-UHFFFAOYSA-N	5.0		Wang et al. (2017)	Q	81, 241
MCM:INAHPCO3H	1.8×10^{12}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_9$	2.5×10^{9}		Wang et al. (2017)	Q	81, 240
ZYWYMWCOZFANRV-UHFFFAOYSA-N	3.8×10^{2}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:INAHPPAN	8.0×10^{10}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_{11}$	1.1×10^{9}		Wang et al. (2017)	Q	81, 240
ZXVKOORKVQYPPA-UHFFFAOYSA-N	3.4		Wang et al. (2017)	Q	81, 241
MCM:INANCO3H	2.7×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_{10}$	2.6×10^{8}		Wang et al. (2017)	Q	81, 240
HKZKRKUNOXITIG-UHFFFAOYSA-N	3.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:INANO3	7.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}N_2O_8$	2.6×10^{7}		Wang et al. (2017)	Q	81, 240
VVVQXVVEBQASSQ-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:INANPAN	1.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_7N_3O_{12}$	3.7×10^{7}		Wang et al. (2017)	Q	81, 240
PTXQCTHWIXKTGJ-UHFFFAOYSA-N	4.7×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:INAOH	4.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_6$	2.9×10^{8}		Wang et al. (2017)	Q	81, 240
KOIOFJRFFFLZDV-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:INAOOH	5.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_7$	4.7×10^{8}		Wang et al. (2017)	Q	81, 240
JIJPRURLLPNXAY-UHFFFAOYSA-N	2.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:INB1HPCO3H	1.5×10^{12}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_9$	1.3×10^{9}		Wang et al. (2017)	Q	81, 240
UQVCIXBCKWUTPD-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:INB1HPPAN	6.9×10^{10}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_{11}$	5.3×10^{8}		Wang et al. (2017)	Q	81, 240
MXDOILKWVFGWCS-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:INB1NACO3H	2.6×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_{10}$	2.5×10^{8}		Wang et al. (2017)	Q	81, 240
IWCHPIGOQCZQCT-UHFFFAOYSA-N	8.3		Wang et al. (2017)	Q	81, 241
MCM:INB1NAPAN	1.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_7N_3O_{12}$	7.1×10^{7}		Wang et al. (2017)	Q	81, 240
NYNQOGZUUKXJDZ-UHFFFAOYSA-N	2.8×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:INB1NBCO3H	2.6×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_{10}$	2.0×10^{8}		Wang et al. (2017)	Q	81, 240
KPBUCMMBNBINOH-UHFFFAOYSA-N	3.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:INB1NBPAN	1.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_7N_3O_{12}$	5.8×10^{7}		Wang et al. (2017)	Q	81, 240
JLOMTJWSNAHKLK-UHFFFAOYSA-N	4.5×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:INB1NO3	7.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}N_2O_8$	1.4×10^{7}		Wang et al. (2017)	Q	81, 240
JJLGQNDDHJZYHP-UHFFFAOYSA-N	8.1×10^{2}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:INB1OH	6.9×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_6$	1.7×10^{8}		Wang et al. (2017)	Q	81, 240
CMMIHJKAMSCCNX-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:INB1OOH	5.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_7$	1.1×10^{8}		Wang et al. (2017)	Q	81, 240
QLIFJAFKYUVUMD-UHFFFAOYSA-N	1.9×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:INB2OOH	5.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_7$	5.6×10^{8}		Wang et al. (2017)	Q	81, 240
KNHLEPZPJYMJKZ-UHFFFAOYSA-N	4.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:INCNCO3H	2.7×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_{10}$	3.0×10^{8}		Wang et al. (2017)	Q	81, 240
OBBLXUYPBVASEH-UHFFFAOYSA-N	8.0		Wang et al. (2017)	Q	81, 241
MCM:INCNO3	7.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}N_2O_8$	2.7×10^{7}		Wang et al. (2017)	Q	81, 240
YANCNBBJBURWKL-UHFFFAOYSA-N	2.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:INCNPAN	1.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_7N_3O_{12}$	5.4×10^{7}		Wang et al. (2017)	Q	81, 240
MINPDRSMAYIHHB-UHFFFAOYSA-N	2.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:INCOH	4.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_6$	2.8×10^{8}		Wang et al. (2017)	Q	81, 240
CLYWBEAWDTVRBE-UHFFFAOYSA-N	4.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:INCOOH	5.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_7$	6.9×10^{8}		Wang et al. (2017)	Q	81, 240
LZOWWVNBCGLMRZ-UHFFFAOYSA-N	2.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:INDHCO3H	3.5×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_8$	5.3×10^{7}		Wang et al. (2017)	Q	81, 240
QUYOEJZVAFIYRP-UHFFFAOYSA-N	5.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:INDHPAN	1.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_{10}$	6.3×10^{8}		Wang et al. (2017)	Q	81, 240
WUJYJPIJVADQSX-UHFFFAOYSA-N	3.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:INDHPCO3H	1.5×10^{12}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_9$	8.9×10^{8}		Wang et al. (2017)	Q	81, 240
XHWXDLVQLOECHL-UHFFFAOYSA-N	6.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:INDHPPAN	6.9×10^{10}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_{11}$	4.4×10^{8}		Wang et al. (2017)	Q	81, 240
MNXVJBKQIAYCJC-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	81, 241
MCM:INDOH	6.9×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_6$	1.7×10^{8}		Wang et al. (2017)	Q	81, 240
HMAKIHHEIIANEM-UHFFFAOYSA-N	3.7×10^{4}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:INDOOH	5.3×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_7$	1.1×10^{8}		Wang et al. (2017)	Q	81, 240
MAYHMSJZSHQSOH-UHFFFAOYSA-N	7.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:ISOPANO3	6.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	1.9×10^{3}		Wang et al. (2017)	Q	81, 240
ISDFXKLTMWDHJL-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ISOPBNO3	5.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
CIXVZPWFWFMUOH-UHFFFAOYSA-N	3.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:ISOPCNO3	6.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	1.9×10^{3}		Wang et al. (2017)	Q	81, 240
IDJHVSOIJITEQU-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ISOPDNO3	5.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	1.8×10^{2}		Wang et al. (2017)	Q	81, 240
PYTOMGVARIWPAT-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
MCM:M2BU2OLNO3	2.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	9.1×10^{1}		Wang et al. (2017)	Q	81, 240
AGMVBVSNQJHQAX-UHFFFAOYSA-N	5.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:M2BUOL2NO3	1.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	7.4×10^{1}		Wang et al. (2017)	Q	81, 240
RQINUHXDGZGUIX-UHFFFAOYSA-N	5.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:M3BU2OLNO3	3.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	1.4×10^{2}		Wang et al. (2017)	Q	81, 240
HJMHUJWXCZNPJL-UHFFFAOYSA-N	3.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:MBOANO3	6.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_5$	1.6×10^{5}		Wang et al. (2017)	Q	81, 240
SMFXIBRHTKUPLI-UHFFFAOYSA-N	5.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MBOBNO3	2.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_5$	1.6×10^{5}		Wang et al. (2017)	Q	81, 240
DYXSFFPMZZUQFC-UHFFFAOYSA-N	4.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:ME2BUOLNO3	2.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	8.1×10^{1}		Wang et al. (2017)	Q	81, 240
SBGDAJKUHMJEMT-UHFFFAOYSA-N	4.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:ME3BUOLNO3	3.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	1.4×10^{2}		Wang et al. (2017)	Q	81, 240
YWTWLHUMBHVVJS-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	81, 241
MCM:NC4OHCO3H	2.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_7$	1.6×10^{6}		Wang et al. (2017)	Q	81, 240
PAYOKBFCVVFNAB-UHFFFAOYSA-N	4.1		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NC4OHCPAN	9.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_9$	4.2×10^{5}		Wang et al. (2017)	Q	81, 240
JNBJPCXCCYUJJV-UHFFFAOYSA-N	2.8×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:NC524NO3	2.7×10^{10}		Wang et al. (2017)	Q	81, 239
$C_5H_{10}N_2O_9$	1.6×10^{10}		Wang et al. (2017)	Q	81, 240
NSZZUBPWOYNZJW-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:NC524OH	1.1×10^{11}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_7$	1.4×10^{11}		Wang et al. (2017)	Q	81, 240
ZZGZKDXCMVGDSK-UHFFFAOYSA-N	5.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:NC524OOH	1.8×10^{13}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_8$	1.7×10^{11}		Wang et al. (2017)	Q	81, 240
IVLBZHUBMDVGDP-UHFFFAOYSA-N	9.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:NMBOAOOH	1.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_6$	9.8×10^{4}		Wang et al. (2017)	Q	81, 240
JWWMAKNKCQEFPZ-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NMBOBOOH	1.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_6$	4.3×10^{4}		Wang et al. (2017)	Q	81, 240
ZVOCBPRLBFFNTM-UHFFFAOYSA-N	3.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PE1ENEANO3	2.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
VVLSYMLJBKJHQI-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	81, 241
MCM:PE1ENEBNO3	2.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	1.3×10^{2}		Wang et al. (2017)	Q	81, 240
ZAYLQHAUCSLXCO-UHFFFAOYSA-N	6.5×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:PE2ENEANO3	3.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	1.2×10^{2}		Wang et al. (2017)	Q	81, 240
SNSYWPGYFWSVQC-UHFFFAOYSA-N	6.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:PE2ENEBNO3	3.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
FSHUAFNCTFMDNJ-UHFFFAOYSA-N	2.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:PROL11MNO3	1.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	8.5×10^{1}		Wang et al. (2017)	Q	81, 240
XLOGQOLFBMMDEL-UHFFFAOYSA-N	5.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:PROL1MPAN	3.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	2.5×10^{3}		Wang et al. (2017)	Q	81, 240
KGIFHBAEXLJKCU-UHFFFAOYSA-N	1.5×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:BZBIPERNO3	1.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_6$	8.7×10^{4}		Wang et al. (2017)	Q	81, 240
RBJPNJQUNYROJW-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C4ME2OHNO3	1.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	5.1×10^{1}		Wang et al. (2017)	Q	81, 240
KWGTWPROGIVFDL-UHFFFAOYSA-N	1.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C518PAN	1.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_6$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
SMGAVNKPBYTONP-UHFFFAOYSA-N	4.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C622NO3	3.5×10^{1}	11000	Wieser et al. (2023)	Q	439
$C_6H_{11}NO_4$	4.0×10^{1}		Wang et al. (2017)	Q	81, 239
UCAFMJJTBHTENA-UHFFFAOYSA-N	6.6×10^{2}		Wang et al. (2017)	Q	81, 240
	2.0		Wang et al. (2017)	Q	81, 241
MCM:C624NO3	4.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_4$	3.8×10^{2}		Wang et al. (2017)	Q	81, 240
NPRBCQJDIIBUMY-UHFFFAOYSA-N	5.4		Wang et al. (2017)	Q	81, 241
MCM:C64OH5NO3	2.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	7.8×10^{1}		Wang et al. (2017)	Q	81, 240
SZVWRLIYDKPIRS-UHFFFAOYSA-N	2.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C65OH4NO3	2.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	8.7×10^{1}		Wang et al. (2017)	Q	81, 240
ZZPOFDLVCBSRPC-UHFFFAOYSA-N	5.5×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C66NO35OH	2.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	8.9×10^{1}		Wang et al. (2017)	Q	81, 240
FGVUHVRIXFWTDQ-UHFFFAOYSA-N	5.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6OH5NO3	2.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	8.1×10^{1}		Wang et al. (2017)	Q	81, 240
WNZDORMXFCCFFY-UHFFFAOYSA-N	8.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN11	7.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	2.8×10^{4}		Wang et al. (2017)	Q	81, 240
MMZOJEONIKVQSZ-UHFFFAOYSA-N	6.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN13	4.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	1.8×10^{4}		Wang et al. (2017)	Q	81, 240
UVFJOYDNGFNBNV-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	81, 241
MCM:C6PAN14	4.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	1.9×10^{4}		Wang et al. (2017)	Q	81, 240
OFISHWPBQMHPEB-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN19	7.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	2.6×10^{4}		Wang et al. (2017)	Q	81, 240
ZTVAXWHNQKLGPW-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C6PAN1	6.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	2.6×10^{4}		Wang et al. (2017)	Q	81, 240
INIWXNWKFGUMOJ-UHFFFAOYSA-N	6.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN20	7.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	1.5×10^{4}		Wang et al. (2017)	Q	81, 240
HBAXDJNNSYEITK-UHFFFAOYSA-N	4.8×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN21	4.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	1.6×10^{4}		Wang et al. (2017)	Q	81, 240
PXGXPDBWNDXFTJ-UHFFFAOYSA-N	3.0×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN22	6.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	1.3×10^{4}		Wang et al. (2017)	Q	81, 240
YIFZDOMLXOKIHL-UHFFFAOYSA-N	1.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN23	3.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	2.6×10^{3}		Wang et al. (2017)	Q	81, 240
OODNPGDDVDMKSB-UHFFFAOYSA-N	4.2×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN4	7.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	2.1×10^{4}		Wang et al. (2017)	Q	81, 240
ZWWUNLHZACGCEV-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
MCM:C6PAN8	4.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	2.8×10^{4}		Wang et al. (2017)	Q	81, 240
UOLRWSMDFSCHJH-UHFFFAOYSA-N	7.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:CYHXOLANO3	8.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_4$	4.6×10^{2}		Wang et al. (2017)	Q	81, 240
GVSCAKVHXWAQQJ-UHFFFAOYSA-N	4.7		Wang et al. (2017)	Q	81, 241
MCM:H13M3C5NO3	4.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_5$	2.8×10^{5}		Wang et al. (2017)	Q	81, 240
ZRQJKBICSYYJDC-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:H1MC5NO3	1.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	3.6×10^{2}		Wang et al. (2017)	Q	81, 240
YQESDLQNDPCVPT-UHFFFAOYSA-N	8.7		Wang et al. (2017)	Q	81, 241
MCM:H2MC5NO3	1.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	4.3×10^{2}		Wang et al. (2017)	Q	81, 240
OQOPDPWKHFKGPO-UHFFFAOYSA-N	4.7		Wang et al. (2017)	Q	81, 241
MCM:H3M3C5NO3	1.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	2.5×10^{2}		Wang et al. (2017)	Q	81, 240
KFPWVQORUDKTSF-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
MCM:HM22C4NO3	1.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	3.0×10^{2}		Wang et al. (2017)	Q	81, 240
VALJBIPPHZOXME-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:HM23C4NO3	1.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	4.8×10^{2}		Wang et al. (2017)	Q	81, 240
VYFSYIPQAVXJDI-UHFFFAOYSA-N	4.5		Wang et al. (2017)	Q	81, 241
MCM:HM33C4NO3	1.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	3.2×10^{2}		Wang et al. (2017)	Q	81, 240
HUEIARDLQBFSAX-UHFFFAOYSA-N	4.9		Wang et al. (2017)	Q	81, 241
MCM:HO1C6NO3	1.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	2.5×10^{2}		Wang et al. (2017)	Q	81, 240
ITCMBKDCMKPMFX-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	81, 241
MCM:HO1MC5NO3	1.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	2.4×10^{2}		Wang et al. (2017)	Q	81, 240
HKEZUADWXQLOIL-UHFFFAOYSA-N	4.9		Wang et al. (2017)	Q	81, 241
MCM:HO2C6NO3	1.6×10^{1}	10000	Wieser et al. (2023)	Q	439
$C_6H_{13}NO_4$	1.9×10^{1}		Wang et al. (2017)	Q	81, 239
PAWWQEMXBSLVJC-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	81, 240
	4.2		Wang et al. (2017)	Q	81, 241
MCM:HO2M2C5NO3	1.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	2.9×10^{2}		Wang et al. (2017)	Q	81, 240
VYPLOHRVLBPDEY-UHFFFAOYSA-N	5.0		Wang et al. (2017)	Q	81, 241
MCM:HO2MC5NO3	1.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	3.1×10^{2}		Wang et al. (2017)	Q	81, 240
HYCOTEZKEHIINQ-UHFFFAOYSA-N	3.5		Wang et al. (2017)	Q	81, 241
MCM:HO3C6NO3	1.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	3.0×10^{2}		Wang et al. (2017)	Q	81, 240
DLCRGHMYOOYQLW-UHFFFAOYSA-N	2.8		Wang et al. (2017)	Q	81, 241
MCM:NDNPHENOOH	1.2×10^{15}		Wang et al. (2017)	Q	81, 239
$C_6H_5N_3O_{12}$	3.2×10^{9}		Wang et al. (2017)	Q	81, 240
CXGWHQULUCBXTG-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NNCATECOOH	1.4×10^{16}		Wang et al. (2017)	Q	81, 239
$C_6H_6N_2O_{11}$	5.9×10^{8}		Wang et al. (2017)	Q	81, 240
SEZKEDQZGXKDIE-UHFFFAOYSA-N	1.0×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:NPHENOH	1.8×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_7$	8.5×10^{6}		Wang et al. (2017)	Q	81, 240
RMHIEAGXGVAIOV-UHFFFAOYSA-N	4.8×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:NPHENOOH	4.7×10^{10}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_8$	5.8×10^{6}		Wang et al. (2017)	Q	81, 240
AMKSGTJAMDYUMG-UHFFFAOYSA-N	4.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C622PAN	1.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{11}NO_6$	2.8×10^{4}		Wang et al. (2017)	Q	81, 240
YZCFVDKMDQZEJM-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C624PAN	1.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{11}NO_6$	2.0×10^{4}		Wang et al. (2017)	Q	81, 240
GVGFFJILZZBAQC-UHFFFAOYSA-N	2.3		Wang et al. (2017)	Q	81, 241
MCM:C720NO3	1.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_7H_{11}NO_4$	1.7×10^{3}		Wang et al. (2017)	Q	81, 240
VRUSDNGIDALYSE-UHFFFAOYSA-N	3.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C7PAN1	3.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{13}NO_6$	2.1×10^{4}		Wang et al. (2017)	Q	81, 240
HWQKKNUBUUPBAM-UHFFFAOYSA-N	2.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C7PAN2	6.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{13}NO_6$	9.8×10^{3}		Wang et al. (2017)	Q	81, 240
LEPHBBVBSNQAKS-UHFFFAOYSA-N	6.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:H2M2C65NO3	1.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{15}NO_4$	1.4×10^{2}		Wang et al. (2017)	Q	81, 240
CAEJQFHLOCBFOE-UHFFFAOYSA-N	3.7		Wang et al. (2017)	Q	81, 241
MCM:H2M4C65NO3	1.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{15}NO_4$	2.1×10^{2}		Wang et al. (2017)	Q	81, 240
GNQNFXQMHRYYMA-UHFFFAOYSA-N	3.2		Wang et al. (2017)	Q	81, 241
MCM:H2M5C65NO3	1.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{15}NO_4$	9.6×10^{1}		Wang et al. (2017)	Q	81, 240
JWGQNCMAKPVWAL-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:H3M3C6NO3	1.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{15}NO_4$	2.3×10^{2}		Wang et al. (2017)	Q	81, 240
HWCRTHIHVAVLJX-UHFFFAOYSA-N	2.3		Wang et al. (2017)	Q	81, 241
MCM:HO3C76NO3	1.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{15}NO_4$	1.5×10^{2}		Wang et al. (2017)	Q	81, 240
FLDFLEPRHCTYNR-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	81, 241
MCM:MNNCATCOOH	1.0×10^{16}		Wang et al. (2017)	Q	81, 239
$C_7H_8N_2O_{11}$	5.5×10^{9}		Wang et al. (2017)	Q	81, 240
QARZHCGSBCBWKI-UHFFFAOYSA-N	1.2×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:NCRESOH	9.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_7$	3.4×10^{6}		Wang et al. (2017)	Q	81, 240
DNQMNVUMZARJRH-UHFFFAOYSA-N	7.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:NCRESOOH	2.6×10^{10}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_8$	2.1×10^{6}		Wang et al. (2017)	Q	81, 240
CBYLLFTZDVJCIH-UHFFFAOYSA-N	6.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NDNCRESOOH	7.1×10^{14}		Wang et al. (2017)	Q	81, 239
$C_7H_7N_3O_{12}$	1.4×10^{9}		Wang et al. (2017)	Q	81, 240
LRLYMWFOIDHJSH-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:TLBIPERNO3	5.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_6$	2.5×10^{4}		Wang et al. (2017)	Q	81, 240
BBVQCFWACDVWPL-UHFFFAOYSA-N	4.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C8PAN1	4.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{15}NO_6$	8.0×10^{3}		Wang et al. (2017)	Q	81, 240
JRARROZAJMGAPP-UHFFFAOYSA-N	7.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:EBZBPERNO3	5.4×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_6$	1.6×10^{4}		Wang et al. (2017)	Q	81, 240
GVVNXZZYBMLIBS-UHFFFAOYSA-N	1.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:ENNCATCOOH	8.7×10^{15}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}N_2O_{11}$	3.2×10^{9}		Wang et al. (2017)	Q	81, 240
SUCBZAKUUVBJMN-UHFFFAOYSA-N	5.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HO3C86NO3	1.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_8H_{17}NO_4$	1.2×10^{2}		Wang et al. (2017)	Q	81, 240
WNECKFLKAYSMQF-UHFFFAOYSA-N	1.8		Wang et al. (2017)	Q	81, 241
MCM:MXNNCATOOH	5.4×10^{15}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}N_2O_{11}$	2.0×10^{9}		Wang et al. (2017)	Q	81, 240
SNJAPGUPFXVMJK-UHFFFAOYSA-N	4.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:MXYBIPENO3	3.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_6$	8.9×10^{3}		Wang et al. (2017)	Q	81, 240
QFCKPTYGEYQVET-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NDNEBZLOOH	6.3×10^{14}		Wang et al. (2017)	Q	81, 239
$C_8H_9N_3O_{12}$	8.5×10^{8}		Wang et al. (2017)	Q	81, 240
XZASAIPCUIAVQG-UHFFFAOYSA-N	4.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NDNMXYLOOH	4.6×10^{14}		Wang et al. (2017)	Q	81, 239
$C_8H_9N_3O_{12}$	8.0×10^{9}		Wang et al. (2017)	Q	81, 240
AAXPRTISYYDKLT-UHFFFAOYSA-N	1.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NDNOXYLOOH	8.5×10^{14}		Wang et al. (2017)	Q	81, 239
$C_8H_9N_3O_{12}$	2.3×10^{9}		Wang et al. (2017)	Q	81, 240
SEMBUWBKKSEFTL-UHFFFAOYSA-N	9.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NDNPXYLOOH	4.6×10^{14}		Wang et al. (2017)	Q	81, 239
$C_8H_9N_3O_{12}$	1.2×10^{9}		Wang et al. (2017)	Q	81, 240
YXONGYHUJBRFJO-UHFFFAOYSA-N	4.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NEBNZOLOH	7.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_7$	2.1×10^{6}		Wang et al. (2017)	Q	81, 240
GKEIZOZEJLMBMT-UHFFFAOYSA-N	2.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:NEBNZOLOOH	2.0×10^{10}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_8$	1.3×10^{6}		Wang et al. (2017)	Q	81, 240
DZFBJORWJYJOSR-UHFFFAOYSA-N	3.9×10^{4}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:NMXYOLOH	5.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_7$	1.4×10^{6}		Wang et al. (2017)	Q	81, 240
SFEIDLQIDXHPNL-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NMXYOLOOH	1.4×10^{10}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_8$	8.1×10^{5}		Wang et al. (2017)	Q	81, 240
ZTRVHLWFIBLUPT-UHFFFAOYSA-N	6.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NOXYOLOH	6.6×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_7$	2.3×10^{6}		Wang et al. (2017)	Q	81, 240
UBRWKHDWLQNZCI-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:NOXYOLOOH	1.7×10^{10}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_8$	1.5×10^{6}		Wang et al. (2017)	Q	81, 240
UHJNRWMXKFNWGQ-UHFFFAOYSA-N	2.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NPXYOLOH	6.6×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_7$	3.0×10^{6}		Wang et al. (2017)	Q	81, 240
DMOUSJNYQFTOEV-UHFFFAOYSA-N	2.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NPXYOLOOH	1.7×10^{10}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_8$	1.8×10^{6}		Wang et al. (2017)	Q	81, 240
XNVGITFEYRRJBZ-UHFFFAOYSA-N	3.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:OXNNCATOOH	1.0×10^{16}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}N_2O_{11}$	3.5×10^{8}		Wang et al. (2017)	Q	81, 240
GYUDSTHOULZHIU-UHFFFAOYSA-N	3.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:OXYBIPENO3	3.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_6$	9.1×10^{3}		Wang et al. (2017)	Q	81, 240
QQSYVIZUYAXYBZ-UHFFFAOYSA-N	2.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:PXNNCATOOH	5.4×10^{15}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}N_2O_{11}$	2.0×10^{8}		Wang et al. (2017)	Q	81, 240
PMLOPKQQVRFHBT-UHFFFAOYSA-N	4.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:PXYBIPENO3	3.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_6$	9.3×10^{3}		Wang et al. (2017)	Q	81, 240
DHJHBQWQGWNRCX-UHFFFAOYSA-N	2.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C9PAN1	3.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{17}NO_6$	6.8×10^{3}		Wang et al. (2017)	Q	81, 240
XXDOIRAKHRPRCF-UHFFFAOYSA-N	6.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:HO3C96NO3	1.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{19}NO_4$	9.3×10^{1}		Wang et al. (2017)	Q	81, 240
IBTJZAOBCFQTAU-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
MCM:IPBZBPRNO3	5.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_6$	1.5×10^{4}		Wang et al. (2017)	Q	81, 240
VLTHUNWGYHRCPS-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:IPNNCATOOH	8.1×10^{15}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}N_2O_{11}$	2.9×10^{9}		Wang et al. (2017)	Q	81, 240
QCQAPHFHFZPQHQ-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:METLBIPNO3	2.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_6$	5.9×10^{3}		Wang et al. (2017)	Q	81, 240
VQZACYIDHNLNBQ-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MTNNCATOOH	4.8×10^{15}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}N_2O_{11}$	1.2×10^{9}		Wang et al. (2017)	Q	81, 240
ILPSXJBNDMCAEH-UHFFFAOYSA-N	9.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NDNIPBLOOH	5.9×10^{14}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}N_3O_{12}$	8.0×10^{8}		Wang et al. (2017)	Q	81, 240
HEZPBZRCUHPAHJ-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NDNMETLOOH	3.8×10^{14}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}N_3O_{12}$	4.9×10^{9}		Wang et al. (2017)	Q	81, 240
GVOHWVMFRUNQQB-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NDNOETLOOH	6.9×10^{14}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}N_3O_{12}$	1.4×10^{9}		Wang et al. (2017)	Q	81, 240
DLTVFZDBANLVJD-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NDNPBZLOOH	5.1×10^{14}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}N_3O_{12}$	6.8×10^{8}		Wang et al. (2017)	Q	81, 240
JBFCRLZRPRJLGG-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NDNPETLOOH	3.8×10^{14}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}N_3O_{12}$	6.8×10^{8}		Wang et al. (2017)	Q	81, 240
HIQGLTMZAYSJOX-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NDNT123OOH	4.8×10^{14}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}N_3O_{12}$	1.1×10^{9}		Wang et al. (2017)	Q	81, 240
UGLBOUATFGGZQD-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NDNT124OOH	2.6×10^{14}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}N_3O_{12}$	5.5×10^{8}		Wang et al. (2017)	Q	81, 240
JFYUNHMAYFMSCF-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NIPBNZOLOH	7.3×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	2.1×10^{6}		Wang et al. (2017)	Q	81, 240
IAYADIRZIVDBNK-UHFFFAOYSA-N	6.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:NIPBZOLOOH	1.9×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_8$	1.2×10^{6}		Wang et al. (2017)	Q	81, 240
UJRLUYDBOZESDX-UHFFFAOYSA-N	2.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NMETOLOH	4.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	9.8×10^{5}		Wang et al. (2017)	Q	81, 240
JUUDFVZFULKTPV-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\ Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:NMETOLOOH	1.1×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_8$	5.5×10^{5}		Wang et al. (2017)	Q	81, 240
CCCPQNSHVNXETJ-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NOETOLOH	6.5×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	2.9×10^{6}		Wang et al. (2017)	Q	81, 240
RRTVORKFFCXYCH-UHFFFAOYSA-N	4.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NOETOLOOH	1.7×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_8$	1.7×10^{6}		Wang et al. (2017)	Q	81, 240
CGRZNCSNBNPNBR-UHFFFAOYSA-N	2.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NPBNZOLOH	7.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	1.6×10^{6}		Wang et al. (2017)	Q	81, 240
PSGNFPQCVGIEDF-UHFFFAOYSA-N	2.9×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:NPBNZOLOOH	1.9×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_8$	9.8×10^{5}		Wang et al. (2017)	Q	81, 240
SNFHXCYEBCZPSO-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NPETOLOH	5.3×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	1.8×10^{6}		Wang et al. (2017)	Q	81, 240
ILVSHXKPUYWBMX-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NPETOLOOH	1.4×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_8$	8.9×10^{5}		Wang et al. (2017)	Q	81, 240
BKSLAYLCQMXSES-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NTM123LOOH	1.1×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_8$	9.1×10^{5}		Wang et al. (2017)	Q	81, 240
BTWUGVBELCWISQ-UHFFFAOYSA-N	5.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NTM123OLOH	4.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	1.6×10^{6}		Wang et al. (2017)	Q	81, 240
DXGFZPSQDYIOOU-UHFFFAOYSA-N	7.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NTM124LOOH	1.1×10^{10}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_8$	1.3×10^{6}		Wang et al. (2017)	Q	81, 240
JDMNMHRINWGUFB-UHFFFAOYSA-N	3.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NTM124OLOH	4.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	2.3×10^{6}		Wang et al. (2017)	Q	81, 240
RASHBSOBGFFOLP-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NTM135LOOH	9.6×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_8$	5.1×10^{5}		Wang et al. (2017)	Q	81, 240
AUGMYCIDZMPUKI-UHFFFAOYSA-N	3.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NTM135OLOH	3.6×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
RAAKFDOLNJCXRG-UHFFFAOYSA-N	2.7×10^{3}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:OETLBIPNO3	2.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_6$	6.2×10^{3}		Wang et al. (2017)	Q	81, 240
FQBYEMVYEQQXMF-UHFFFAOYSA-N	6.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:OTNNCATOOH	8.9×10^{15}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}N_2O_{11}$	2.1×10^{8}		Wang et al. (2017)	Q	81, 240
QVFSJCAPJVJPQJ-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:PBZBPERNO3	4.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_6$	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
XWXMYNZXCPDSAQ-UHFFFAOYSA-N	2.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PETLBIPNO3	2.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_6$	6.2×10^{3}		Wang et al. (2017)	Q	81, 240
SOIPWHDZHXSJJN-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PNNCATCOOH	6.9×10^{15}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}N_2O_{11}$	2.5×10^{9}		Wang et al. (2017)	Q	81, 240
VZHROOMDTDJZFR-UHFFFAOYSA-N	4.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:PTNNCATOOH	4.8×10^{15}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}N_2O_{11}$	1.2×10^{8}		Wang et al. (2017)	Q	81, 240
DSPOEZNZVSBNSI-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:T123NCTOOH	9.3×10^{16}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_9$	3.4×10^{10}		Wang et al. (2017)	Q	81, 240
QTWHDHJHZAXHRP-UHFFFAOYSA-N	2.6×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:T123NNCOOH	3.0×10^{15}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}N_2O_{11}$	8.9×10^{8}		Wang et al. (2017)	Q	81, 240
DNVSLQYQQCSWFT-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:T124NCTOOH	1.7×10^{17}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_9$	3.4×10^{9}		Wang et al. (2017)	Q	81, 240
TXEYLBVXEVQRAA-UHFFFAOYSA-N	6.9×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:T124NNCOOH	3.0×10^{15}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}N_2O_{11}$	1.0×10^{8}		Wang et al. (2017)	Q	81, 240
ATYVZJLHFNLHKS-UHFFFAOYSA-N	7.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:TM123BPNO3	1.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_6$	4.9×10^{3}		Wang et al. (2017)	Q	81, 240
RQYOJMSOWIZBID-UHFFFAOYSA-N	2.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:TM124BPNO3	1.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_6$	3.8×10^{3}		Wang et al. (2017)	Q	81, 240
KUPKWWJOBRXSMW-UHFFFAOYSA-N	9.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:TM135BPNO3	2.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_6$	6.2×10^{3}		Wang et al. (2017)	Q	81, 240
VYQMVFHQGVVJTP-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:APINANO3	6.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_4$	7.3×10^{1}		Wang et al. (2017)	Q	81, 240
YITBNQHGOKCTCE-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	81, 241
MCM:APINBNO3	6.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_4$	9.3×10^{1}		Wang et al. (2017)	Q	81, 240
AFJBVFUZFQZZRG-UHFFFAOYSA-N	2.9		Wang et al. (2017)	Q	81, 241
MCM:APINCNO3	7.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_4$	9.3×10^{2}		Wang et al. (2017)	Q	81, 240
IHZLDCJLQGWYSD-UHFFFAOYSA-N	4.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:BPINANO3	6.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_4$	9.6×10^{1}		Wang et al. (2017)	Q	81, 240
LIKORQJDVXFFRR-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	81, 241
MCM:BPINBNO3	6.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_4$	1.5×10^{2}		Wang et al. (2017)	Q	81, 240
PIICVRQEXAAMFO-UHFFFAOYSA-N	2.7		Wang et al. (2017)	Q	81, 241
MCM:BPINCNO3	6.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_4$	1.7×10^{3}		Wang et al. (2017)	Q	81, 240
IVSZOCZGKNSHLW-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C10PAN1	3.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{19}NO_6$	6.0×10^{3}		Wang et al. (2017)	Q	81, 240
PVQDOCOVRZVCAL-UHFFFAOYSA-N	6.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C918PAN	8.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_6$	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
GIWCNEZLGDWGNI-UHFFFAOYSA-N	6.5×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:DMEBIPNO3	1.7×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_6$	4.2×10^{3}		Wang et al. (2017)	Q	81, 240
LWYZBKFMLLCHQU-UHFFFAOYSA-N	7.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO3C106NO3	1.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{21}NO_4$	7.6×10^{1}		Wang et al. (2017)	Q	81, 240
LRSOGLAVONYUMB-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	81, 241
MCM:LIMANO3	8.4×10^{1}	12000	Wieser et al. (2023)	Q	439
$C_{10}H_{17}NO_4$	6.5×10^{1}		Wang et al. (2017)	Q	81, 239
LZDKYYHMAURBIK-UHFFFAOYSA-N	1.8×10^{2}		Wang et al. (2017)	Q	81, 240
	2.8		Wang et al. (2017)	Q	81, 241
MCM:LIMBNO3	6.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_4$	2.3×10^{2}		Wang et al. (2017)	Q	81, 240
WIRXFNWUDJEZSG-UHFFFAOYSA-N	5.5		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:LIMCNO3	8.6×10^{1}	19000	Wieser et al. (2023)	Q	439
$C_{10}H_{17}NO_4$	8.1×10^{1}		Wang et al. (2017)	Q	81, 239
ZELLOEPLERCREX-UHFFFAOYSA-N	6.2×10^{2}		Wang et al. (2017)	Q	81, 240
	8.1		Wang et al. (2017)	Q	81, 241
MCM:NDMEPHOLOH	3.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_7$	7.4×10^{5}		Wang et al. (2017)	Q	81, 240
XEZYIWLRTFENIO-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NDMEPLOOH	7.4×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_8$	3.4×10^{5}		Wang et al. (2017)	Q	81, 240
CUWVWZNCHDONFF-UHFFFAOYSA-N	7.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DETLBIPNO3	1.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{17}NO_6$	3.1×10^{3}		Wang et al. (2017)	Q	81, 240
HUKONYHKUULPQM-UHFFFAOYSA-N	4.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HO3C116NO3	8.0		Wang et al. (2017)	Q	81, 239
$C_{11}H_{23}NO_4$	6.2×10^{1}		Wang et al. (2017)	Q	81, 240
ZSRHOFPLHKNYIP-UHFFFAOYSA-N	9.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:NDEMPHOLOH	2.6×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{17}NO_7$	4.7×10^{5}		Wang et al. (2017)	Q	81, 240
SFAWLNJVZQJDAW-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NDEMPLOOH	6.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{17}NO_8$	2.4×10^{5}		Wang et al. (2017)	Q	81, 240
KQXYYOILDOZYPH-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HO3C126NO3	6.5		Wang et al. (2017)	Q	81, 239
$C_{12}H_{25}NO_4$	4.8×10^{1}		Wang et al. (2017)	Q	81, 240
NBVYOETUGSGBPE-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
MCM:BCANO3	6.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{25}NO_4$	1.1×10^{3}		Wang et al. (2017)	Q	81, 240
DXJZLWPVAKABFC-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:BCBNO3	6.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{25}NO_4$	1.7×10^{3}		Wang et al. (2017)	Q	81, 240
GGDFBGYMWXIISJ-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:BCCNO3	8.5×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{25}NO_4$	2.0×10^{3}		Wang et al. (2017)	Q	81, 240
AJHNYRDSMBHFTD-UHFFFAOYSA-N	1.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:GLYPAN	4.5×10^{3}		Wang et al. (2017)	Q	81, 239
C_2HNO_6	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
WWNQODGUPABTBB-UHFFFAOYSA-N	4.2×10^{-4}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NO3CH2CHO	1.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_2H_3NO_4$	9.3×10^{1}		Wang et al. (2017)	Q	81, 240
ABUBKAMLUVOXSP-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C3PAN2	3.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_3NO_6$	4.0×10^{3}		Wang et al. (2017)	Q	81, 240
JCWPFKBPQPIIIA-UHFFFAOYSA-N	5.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:CHOPRNO3	1.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_3H_5NO_4$	3.9×10^{1}		Wang et al. (2017)	Q	81, 240
IIFXHQMWCHWMFS-UHFFFAOYSA-N	3.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:BUTAL2NO3	8.1		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_4$	1.9×10^{1}		Wang et al. (2017)	Q	81, 240
JTMAFXAEAWTSPM-UHFFFAOYSA-N	1.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:BUTALNO3	8.1		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_4$	4.6×10^{1}		Wang et al. (2017)	Q	81, 240
YGQOBBYMNDZOFN-UHFFFAOYSA-N	1.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C4CONO3OOH	7.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	2.1×10^{5}		Wang et al. (2017)	Q	81, 240
OPYZRKWHBYWVFV-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C4NO3COOOH	7.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
LPNJZRUFCUXQKM-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	81, 241
MCM:CHOC2PAN	2.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_6$	9.3×10^{3}		Wang et al. (2017)	Q	81, 240
RNHARUXEGCOCNU-UHFFFAOYSA-N	2.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:CONM2CHO	5.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_5$	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
UXLHNUQVUCPVFF-UHFFFAOYSA-N	4.5×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:CONM2CO3H	5.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_7$	1.0×10^{5}		Wang et al. (2017)	Q	81, 240
KDPSYMPAERQTCV-UHFFFAOYSA-N	1.6		Wang et al. (2017)	Q	81, 241
MCM:CONM2PAN	2.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_4N_2O_9$	4.5×10^{4}		Wang et al. (2017)	Q	81, 240
PRUSZGKEVUCSBM-UHFFFAOYSA-N	2.8×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:IBUALANO3	8.1		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_4$	6.0×10^{1}		Wang et al. (2017)	Q	81, 240
BBEYVRKCPRBWGK-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:IBUDIALPAN	3.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_6$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
ANKFJODHGNELSW-UHFFFAOYSA-N	6.0×10^{-3}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:MALDIALPAN	1.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_3NO_6$	2.3×10^{4}		Wang et al. (2017)	Q	81, 240
JVYQADFHFGBZRY-UHFFFAOYSA-N	2.2×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:MPRBNO3CHO	5.6		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_4$	7.8		Wang et al. (2017)	Q	81, 240
ZFRSNPXDNOXJAQ-UHFFFAOYSA-N	1.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:NC3CHO	3.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_4$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
IRCIUAVPVOGPAB-UHFFFAOYSA-N	3.7		Wang et al. (2017)	Q	81, 241
MCM:C3M3CHONO3	4.7		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	1.6×10^{1}		Wang et al. (2017)	Q	81, 240
FSONNVXXYIKSKL-UHFFFAOYSA-N	1.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C3MCODBPAN	7.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_5NO_6$	2.2×10^{4}		Wang et al. (2017)	Q	81, 240
ABUKHSDGKGHQTM-UHFFFAOYSA-N	6.8×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:C3MNO3CHO	7.6		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	1.4×10^{1}		Wang et al. (2017)	Q	81, 240
IIGIHDSEOSVDKL-UHFFFAOYSA-N	1.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C4CHOBNO3	6.8		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	2.5×10^{1}		Wang et al. (2017)	Q	81, 240
IRTPVYBICUATCF-UHFFFAOYSA-N	9.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C4NO3CHO	4.7		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	5.0		Wang et al. (2017)	Q	81, 240
WGTULXFSTHCAFV-UHFFFAOYSA-N	1.0×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C514NO3	6.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_5$	3.6×10^{4}		Wang et al. (2017)	Q	81, 240
CEGGSEAULUFJEH-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C52NO31CO	6.8		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	1.2×10^{1}		Wang et al. (2017)	Q	81, 240
OIPNOUWHATXHHM-UHFFFAOYSA-N	1.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:CO1M22PAN	1.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_6$	6.0×10^{2}		Wang et al. (2017)	Q	81, 240
JNBWLVYXFYINSW-UHFFFAOYSA-N	4.4×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:MC3CODBPAN	7.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_5NO_6$	1.9×10^{4}		Wang et al. (2017)	Q	81, 240
AENWJVOXGCGHKR-UHFFFAOYSA-N	4.1×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:NC4CHO	2.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_4$	9.8×10^{1}		Wang et al. (2017)	Q	81, 240
FHQODWHGFJXLCS-UHFFFAOYSA-N	6.3		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C522PAN	4.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_6$	4.6×10^{3}		Wang et al. (2017)	Q	81, 240
BLDVCFQHUDZGIY-UHFFFAOYSA-N	9.8×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C65NO36CHO	5.9		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_4$	8.9		Wang et al. (2017)	Q	81, 240
AWOTULOVYXZRSX-UHFFFAOYSA-N	1.4×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:CHOC4PAN	2.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_6$	3.6×10^{3}		Wang et al. (2017)	Q	81, 240
LKJHECXHBJSEQK-UHFFFAOYSA-N	3.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:CO1C6NO3	5.3		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_4$	2.9×10^{1}		Wang et al. (2017)	Q	81, 240
BSOUFWBHIRXMPX-UHFFFAOYSA-N	1.8		Wang et al. (2017)	Q	81, 241
MCM:C615PAN	1.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_7$	2.3×10^{5}		Wang et al. (2017)	Q	81, 240
QXDOZRAOCVERTF-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C729NO3	1.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_7H_{11}NO_4$	3.2×10^{1}		Wang et al. (2017)	Q	81, 240
IVMGVFSKIJXXOW-UHFFFAOYSA-N	4.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C729PAN	3.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_6$	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
UQYKHYVNMQUYAN-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C810NO3	2.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{13}NO_5$	7.3×10^{3}		Wang et al. (2017)	Q	81, 240
CHBSGOHAWLCLGZ-UHFFFAOYSA-N	4.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C822NO3	2.9×10^{1}	10000	Wieser et al. (2023)	Q	439
$C_8H_{13}NO_4$	8.9		Wang et al. (2017)	Q	81, 239
JWAJNALJDDSHOA-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	81, 240
	1.1		Wang et al. (2017)	Q	81, 241
MCM:C830NO3	1.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_8H_{13}NO_4$	2.8×10^{1}		Wang et al. (2017)	Q	81, 240
FXBNRUYCAFEPCZ-UHFFFAOYSA-N	7.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C831NO3	2.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{13}NO_5$	9.3×10^{3}		Wang et al. (2017)	Q	81, 240
OVEOYJGENOZMLJ-UHFFFAOYSA-N	5.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C89NO3	1.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_8H_{13}NO_4$	2.8×10^{1}		Wang et al. (2017)	Q	81, 240
JVGNHSSLWSUTIF-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NC826OOH	1.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{13}NO_7$	5.1×10^{7}		Wang et al. (2017)	Q	81, 240
LIEZCAAIBRALIF-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C822PAN	2.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_6$	1.1×10^{3}		Wang et al. (2017)	Q	81, 240
AEOJBADXVLGVNE-UHFFFAOYSA-N	3.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C830PAN	3.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_6$	2.4×10^{3}		Wang et al. (2017)	Q	81, 240
NSAJKAFLWKCEMC-UHFFFAOYSA-N	1.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C89PAN	3.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_6$	2.5×10^{3}		Wang et al. (2017)	Q	81, 240
MAIUDZACSGCMBD-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	81, 241
MCM:NC91CHO	1.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_4$	1.4×10^{1}		Wang et al. (2017)	Q	81, 240
AVQCYYCZMFYNOE-UHFFFAOYSA-N	8.1×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C126NO3	1.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{19}NO_4$	3.4×10^{1}		Wang et al. (2017)	Q	81, 240
LCRFSVKVQOPOBC-UHFFFAOYSA-N	7.3		Wang et al. (2017)	Q	81, 241
MCM:C126PAN	3.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{19}NO_6$	1.8×10^{3}		Wang et al. (2017)	Q	81, 240
TVUSLNPYCCAOKX-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	81, 241
MCM:C136NO3	8.7		Wang et al. (2017)	Q	81, 239
$C_{13}H_{21}NO_4$	3.0×10^{1}		Wang et al. (2017)	Q	81, 240
FAQBCXSJSFDOSN-UHFFFAOYSA-N	8.0		Wang et al. (2017)	Q	81, 241
MCM:NC1313OOH	2.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{21}NO_7$	9.1×10^{7}		Wang et al. (2017)	Q	81, 240
AIWUKZRYSUWIQN-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C136PAN	3.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{21}NO_6$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
HVYQJFOLIDVKQK-UHFFFAOYSA-N	4.1		Wang et al. (2017)	Q	81, 241
MCM:C42AOH	1.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_5NO_5$	1.6×10^{4}		Wang et al. (2017)	Q	81, 240
CQVFGUOZVNZZAM-UHFFFAOYSA-N	5.5		Wang et al. (2017)	Q	81, 241
MCM:HCOCOHPAN	1.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_3H_3NO_7$	5.4×10^{5}		Wang et al. (2017)	Q	81, 240
GGQYFRDCXKQQIA-UHFFFAOYSA-N	2.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C41NO3	5.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	1.4×10^{7}		Wang et al. (2017)	Q	81, 240
SGYMVPWBXCYWGY-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C42OH	1.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	1.6×10^{7}		Wang et al. (2017)	Q	81, 240
OIAGCOLJHCONRV-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C42OOH	1.3×10^{8}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_7$	1.4×10^{7}		Wang et al. (2017)	Q	81, 240
KUKJNXCETLVUQA-UHFFFAOYSA-N	1.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C4OCCOHNO3	1.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_5$	9.8×10^{3}		Wang et al. (2017)	Q	81, 240
NEHFOAWUQWHZTI-UHFFFAOYSA-N	1.6		Wang et al. (2017)	Q	81, 241
MCM:COCCOHNO3	3.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_5$	3.2×10^{4}		Wang et al. (2017)	Q	81, 240
HMCDHWALZVCNKO-UHFFFAOYSA-N	6.8		Wang et al. (2017)	Q	81, 241
MCM:COHM2PAN	6.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_7$	2.2×10^{5}		Wang et al. (2017)	Q	81, 240
UXUAXYPQPQSXRR-UHFFFAOYSA-N	5.0×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:MACRNB	1.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_5$	1.3×10^{4}		Wang et al. (2017)	Q	81, 240
DLZDCWJOERFHAS-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
MCM:MACRNO3	2.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_5$	7.1×10^{3}		Wang et al. (2017)	Q	81, 240
ALINXPRBVMXOGH-UHFFFAOYSA-N	3.2		Wang et al. (2017)	Q	81, 241
MCM:C4M2ALOHNO3	8.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_6$	1.4×10^{6}		Wang et al. (2017)	Q	81, 240
UOGOTHSJBRKVRR-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	81, 241
MCM:C510OH	1.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	1.2×10^{7}		Wang et al. (2017)	Q	81, 240
ZCOZZYNQPKXJEJ-UHFFFAOYSA-N	8.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C510OOH	7.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_7$	1.4×10^{7}		Wang et al. (2017)	Q	81, 240
GGBWELVRYZRQMP-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C57NO3	2.0×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	1.3×10^{7}		Wang et al. (2017)	Q	81, 240
KHAJTJUOMDNQGW-UHFFFAOYSA-N	6.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C58NO3	2.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	1.0×10^{7}		Wang et al. (2017)	Q	81, 240
UZUIBKBJXOKLGO-UHFFFAOYSA-N	5.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DNC524CO	7.1×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_9$	9.6×10^{8}		Wang et al. (2017)	Q	81, 240
WXHJTLSKHGDJHS-UHFFFAOYSA-N	1.9×10^{4}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HNC524CO	2.9×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_7$	1.5×10^{10}		Wang et al. (2017)	Q	81, 240
UHQMTOKWUFCERL-UHFFFAOYSA-N	5.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:HPNC524CO	4.7×10^{12}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_8$	1.7×10^{10}		Wang et al. (2017)	Q	81, 240
QASKBBWYYSGCPQ-UHFFFAOYSA-N	1.9×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:INAHCHO	1.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	1.5×10^{7}		Wang et al. (2017)	Q	81, 240
GJDCYRXOLZPRRL-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:INAHPCHO	1.6×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_7$	2.6×10^{7}		Wang et al. (2017)	Q	81, 240
WOIAKHQAPCBXNP-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:INANCHO	2.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_8$	1.7×10^{6}		Wang et al. (2017)	Q	81, 240
AOWQROMNZIXQRL-UHFFFAOYSA-N	6.3		Wang et al. (2017)	Q	81, 241
MCM:INB1HPCHO	1.4×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_7$	1.9×10^{7}		Wang et al. (2017)	Q	81, 240
PPUPDRIHXISUBS-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:INB1NACHO	2.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_8$	7.4×10^{6}		Wang et al. (2017)	Q	81, 240
FPDRKJBIBBHIBW-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:INB1NBCHO	2.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_8$	5.4×10^{6}		Wang et al. (2017)	Q	81, 240
DIJODJNNHWDXRN-UHFFFAOYSA-N	2.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:INCNCHO	2.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_8$	3.4×10^{6}		Wang et al. (2017)	Q	81, 240
QYWHAZCEYLWYSZ-UHFFFAOYSA-N	3.1		Wang et al. (2017)	Q	81, 241
MCM:INDHCHO	2.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	1.6×10^{7}		Wang et al. (2017)	Q	81, 240
LXJORHVMGZGMRK-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:INDHPCHO	1.4×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_7$	1.3×10^{7}		Wang et al. (2017)	Q	81, 240
NKPKKBYOCYFEQQ-UHFFFAOYSA-N	4.0×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:MMALNACO3H	9.3×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_8$	2.0×10^{6}		Wang et al. (2017)	Q	81, 240
WWJYGONDDIBFHK-UHFFFAOYSA-N	8.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MMALNAPAN	4.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_6N_2O_{10}$	6.0×10^{7}		Wang et al. (2017)	Q	81, 240
JNHZFZYBXYVXPX-UHFFFAOYSA-N	2.3×10^{-2}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MMALNBCO3H	9.3×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_8$	3.9×10^{7}		Wang et al. (2017)	Q	81, 240
ASZGKTQVJXPLHM-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MMALNBPAN	4.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_6N_2O_{10}$	1.3×10^{7}		Wang et al. (2017)	Q	81, 240
QNDDWZGVLTYMIK-UHFFFAOYSA-N	1.1×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:NMBOBCO	1.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	2.2×10^{4}		Wang et al. (2017)	Q	81, 240
ZWLCCOCHHFERQT-UHFFFAOYSA-N	1.6		Wang et al. (2017)	Q	81, 241
MCM:C1H4C5PAN	5.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_7$	2.5×10^{7}		Wang et al. (2017)	Q	81, 240
XKXYOEFJYDLELH-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C623NO3	4.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	6.0×10^{7}		Wang et al. (2017)	Q	81, 240
UTKYBRKMQKBGOV-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C67NO3	1.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	6.9×10^{4}		Wang et al. (2017)	Q	81, 240
MTROCBFSNOSSFX-UHFFFAOYSA-N	4.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C68NO3	1.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	6.8×10^{4}		Wang et al. (2017)	Q	81, 240
DFCRZDMTYDUCKH-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO1H63NO3	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	6.0×10^{5}		Wang et al. (2017)	Q	81, 240
QWPYKWKOPQKYFO-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NC623OH	4.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	2.7×10^{8}		Wang et al. (2017)	Q	81, 240
LIALSLHETRNECK-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NC623OOH	1.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_7$	6.0×10^{7}		Wang et al. (2017)	Q	81, 240
LUCHFEJMQFYPEG-UHFFFAOYSA-N	6.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C728NO3	1.5×10^{8}	17000	Wieser et al. (2023)	Q	439
$C_7H_{13}NO_6$	3.2×10^{7}		Wang et al. (2017)	Q	81, 239
CDBHNFBQKSTCON-UHFFFAOYSA-N	2.0×10^{8}		Wang et al. (2017)	Q	81, 240
	3.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C730NO3	3.5×10^{9}	17000	Wieser et al. (2023)	Q	439
$C_7H_{13}NO_6$	3.2×10^{7}		Wang et al. (2017)	Q	81, 239
RVWIAVBELSCRER-UHFFFAOYSA-N	1.4×10^{9}		Wang et al. (2017)	Q	81, 240
	9.8×10^{4}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:NC728OH	3.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_{13}NO_6$	5.4×10^{8}		Wang et al. (2017)	Q	81, 240
RMGZPHZIJLBXBA-UHFFFAOYSA-N	9.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NC728OOH	7.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{13}NO_7$	2.0×10^{8}		Wang et al. (2017)	Q	81, 240
NMPAVXKBWDGSMK-UHFFFAOYSA-N	2.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:NC730OH	3.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_{13}NO_6$	2.4×10^{8}		Wang et al. (2017)	Q	81, 240
ZPFRZNAADTZJOS-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NC730OOH	7.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{13}NO_7$	2.7×10^{9}		Wang et al. (2017)	Q	81, 240
LJYXGYOAXKBDIY-UHFFFAOYSA-N	6.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C826NO3	9.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{13}NO_6$	4.6×10^{7}		Wang et al. (2017)	Q	81, 240
HYUHCBAMOFNBPC-UHFFFAOYSA-N	5.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NC826OH	9.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{13}NO_6$	6.2×10^{7}		Wang et al. (2017)	Q	81, 240
UXZRCYKYQRKKOI-UHFFFAOYSA-N	3.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C127NO3	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{19}NO_5$	1.7×10^{5}		Wang et al. (2017)	Q	81, 240
RZJFRKYKWJUXLW-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C1311NO3	1.7×10^{4}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{21}NO_5$	1.4×10^{5}		Wang et al. (2017)	Q	81, 240
HIIZKUNLVYOKLJ-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C1313NO3	9.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{21}NO_6$	5.8×10^{7}		Wang et al. (2017)	Q	81, 240
SXMORIYKGFOKAB-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NC1313OH	9.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{21}NO_6$	6.8×10^{7}		Wang et al. (2017)	Q	81, 240
RAUQQNONBFDDJB-UHFFFAOYSA-N	5.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C3NO3COOOH	5.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_3H_5NO_6$	4.0×10^{4}		Wang et al. (2017)	Q	81, 240
JXBSDKIVLYRFTK-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CH3COPAN	2.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_3NO_6$	2.1×10^{3}		Wang et al. (2017)	Q	81, 240
BNYSUSDQQIWDSZ-UHFFFAOYSA-N	2.2×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:BUTONENO3	7.1		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_4$	3.5×10^{1}		Wang et al. (2017)	Q	81, 240
KFRUNLQRYXGRRS-UHFFFAOYSA-N	7.4×10^{-2}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CO23C4NO3	3.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_5$	4.3×10^{3}		Wang et al. (2017)	Q	81, 240
RSORCZUYAJEINP-UHFFFAOYSA-N	7.1×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:CO2C3PAN	2.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_6$	4.0×10^{3}		Wang et al. (2017)	Q	81, 240
VXGDXYQGFKIYIJ-UHFFFAOYSA-N	1.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:CO2N3CO3H	6.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_7$	5.5×10^{5}		Wang et al. (2017)	Q	81, 240
PLOOSZKRSUJKKF-UHFFFAOYSA-N	4.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CO2N3PAN	3.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_4N_2O_9$	2.3×10^{5}		Wang et al. (2017)	Q	81, 240
RXUYCSQEPKEYNB-UHFFFAOYSA-N	2.3×10^{-3}		Wang et al. (2017)	Q	81, 241
2-oxobutyl nitrate	5.9		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_4$	5.9×10^{1}		Wang et al. (2017)	Q	81, 240
[138779-12-1]	3.1×10^{-1}		Wang et al. (2017)	Q	81, 241
OVISQPFXRZOZFI-UHFFFAOYSA-N					
MCM:COC4NO3OOH	5.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	1.8×10^{4}		Wang et al. (2017)	Q	81, 240
AEHFBVVGPAXMNG-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MEKANO3	5.9		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_4$	1.3×10^{2}		Wang et al. (2017)	Q	81, 240
SQFMCLNZTZWUJY-UHFFFAOYSA-N	8.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:NMVK	1.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_4$	1.0×10^{2}		Wang et al. (2017)	Q	81, 240
YTEQPVIDLVIVHW-UHFFFAOYSA-N	3.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C4M2NO3ONE	3.8		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	7.3		Wang et al. (2017)	Q	81, 240
DIMIHFOKCQZMGY-UHFFFAOYSA-N	5.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C4M3NO3ONE	5.5		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	3.4×10^{1}		Wang et al. (2017)	Q	81, 240
SAHLZHFOPIFWKH-UHFFFAOYSA-N	1.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C4MCNO3OOH	2.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	8.3×10^{4}		Wang et al. (2017)	Q	81, 240
AOCDDMVLVLTZNT-UHFFFAOYSA-N	2.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C51NO324CO	3.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_5$	2.0×10^{4}		Wang et al. (2017)	Q	81, 240
KIDZPQUIRFWTHY-UHFFFAOYSA-N	8.0		Wang et al. (2017)	Q	81, 241
MCM:C51NO32CO	4.9		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	3.2×10^{1}		Wang et al. (2017)	Q	81, 240
TTZVKGPORDTQGG-UHFFFAOYSA-N	2.6×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C52NO33CO	5.5		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	1.6×10^{1}		Wang et al. (2017)	Q	81, 240
VOCQUTRGVIAJPG-UHFFFAOYSA-N	6.2×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C53NO324CO	3.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_5$	7.4×10^{3}		Wang et al. (2017)	Q	81, 240
QYJXVKSLJJQONK-UHFFFAOYSA-N	1.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C53NO32CO	5.5		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	1.7×10^{1}		Wang et al. (2017)	Q	81, 240
LVGYWFUEHRGRSS-UHFFFAOYSA-N	6.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C5CONO3OOH	2.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	3.7×10^{3}		Wang et al. (2017)	Q	81, 240
ZDTBCADGPXXLKE-UHFFFAOYSA-N	3.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C5COO2NO2	7.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_5NO_6$	3.9×10^{4}		Wang et al. (2017)	Q	81, 240
BZPLAICQOBBIOR-UHFFFAOYSA-N	4.7×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C5NO3O4OOH	4.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	4.6×10^{3}		Wang et al. (2017)	Q	81, 240
CASCWEIOXSCVGJ-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C5NO3OAOOH	4.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	5.3×10^{5}		Wang et al. (2017)	Q	81, 240
FLHIUJMTRYIPLY-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C5ONO34OOH	4.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	1.5×10^{5}		Wang et al. (2017)	Q	81, 240
LOZNRBAEPWQBFW-UHFFFAOYSA-N	2.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C5PAN16	1.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_6$	2.0×10^{3}		Wang et al. (2017)	Q	81, 240
IZEBTYZDWKBBFQ-UHFFFAOYSA-N	5.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C5PAN2	1.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_6$	9.6×10^{3}		Wang et al. (2017)	Q	81, 240
XMORPXKVSPHXDA-UHFFFAOYSA-N	5.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C5PAN7	2.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_6$	1.5×10^{3}		Wang et al. (2017)	Q	81, 240
VONRVKPFQAOOPX-UHFFFAOYSA-N	3.0×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C5PAN9	1.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_5NO_7$	2.5×10^{5}		Wang et al. (2017)	Q	81, 240
HJZPHZLLKGPYCO-UHFFFAOYSA-N	5.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:DIEKBNO3	4.9		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	5.5×10^{1}		Wang et al. (2017)	Q	81, 240
WKTFKAAKLZJYGP-UHFFFAOYSA-N	5.9×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:INANCOCO3H	4.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_6N_2O_{10}$	1.4×10^{7}		Wang et al. (2017)	Q	81, 240
OKQCOTADQFFQES-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	81, 241
MCM:INANCOPAN	1.9×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_5N_3O_{12}$	5.3×10^{6}		Wang et al. (2017)	Q	81, 240
OHHXWPYTKFCNFA-UHFFFAOYSA-N	8.0×10^{-5}		Wang et al. (2017)	Q	81, 241
MCM:MIPKBNO3	5.5		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	5.5×10^{1}		Wang et al. (2017)	Q	81, 240
PNKPSVUHDDVFRC-UHFFFAOYSA-N	6.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:MPRKNO3	5.5		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_4$	3.9×10^{1}		Wang et al. (2017)	Q	81, 240
GMHWHQCXUOCSQQ-UHFFFAOYSA-N	4.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C3COCPAN	1.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_6$	1.1×10^{3}		Wang et al. (2017)	Q	81, 240
QAGGXZNGFPYUOO-UHFFFAOYSA-N	4.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C4MCODBPAN	5.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_6$	3.3×10^{4}		Wang et al. (2017)	Q	81, 240
OBEVNDXPXGMJPT-UHFFFAOYSA-N	1.4×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C62NO335CO	3.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_5$	6.0×10^{3}		Wang et al. (2017)	Q	81, 240
ABDNFJAHWTWRFH-UHFFFAOYSA-N	3.9		Wang et al. (2017)	Q	81, 241
MCM:C62NO33CO	4.6		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_4$	9.8		Wang et al. (2017)	Q	81, 240
OBVLXHVNJQTRAU-UHFFFAOYSA-N	4.5×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C63NO32CO	4.6		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_4$	1.1×10^{1}		Wang et al. (2017)	Q	81, 240
QSKMGJAWRGUYGL-UHFFFAOYSA-N	5.5×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C64NO335CO	3.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_5$	4.2×10^{3}		Wang et al. (2017)	Q	81, 240
CHGSCHAFWLLPDM-UHFFFAOYSA-N	8.0×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C66NO35CO	4.3		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_4$	2.2×10^{1}		Wang et al. (2017)	Q	81, 240
NNYDFJRPKYRBEY-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6CO134PAN	1.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_7$	1.4×10^{5}		Wang et al. (2017)	Q	81, 240
OIZONYBQGYIWDV-UHFFFAOYSA-N	2.2×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C6CONO3OOH	3.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	1.3×10^{5}		Wang et al. (2017)	Q	81, 240
JAMSWIXAFBYGGR-UHFFFAOYSA-N	3.8×10^{2}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:C6DCARBPAN	7.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_6$	1.8×10^{4}		Wang et al. (2017)	Q	81, 240
QTAROYORLXCHIO-UHFFFAOYSA-N	3.0×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C6NO324CO	2.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_5$	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
ZLHGCQIPJTVAEP-UHFFFAOYSA-N	4.4		Wang et al. (2017)	Q	81, 241
MCM:C6NO3COOOH	3.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	2.6×10^{5}		Wang et al. (2017)	Q	81, 240
HQTZSBFILMVSJZ-UHFFFAOYSA-N	5.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN12	1.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_6$	3.4×10^{3}		Wang et al. (2017)	Q	81, 240
LSIJQLAUAXHOJI-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN16	1.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_6$	5.3×10^{2}		Wang et al. (2017)	Q	81, 240
JDUNWYCOIXFXGK-UHFFFAOYSA-N	1.8×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN2	1.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_6$	4.9×10^{3}		Wang et al. (2017)	Q	81, 240
BSRDZZSTWMTZHH-UHFFFAOYSA-N	4.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN5	1.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_6$	3.4×10^{3}		Wang et al. (2017)	Q	81, 240
AYORGEAGFIRFHW-UHFFFAOYSA-N	4.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN6	1.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_6$	6.6×10^{2}		Wang et al. (2017)	Q	81, 240
STXATUQYWORJHN-UHFFFAOYSA-N	1.5×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN7	1.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_7$	1.0×10^{5}		Wang et al. (2017)	Q	81, 240
FEUNFERSGUKVTQ-UHFFFAOYSA-N	2.7×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:CONO3C6OOH	3.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	7.3×10^{4}		Wang et al. (2017)	Q	81, 240
BPHZXGKZHPQLPB-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CYHXONANO3	1.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_4$	3.6×10^{2}		Wang et al. (2017)	Q	81, 240
VLCBNIODXGFPBM-UHFFFAOYSA-N	9.8		Wang et al. (2017)	Q	81, 241
MCM:ECO3PAN	7.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_5NO_8$	4.0×10^{7}		Wang et al. (2017)	Q	81, 240
GLZSBLKUFXIYNN-UHFFFAOYSA-N	3.4×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:EIPKBNO3	4.6		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_4$	2.7×10^{1}		Wang et al. (2017)	Q	81, 240
QPLZWEVCYZLYTL-UHFFFAOYSA-N	2.7×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HEX2ONANO3	4.6		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_4$	2.2×10^{1}		Wang et al. (2017)	Q	81, 240
OZSNHPHDGAJMHG-UHFFFAOYSA-N	2.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:HEX2ONBNO3	4.6		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_4$	3.0×10^{1}		Wang et al. (2017)	Q	81, 240
JYVFNKYOALTNTA-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	81, 241
MCM:HEX3ONANO3	4.6		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_4$	2.0×10^{1}		Wang et al. (2017)	Q	81, 240
KTYGBCIWLHIEKP-UHFFFAOYSA-N	4.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:HEX3ONDNO3	4.3		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_4$	3.6×10^{1}		Wang et al. (2017)	Q	81, 240
PRTKDFINSKNZSU-UHFFFAOYSA-N	6.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:M2BKANO3	5.1		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_4$	2.6×10^{1}		Wang et al. (2017)	Q	81, 240
NYAAKBDXIQFYDD-UHFFFAOYSA-N	3.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:MC4CODBPAN	5.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_6$	3.3×10^{4}		Wang et al. (2017)	Q	81, 240
WHFHKQLMYAOVSY-UHFFFAOYSA-N	2.2×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:MIBKANO3	3.0		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_4$	1.5×10^{1}		Wang et al. (2017)	Q	81, 240
PKJJSCYTBLHEMI-UHFFFAOYSA-N	1.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:MTBKNO3	3.0		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_4$	2.6×10^{1}		Wang et al. (2017)	Q	81, 240
OYSBYTCKEAIMOW-UHFFFAOYSA-N	5.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:NBZQOOH	3.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_5NO_7$	5.6×10^{8}		Wang et al. (2017)	Q	81, 240
NXGPVQDYDGLWQQ-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C627PAN	9.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_7$	3.0×10^{6}		Wang et al. (2017)	Q	81, 240
FQVTWXYWQQSSRX-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C7ADCPAN	3.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_6$	4.3×10^{4}		Wang et al. (2017)	Q	81, 240
OFKNKTFVVCSQBW-UHFFFAOYSA-N	8.1×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C7DCPAN	5.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_6$	9.6×10^{3}		Wang et al. (2017)	Q	81, 240
ZGBUEZLBCHGZPP-UHFFFAOYSA-N	1.4×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C7DDCPAN	4.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_6$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
WCHGYJHJZMHIAR-UHFFFAOYSA-N	5.5×10^{-3}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:C7PAN3	6.3×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_7NO_8$	1.7×10^{7}		Wang et al. (2017)	Q	81, 240
XMNXEIJPBOBVEP-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	81, 241
MCM:IC7DCPAN	6.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_6$	1.0×10^{4}		Wang et al. (2017)	Q	81, 240
NZLPHNCQTJFNGH-UHFFFAOYSA-N	8.1×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:NC71CO	3.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_7NO_6$	2.5×10^{7}		Wang et al. (2017)	Q	81, 240
CDHAVACRDDMHGZ-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NC71OOH	4.5×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_7$	1.6×10^{9}		Wang et al. (2017)	Q	81, 240
CIJBWMVCSXGACJ-UHFFFAOYSA-N	5.6×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:NC72OOH	3.0×10^{11}		Wang et al. (2017)	Q	81, 239
$C_7H_7NO_8$	3.6×10^{10}		Wang et al. (2017)	Q	81, 240
RYHDNZNGTUJGAD-UHFFFAOYSA-N	5.8×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:NPTLQOOH	2.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_7H_7NO_7$	4.8×10^{8}		Wang et al. (2017)	Q	81, 240
WIZJVJIMHIROQF-UHFFFAOYSA-N	6.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C5DBEPAN	2.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_7$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
OYOZKJOWUFGKRQ-UHFFFAOYSA-N	9.6×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:C5EDBPAN	2.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_7$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
KNPMBKOCKIUXFV-UHFFFAOYSA-N	7.6×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:C727PAN	8.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_7$	6.9×10^{5}		Wang et al. (2017)	Q	81, 240
WBGZRMCIPBEEGH-UHFFFAOYSA-N	4.1		Wang et al. (2017)	Q	81, 241
MCM:C7CODBPAN	3.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_6$	7.6×10^{3}		Wang et al. (2017)	Q	81, 240
QVHZZCVTEAGIPK-UHFFFAOYSA-N	3.8×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:C817NO3	3.9×10^{4}	12000	Wieser et al. (2023)	Q	439
$C_8H_{13}NO_5$	2.2×10^{3}		Wang et al. (2017)	Q	81, 239
ZONZWPKPCIWKRN-UHFFFAOYSA-N	3.8×10^{4}		Wang et al. (2017)	Q	81, 240
	3.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NMXYQOOH	1.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_7$	9.6×10^{7}		Wang et al. (2017)	Q	81, 240
MDRQMTCFLWPCNU-UHFFFAOYSA-N	4.0×10^{2}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NOXYQOOH	1.5×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_7$	3.8×10^{8}		Wang et al. (2017)	Q	81, 240
SFYCEAPRSKIFCS-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NPEBQOOH	2.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_7$	2.6×10^{8}		Wang et al. (2017)	Q	81, 240
HZFUWULOZSGVHH-UHFFFAOYSA-N	5.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NPXYQOOH	1.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_7$	9.3×10^{7}		Wang et al. (2017)	Q	81, 240
LMPSHWMXIGVDOI-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C816PAN	2.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_6$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
JXXOSNUALVJMQL-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C817PAN	6.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	1.6×10^{6}		Wang et al. (2017)	Q	81, 240
AGDIJRUETYYZKI-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C827PAN	4.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	5.3×10^{5}		Wang et al. (2017)	Q	81, 240
QMDLSNSKOZAILD-UHFFFAOYSA-N	2.3		Wang et al. (2017)	Q	81, 241
MCM:C828PAN	3.6×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_8$	1.1×10^{7}		Wang et al. (2017)	Q	81, 240
LCFHBKSAGMTDCX-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
MCM:C88PAN	1.7×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_7$	1.4×10^{7}		Wang et al. (2017)	Q	81, 240
KLGKHKJTYFCRCN-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C917NO3	4.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_5$	2.5×10^{5}		Wang et al. (2017)	Q	81, 240
KVWUPUMJPKRVQS-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C923NO3	3.2×10^{1}	11000	Wieser et al. (2023)	Q	439
$C_9H_{15}NO_4$	6.0		Wang et al. (2017)	Q	81, 239
JEWJQSHMOKPQHI-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	81, 240
	4.1		Wang et al. (2017)	Q	81, 241
MCM:C928NO3	1.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{15}NO_5$	3.2×10^{4}		Wang et al. (2017)	Q	81, 240
HCHMIBGRYQMLLZ-UHFFFAOYSA-N	6.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C96NO3	6.6		Wang et al. (2017)	Q	81, 239
$C_9H_{15}NO_4$	5.0×10^{1}		Wang et al. (2017)	Q	81, 240
MMTOEOITRCIZDG-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C9DCNO3	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_5$	7.3×10^{5}		Wang et al. (2017)	Q	81, 240
TURIVFFHDFEFMU-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C9PAN2	2.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_6$	3.2×10^{3}		Wang et al. (2017)	Q	81, 240
VXDDXZNSSANCGN-UHFFFAOYSA-N	8.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:NIPRBQOOH	1.8×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_7$	1.8×10^{8}		Wang et al. (2017)	Q	81, 240
KGZDDJNUZZWZIJ-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NLMKAOOH	5.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{15}NO_6$	8.9×10^{5}		Wang et al. (2017)	Q	81, 240
ZOTFHCKOVMRARL-UHFFFAOYSA-N	5.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NMETLQOOH	1.1×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_7$	5.0×10^{7}		Wang et al. (2017)	Q	81, 240
FSVFAZAPMWXECG-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NOETLQOOH	1.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_7$	2.1×10^{8}		Wang et al. (2017)	Q	81, 240
GHGZYHLEQYQZHR-UHFFFAOYSA-N	3.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NOPINANO3	2.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_4$	2.3×10^{2}		Wang et al. (2017)	Q	81, 240
JEOFIBHUYPQAJL-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NOPINBNO3	2.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_4$	3.1×10^{2}		Wang et al. (2017)	Q	81, 240
QGVNTXJLRAHBMW-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NOPINCNO3	1.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_4$	8.1×10^{1}		Wang et al. (2017)	Q	81, 240
CLMUTFVSCXCGKI-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NPETLQOOH	1.1×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_7$	4.8×10^{7}		Wang et al. (2017)	Q	81, 240
IMJMJNZTMWKOFO-UHFFFAOYSA-N	2.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NPPRBQOOH	1.6×10^{9}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_7$	1.8×10^{8}		Wang et al. (2017)	Q	81, 240
MMAZKJNYHBQGDL-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NTM124QOOH	8.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_7$	6.9×10^{7}		Wang et al. (2017)	Q	81, 240
ZMXXAPJGXNLYQU-UHFFFAOYSA-N	5.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C1011NO3	5.4		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_4$	2.5×10^{1}		Wang et al. (2017)	Q	81, 240
KLQCUGBDZZARMU-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C10PAN2	2.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_6$	2.6×10^{3}		Wang et al. (2017)	Q	81, 240
XGWGKMXMXMPDAK-UHFFFAOYSA-N	4.7		Wang et al. (2017)	Q	81, 241
MCM:C923PAN	2.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_6$	1.0×10^{3}		Wang et al. (2017)	Q	81, 240
ZVYIPTRRRFMSSU-UHFFFAOYSA-N	2.3		Wang et al. (2017)	Q	81, 241
MCM:C928PAN	3.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_7$	1.5×10^{6}		Wang et al. (2017)	Q	81, 240
MIISGCVMOACDOR-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NC101CO	1.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_4$	4.4×10^{1}		Wang et al. (2017)	Q	81, 240
BCIULZBFFUODJR-UHFFFAOYSA-N	4.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:NC101OOH	6.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_6$	3.4×10^{5}		Wang et al. (2017)	Q	81, 240
AQVSRLWLNUXIOL-UHFFFAOYSA-N	5.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NC102OOH	1.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_7$	4.0×10^{8}		Wang et al. (2017)	Q	81, 240
ZNOCONLMTXMLFU-UHFFFAOYSA-N	4.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C1011PAN	1.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{17}NO_6$	2.2×10^{3}		Wang et al. (2017)	Q	81, 240
PRDFPHJPDVZXHH-UHFFFAOYSA-N	2.9		Wang et al. (2017)	Q	81, 241
MCM:C131NO3	2.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{21}NO_5$	3.5×10^{4}		Wang et al. (2017)	Q	81, 240
HFRDBZMTZNPZMV-UHFFFAOYSA-N	2.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C131PAN	7.3×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{21}NO_7$	2.0×10^{6}		Wang et al. (2017)	Q	81, 240
YHMAABVAIQVHRP-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C141NO3	5.9		Wang et al. (2017)	Q	81, 239
$C_{14}H_{23}NO_4$	3.3×10^{1}		Wang et al. (2017)	Q	81, 240
JPXQKVXALDMDKF-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NBCKOOH	4.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{23}NO_6$	4.4×10^{5}		Wang et al. (2017)	Q	81, 240
IMGMBHKHHVQTQK-UHFFFAOYSA-N	1.5×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C141PAN	1.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{23}NO_6$	1.8×10^{3}		Wang et al. (2017)	Q	81, 240
PGNAVHCNSKAOHZ-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C4PAN10	5.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_8$	1.9×10^{7}		Wang et al. (2017)	Q	81, 240
JOAGXXIRMSWAAZ-UHFFFAOYSA-N	2.4×10^{1}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C4PAN6	8.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_7$	5.4×10^{5}		Wang et al. (2017)	Q	81, 240
QRAIBPAZBCTEOB-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:CO3C4NO3OH	8.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_5$	3.2×10^{4}		Wang et al. (2017)	Q	81, 240
HZFDSYFRCPAXEA-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:HMVKANO3	1.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_5$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
UFDPWCOBIOWDKA-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	81, 241
MCM:HMVKNO3	3.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	3.5×10^{7}		Wang et al. (2017)	Q	81, 240
NCLLRWDJHCXXDR-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HNBIACET	5.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_6$	1.4×10^{6}		Wang et al. (2017)	Q	81, 240
HPGBXXMJBUDRLY-UHFFFAOYSA-N	4.7		Wang et al. (2017)	Q	81, 241
MCM:HNMVKOH	1.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	6.8×10^{6}		Wang et al. (2017)	Q	81, 240
KPZZNRQGHDTQNJ-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HNMVKOOH	1.8×10^{9}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_7$	2.4×10^{7}		Wang et al. (2017)	Q	81, 240
CTKAFSDGNPEZFZ-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:MVKNO3	2.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_5$	2.0×10^{4}		Wang et al. (2017)	Q	81, 240
SCJOQBCZNBCTOQ-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MVKOHANO3	6.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	5.5×10^{5}		Wang et al. (2017)	Q	81, 240
DMSMZXCVKMBQGA-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C4MCONO3OH	4.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	1.5×10^{4}		Wang et al. (2017)	Q	81, 240
VRAOJUVNSLNISW-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C517NO3	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	1.9×10^{5}		Wang et al. (2017)	Q	81, 240
DLLRFAPEEPVGBN-UHFFFAOYSA-N	7.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C51NO3	1.9×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	2.3×10^{5}		Wang et al. (2017)	Q	81, 240
OMTWKQRBUUWUQB-UHFFFAOYSA-N	2.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C5NO3CO4OH	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	3.1×10^{5}		Wang et al. (2017)	Q	81, 240
GEKIHWHZVPPEBT-UHFFFAOYSA-N	9.6×10^{1}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CO2OH3MPAN	4.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_7$	1.6×10^{5}		Wang et al. (2017)	Q	81, 240
KOFNDQLSBTYFBZ-UHFFFAOYSA-N	6.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:CO3H4PAN	6.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_7$	2.8×10^{5}		Wang et al. (2017)	Q	81, 240
KVXLZPRANFUVNJ-UHFFFAOYSA-N	1.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:H1C23C4PAN	1.9×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_5NO_8$	7.4×10^{7}		Wang et al. (2017)	Q	81, 240
ZNIKVNWPMOTSJK-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	81, 241
MCM:H3C2C4PAN	2.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_7$	2.2×10^{6}		Wang et al. (2017)	Q	81, 240
UDPFGHOTTZCMEQ-UHFFFAOYSA-N	4.1		Wang et al. (2017)	Q	81, 241
MCM:HMVKBPAN	5.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_7$	3.6×10^{6}		Wang et al. (2017)	Q	81, 240
VVIGYLNPENSKGX-UHFFFAOYSA-N	3.0		Wang et al. (2017)	Q	81, 241
MCM:INANCO	1.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_8$	1.2×10^{6}		Wang et al. (2017)	Q	81, 240
IESHUNGXVKLDSS-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	81, 241
MCM:INB1CO	1.7×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	1.8×10^{7}		Wang et al. (2017)	Q	81, 240
ASROEBVFUUHBLI-UHFFFAOYSA-N	2.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:INCCO	3.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	2.9×10^{5}		Wang et al. (2017)	Q	81, 240
HXWBEXHMXOXGKY-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C4COMOHPAN	2.8×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_8$	9.3×10^{6}		Wang et al. (2017)	Q	81, 240
KHOZKKAVCHSHMN-UHFFFAOYSA-N	3.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C4MOHOPAN	6.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_7$	1.9×10^{5}		Wang et al. (2017)	Q	81, 240
LVRCIQOIMYLYHB-UHFFFAOYSA-N	3.8×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C517PAN	4.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_7$	9.1×10^{6}		Wang et al. (2017)	Q	81, 240
BRUHFHISVNPPNB-UHFFFAOYSA-N	4.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C519PAN	4.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_7$	9.6×10^{6}		Wang et al. (2017)	Q	81, 240
QFUOUYQJXYVTOO-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C5O45OHPAN	5.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_7$	1.7×10^{5}		Wang et al. (2017)	Q	81, 240
VCYALMFEDUSLKE-UHFFFAOYSA-N	5.1×10^{-2}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C610NO3	1.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	1.5×10^{5}		Wang et al. (2017)	Q	81, 240
KOUUCDJHLKRSEQ-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C614NO3	1.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_6$	8.9×10^{6}		Wang et al. (2017)	Q	81, 240
QPXWFZAVXNBNFW-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C61NO3	1.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	1.4×10^{5}		Wang et al. (2017)	Q	81, 240
SYDWDJOZRNVKSU-UHFFFAOYSA-N	6.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C63NO3	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	9.8×10^{4}		Wang et al. (2017)	Q	81, 240
RHTCZESJRHZQFA-UHFFFAOYSA-N	3.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C64NO3	1.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	8.3×10^{4}		Wang et al. (2017)	Q	81, 240
IYYWGRLOLOMZAZ-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C6CONO34OH	1.8×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	1.6×10^{4}		Wang et al. (2017)	Q	81, 240
OLTUAQAPCXKDOJ-UHFFFAOYSA-N	2.7		Wang et al. (2017)	Q	81, 241
MCM:C6NO3CO4OH	1.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	1.8×10^{5}		Wang et al. (2017)	Q	81, 240
WWUUDQUMERSNEM-UHFFFAOYSA-N	4.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C6NO3CO5OH	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	8.1×10^{4}		Wang et al. (2017)	Q	81, 240
IZBQRALUURUKJG-UHFFFAOYSA-N	1.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C6PAN9	1.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_7$	5.1×10^{5}		Wang et al. (2017)	Q	81, 240
NJFFIXOWLQJQIZ-UHFFFAOYSA-N	6.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:MIBKAOHNO3	1.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	6.3×10^{4}		Wang et al. (2017)	Q	81, 240
YCHDRSSXCQCYSO-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C61CPAN	3.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_8$	1.2×10^{7}		Wang et al. (2017)	Q	81, 240
FWCVDVIZOKXUGJ-UHFFFAOYSA-N	1.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C62CPAN	3.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_8$	1.3×10^{7}		Wang et al. (2017)	Q	81, 240
LHOMRHYSYFWOPZ-UHFFFAOYSA-N	7.4×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C712NO3	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{13}NO_5$	5.4×10^{4}		Wang et al. (2017)	Q	81, 240
RPPGGLBPWJPSSV-UHFFFAOYSA-N	7.1		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C719NO3	1.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{11}NO_6$	4.8×10^{9}		Wang et al. (2017)	Q	81, 240
IXGSPJJVHFTXPK-UHFFFAOYSA-N	2.8×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C72NO3	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{13}NO_5$	6.5×10^{4}		Wang et al. (2017)	Q	81, 240
MWIGFUUCEWIWBB-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C77NO3	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_{13}NO_5$	5.0×10^{4}		Wang et al. (2017)	Q	81, 240
KZCKPUAVFWISTB-UHFFFAOYSA-N	7.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:H3C25C6PAN	1.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_8$	6.8×10^{8}		Wang et al. (2017)	Q	81, 240
GUUOCMMOMFUPSI-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C6MOHCOPAN	9.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_8$	1.1×10^{9}		Wang et al. (2017)	Q	81, 240
PDGRPGJWHYLYKK-UHFFFAOYSA-N	6.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C7CO2OHPAN	9.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_8$	1.1×10^{9}		Wang et al. (2017)	Q	81, 240
MICPXOSCTLYWLE-UHFFFAOYSA-N	4.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C829NO3	4.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{13}NO_6$	1.3×10^{6}		Wang et al. (2017)	Q	81, 240
CDMYSTRAPZWSHD-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C82NO3	1.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_8H_{15}NO_5$	4.1×10^{4}		Wang et al. (2017)	Q	81, 240
HUKHBWOLGKLCRF-UHFFFAOYSA-N	7.4		Wang et al. (2017)	Q	81, 241
MCM:C6EO2OHPAN	7.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_8$	6.9×10^{8}		Wang et al. (2017)	Q	81, 240
YGQCKHJQVYPZEV-UHFFFAOYSA-N	3.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C7MJPPAN	7.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_8$	6.5×10^{8}		Wang et al. (2017)	Q	81, 240
XJDHGIQDEMCTOX-UHFFFAOYSA-N	8.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C7MOHCOPAN	5.5×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_8$	1.7×10^{9}		Wang et al. (2017)	Q	81, 240
SORJSZWEJQTGJA-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	81, 241
MCM:C927NO3	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{15}NO_5$	1.1×10^{5}		Wang et al. (2017)	Q	81, 240
RKOGSSYMWVPWJW-UHFFFAOYSA-N	2.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C93NO3	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{17}NO_5$	3.4×10^{4}		Wang et al. (2017)	Q	81, 240
OEEOAFFOONSSLD-UHFFFAOYSA-N	5.1		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:C98NO3	4.0×10^6		Wang et al. (2017)	Q	81, 239
$C_9H_{15}NO_6$	5.6×10^6		Wang et al. (2017)	Q	81, 240
PQCIVFJRBSNULM-UHFFFAOYSA-N	1.8×10^3		Wang et al. (2017)	Q	81, 241
MCM:LMKANO3	2.3×10^4		Wang et al. (2017)	Q	81, 239
$C_9H_{15}NO_5$	2.2×10^5		Wang et al. (2017)	Q	81, 240
OCTKYXAOGSBZDD-UHFFFAOYSA-N	1.3×10^4		Wang et al. (2017)	Q	81, 241
MCM:LMKBNO3	2.3×10^4		Wang et al. (2017)	Q	81, 239
$C_9H_{15}NO_5$	2.6×10^5		Wang et al. (2017)	Q	81, 240
MVWAQQXSBOJSHS-UHFFFAOYSA-N	2.1×10^3		Wang et al. (2017)	Q	81, 241
MCM:C103NO3	8.3×10^3		Wang et al. (2017)	Q	81, 239
$C_{10}H_{19}NO_5$	3.0×10^4		Wang et al. (2017)	Q	81, 240
NTZGBOUJHFKYIP-UHFFFAOYSA-N	4.8		Wang et al. (2017)	Q	81, 241
MCM:C920PAN	3.1×10^5		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_7$	5.9×10^5		Wang et al. (2017)	Q	81, 240
JPFVAVYDZBUWDH-UHFFFAOYSA-N	1.9×10^2		Wang et al. (2017)	Q	81, 241
MCM:C113NO3	7.4×10^3		Wang et al. (2017)	Q	81, 239
$C_{11}H_{21}NO_5$	2.8×10^4		Wang et al. (2017)	Q	81, 240
XIMKJTRLGBXFHP-UHFFFAOYSA-N	9.3		Wang et al. (2017)	Q	81, 241
MCM:C123NO3	6.0×10^3		Wang et al. (2017)	Q	81, 239
$C_{12}H_{23}NO_5$	2.5×10^4		Wang et al. (2017)	Q	81, 240
MVMJPHZGIRWSLB-UHFFFAOYSA-N	3.4		Wang et al. (2017)	Q	81, 241
MCM:C133NO3	1.2×10^9		Wang et al. (2017)	Q	81, 239
$C_{13}H_{21}NO_7$	5.1×10^8		Wang et al. (2017)	Q	81, 240
ODJJFBKGWDLDSF-UHFFFAOYSA-N	1.8×10^5		Wang et al. (2017)	Q	81, 241
MCM:BCKANO3	2.5×10^4		Wang et al. (2017)	Q	81, 239
$C_{14}H_{23}NO_5$	6.0×10^5		Wang et al. (2017)	Q	81, 240
YULYIMMPXZFYHU-UHFFFAOYSA-N	1.8×10^4		Wang et al. (2017)	Q	81, 241
MCM:BCKBNO3	2.5×10^4		Wang et al. (2017)	Q	81, 239
$C_{14}H_{23}NO_5$	1.0×10^6		Wang et al. (2017)	Q	81, 240
VHSFPWDPGIOBJY-UHFFFAOYSA-N	1.9×10^4		Wang et al. (2017)	Q	81, 241
MCM:C142NO3	1.1×10^4		Wang et al. (2017)	Q	81, 239
$C_{14}H_{23}NO_5$	1.9×10^5		Wang et al. (2017)	Q	81, 240
AZGAJOUTVTYWPD-UHFFFAOYSA-N	1.4×10^4		Wang et al. (2017)	Q	81, 241
MCM:C143NO3	3.4×10^6		Wang et al. (2017)	Q	81, 239
$C_{14}H_{23}NO_6$	5.0×10^7		Wang et al. (2017)	Q	81, 240
NNHMCYUMVAAOGX-UHFFFAOYSA-N	1.0×10^5		Wang et al. (2017)	Q	81, 241
MCM:NMGLYOX	6.0×10^3		Wang et al. (2017)	Q	81, 239
$C_3H_3NO_5$	4.1×10^3		Wang et al. (2017)	Q	81, 240
OPXOPVKLHYDIMX-UHFFFAOYSA-N	3.4×10^{-2}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:C312COPAN	2.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_3NO_7$	2.8×10^{5}		Wang et al. (2017)	Q	81, 240
RRBQALAYWSLXKO-UHFFFAOYSA-N	3.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C4CONO3CO	6.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_5$	8.3×10^{3}		Wang et al. (2017)	Q	81, 240
RXLGSPGPVVHCFU-UHFFFAOYSA-N	2.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:NCO23CHO	3.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_3NO_6$	9.8×10^{5}		Wang et al. (2017)	Q	81, 240
VZDGBDWMYVQZKU-UHFFFAOYSA-N	1.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C4CO2DBPAN	6.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_3NO_7$	2.5×10^{6}		Wang et al. (2017)	Q	81, 240
BTFAHSUMXINULH-UHFFFAOYSA-N	4.9×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:C4M22CONO3	3.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_5$	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
FQGALMJVSZOCNN-UHFFFAOYSA-N	5.1×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C512NO3	4.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_5$	2.0×10^{4}		Wang et al. (2017)	Q	81, 240
OAONLGDTCNNTSO-UHFFFAOYSA-N	8.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CHOC3COPAN	1.7×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_5NO_7$	3.8×10^{5}		Wang et al. (2017)	Q	81, 240
MEMYBUIJIAQZMF-UHFFFAOYSA-N	9.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:INANCOCHO	4.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_6N_2O_8$	2.6×10^{5}		Wang et al. (2017)	Q	81, 240
ALBXLNVOOLMBSV-UHFFFAOYSA-N	1.5×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:C511PAN	1.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_7$	8.9×10^{5}		Wang et al. (2017)	Q	81, 240
ADLPISUKTIUEBV-UHFFFAOYSA-N	8.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C5124COPAN	1.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_5NO_8$	1.3×10^{7}		Wang et al. (2017)	Q	81, 240
DHCQJQARWDKNBK-UHFFFAOYSA-N	2.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C512PAN	1.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_7$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
OLSCQSOEJBIJSE-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C515PAN	1.0×10^{9}		Wang et al. (2017)	Q	81, 239
$C_6H_5NO_8$	3.0×10^{7}		Wang et al. (2017)	Q	81, 240
QIUJGMPSWRWOQB-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	81, 241
MCM:C5CO2DBPAN	4.7×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_5NO_7$	2.1×10^{6}		Wang et al. (2017)	Q	81, 240
LCULQJDFGZNNJC-UHFFFAOYSA-N	2.8×10^{-3}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C5DBCO2PAN	4.7×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_5NO_7$	2.1×10^{6}		Wang et al. (2017)	Q	81, 240
QMYFWHUFARKUQS-UHFFFAOYSA-N	3.6×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:C626NO3	4.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_5$	5.1×10^{4}		Wang et al. (2017)	Q	81, 240
OCVBVQJPDKPHST-UHFFFAOYSA-N	1.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C6COCHOPAN	1.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_7$	2.6×10^{6}		Wang et al. (2017)	Q	81, 240
YGLXJUWEIHLTAS-UHFFFAOYSA-N	8.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C4DBM2PAN	3.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_7NO_7$	3.0×10^{6}		Wang et al. (2017)	Q	81, 240
LSIPSXVETZQMNK-UHFFFAOYSA-N	5.4×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:C617PAN	8.7×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_7$	9.6×10^{4}		Wang et al. (2017)	Q	81, 240
PZZHENCPCXAAMZ-UHFFFAOYSA-N	6.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C618PAN	8.7×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_7$	7.8×10^{4}		Wang et al. (2017)	Q	81, 240
TUYXNXVHKYYCNT-UHFFFAOYSA-N	5.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C626PAN	1.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_7$	2.0×10^{6}		Wang et al. (2017)	Q	81, 240
JTOZIQOFBRFINW-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C717NO3	2.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_6$	8.0×10^{5}		Wang et al. (2017)	Q	81, 240
YBNFZHXBUOLIKA-UHFFFAOYSA-N	2.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C718NO3	2.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{11}NO_5$	3.5×10^{3}		Wang et al. (2017)	Q	81, 240
WMUFPKACUPNARK-UHFFFAOYSA-N	3.8		Wang et al. (2017)	Q	81, 241
MCM:C731NO3	3.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_7H_{11}NO_5$	4.5×10^{4}		Wang et al. (2017)	Q	81, 240
WJSMASANGLXUCK-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C7CO2DBPAN	3.7×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_7NO_7$	1.2×10^{6}		Wang et al. (2017)	Q	81, 240
FJSOTAPJABBDID-UHFFFAOYSA-N	2.6×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:NC61CO3H	1.7×10^{12}		Wang et al. (2017)	Q	81, 239
$C_7H_7NO_9$	6.2×10^{8}		Wang et al. (2017)	Q	81, 240
RCADYDMYBSYTRH-UHFFFAOYSA-N	6.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NC6PAN1	6.6×10^{10}		Wang et al. (2017)	Q	81, 239
$C_7H_6N_2O_{11}$	2.4×10^{8}		Wang et al. (2017)	Q	81, 240
LNWBMFOWVOYBBT-UHFFFAOYSA-N	2.0×10^{-2}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C4DBMEPAN	2.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_7$	1.6×10^{6}		Wang et al. (2017)	Q	81, 240
JDCDQJWNYIFIQT-UHFFFAOYSA-N	3.5×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:C718PAN	7.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_7$	2.3×10^{5}		Wang et al. (2017)	Q	81, 240
IZJQRCOOVGKQNV-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	81, 241
MCM:C731PAN	1.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_7$	1.7×10^{6}		Wang et al. (2017)	Q	81, 240
BCDBCVPVNWUZKV-UHFFFAOYSA-N	4.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C8CO2DBPAN	3.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_7$	6.9×10^{5}		Wang et al. (2017)	Q	81, 240
IPAWZRQBQOFPJA-UHFFFAOYSA-N	1.4×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:C8DBCO2PAN	3.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_7$	8.0×10^{5}		Wang et al. (2017)	Q	81, 240
ZDCAPCKMKJMPHV-UHFFFAOYSA-N	1.0×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:C87PAN	6.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_8$	2.8×10^{7}		Wang et al. (2017)	Q	81, 240
KZPDHKTVZKNFJF-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	81, 241
MCM:C915NO3	5.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_5$	3.2×10^{4}		Wang et al. (2017)	Q	81, 240
CFOCUCLSGKHNEG-UHFFFAOYSA-N	5.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C916NO3	1.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_6$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
VOXWFVUGDBUBCW-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C918NO3	5.9×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_5$	5.6×10^{3}		Wang et al. (2017)	Q	81, 240
AMOFMDWAGAYJCS-UHFFFAOYSA-N	5.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C919NO3	1.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_6$	1.0×10^{6}		Wang et al. (2017)	Q	81, 240
DCZHYWWXGROBKB-UHFFFAOYSA-N	8.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C930NO3	1.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_6$	5.6×10^{5}		Wang et al. (2017)	Q	81, 240
DDSHYSHFPVKRPI-UHFFFAOYSA-N	1.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C1010NO3	3.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_5$	8.5×10^{3}		Wang et al. (2017)	Q	81, 240
GVXIDPZAUKXFPR-UHFFFAOYSA-N	4.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C1012NO3	1.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_5$	8.1×10^{3}		Wang et al. (2017)	Q	81, 240
XKIZNDJDYSDNBL-UHFFFAOYSA-N	2.7×10^{2}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C106NO3	1.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_6$	7.3×10^{5}		Wang et al. (2017)	Q	81, 240
DSEFLMWIAZKUSJ-UHFFFAOYSA-N	4.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C108NO3	1.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_6$	2.2×10^{5}		Wang et al. (2017)	Q	81, 240
MVSLQVXNIWKHQS-UHFFFAOYSA-N	6.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NLIMALOOH	1.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_7$	3.4×10^{7}		Wang et al. (2017)	Q	81, 240
NTLQQKIUYMIZPN-UHFFFAOYSA-N	2.8×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PINALNO3	3.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_5$	1.6×10^{4}		Wang et al. (2017)	Q	81, 240
FNTMCASBPWQXGD-UHFFFAOYSA-N	3.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C116NO3	4.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{17}NO_5$	3.7×10^{4}		Wang et al. (2017)	Q	81, 240
AWSJYNTZBDMUKU-UHFFFAOYSA-N	3.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C116PAN	1.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{17}NO_7$	2.3×10^{6}		Wang et al. (2017)	Q	81, 240
IHJLCJPVFFZKMO-UHFFFAOYSA-N	1.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C1210NO3	3.4×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{19}NO_5$	4.1×10^{4}		Wang et al. (2017)	Q	81, 240
IJHSXQWUSMROBJ-UHFFFAOYSA-N	7.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C1210PAN	1.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{19}NO_7$	2.0×10^{6}		Wang et al. (2017)	Q	81, 240
PWZZEUPXUFAYML-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NBCALOOH	1.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{25}NO_7$	8.5×10^{7}		Wang et al. (2017)	Q	81, 240
TUYLAULXHOKFAG-UHFFFAOYSA-N	7.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:H3NCO2CHO	1.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_6$	3.6×10^{6}		Wang et al. (2017)	Q	81, 240
VCTGKRYJUDQYFK-UHFFFAOYSA-N	3.4		Wang et al. (2017)	Q	81, 241
MCM:HMVKNGLYOX	2.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_6$	9.3×10^{5}		Wang et al. (2017)	Q	81, 240
VDDXFUNTPSDTJP-UHFFFAOYSA-N	9.3		Wang et al. (2017)	Q	81, 241
MCM:INB1GLYOX	1.2×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_6$	3.1×10^{5}		Wang et al. (2017)	Q	81, 240
NAZCWKUVRXJZPX-UHFFFAOYSA-N	3.0		Wang et al. (2017)	Q	81, 241
MCM:INCGLYOX	6.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_6$	4.8×10^{5}		Wang et al. (2017)	Q	81, 240
DGCXGPGOOTUCCO-UHFFFAOYSA-N	3.0×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C5CO2OHPAN	2.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_5NO_8$	1.7×10^{9}		Wang et al. (2017)	Q	81, 240
MLSWEUDOYVEBFO-UHFFFAOYSA-N	7.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C6CO2OHPAN	1.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_7NO_8$	1.4×10^{9}		Wang et al. (2017)	Q	81, 240
GITGCCFTTYJWBT-UHFFFAOYSA-N	4.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C5M2OHOPAN	9.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_8$	2.0×10^{9}		Wang et al. (2017)	Q	81, 240
MJYXUWCXTAYXTN-UHFFFAOYSA-N	7.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C7OHCO2PAN	1.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_8$	8.3×10^{8}		Wang et al. (2017)	Q	81, 240
WKRTWLVIFYOGIB-UHFFFAOYSA-N	1.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C5MEJPAN	7.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_8$	1.2×10^{9}		Wang et al. (2017)	Q	81, 240
KTOTUVLJTIGMKC-UHFFFAOYSA-N	5.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C8CO2OHPAN	1.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_8$	6.6×10^{8}		Wang et al. (2017)	Q	81, 240
UEMVFSSSLHUULZ-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:C8OHCO2PAN	9.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_8$	5.8×10^{8}		Wang et al. (2017)	Q	81, 240
GUTUSTBTBKWXHL-UHFFFAOYSA-N	1.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:LIMALNO3	1.3×10^{8}	23000	Wieser et al. (2023)	Q	439
$C_{10}H_{17}NO_6$	5.3×10^{6}		Wang et al. (2017)	Q	81, 239
FDBNDHKWTKEDSC-UHFFFAOYSA-N	3.2×10^{7}		Wang et al. (2017)	Q	81, 240
	3.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NLIMALOH	5.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_6$	4.8×10^{7}		Wang et al. (2017)	Q	81, 240
NNOYMJCUDKQQLW-UHFFFAOYSA-N	2.7×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C117NO3	7.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{17}NO_6$	1.0×10^{7}		Wang et al. (2017)	Q	81, 240
VRGCJRKSASUXOA-UHFFFAOYSA-N	2.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C118NO3	2.2×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{17}NO_7$	6.5×10^{8}		Wang et al. (2017)	Q	81, 240
RHEKUCZWBZRVBN-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C1215NO3	1.8×10^{9}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{19}NO_7$	1.1×10^{10}		Wang et al. (2017)	Q	81, 240
HIFZNEWSKKHKQF-UHFFFAOYSA-N	2.6×10^{5}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:C128NO3	6.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{19}NO_6$	5.3×10^{7}		Wang et al. (2017)	Q	81, 240
XVMHBNQZULJJQH-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C1312NO3	5.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{21}NO_6$	1.4×10^{8}		Wang et al. (2017)	Q	81, 240
LCWPKTPKZZROTF-UHFFFAOYSA-N	3.2×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:BCALNO3	4.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{25}NO_6$	5.3×10^{7}		Wang et al. (2017)	Q	81, 240
KJHBLMRUHUAACD-UHFFFAOYSA-N	8.7×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:NBCALOH	4.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{25}NO_6$	6.2×10^{7}		Wang et al. (2017)	Q	81, 240
YUOPYTDNMDNILJ-UHFFFAOYSA-N	6.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NO3CH2CO2H	1.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_2H_3NO_5$	8.3×10^{4}		Wang et al. (2017)	Q	81, 240
VHOVOPOBBVJMEP-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:PRNO3CO2H	1.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_5NO_5$	9.1×10^{3}		Wang et al. (2017)	Q	81, 240
DVOPCQDTEPKYKW-UHFFFAOYSA-N	7.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MPRNO3CO2H	8.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_5$	3.3×10^{3}		Wang et al. (2017)	Q	81, 240
MSBKTJKUKRRTOZ-UHFFFAOYSA-N	3.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NC3CO2H	4.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_5$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
IYBHCPMQXJSPPT-UHFFFAOYSA-N	4.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C3MNO3CO2H	1.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	2.2×10^{3}		Wang et al. (2017)	Q	81, 240
CCKPHGGNTPAJHG-UHFFFAOYSA-N	2.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C43NO3CO2H	6.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
PAJLSJNKCRUQAA-UHFFFAOYSA-N	2.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C4NO3CO2H	9.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	2.0×10^{3}		Wang et al. (2017)	Q	81, 240
LHOHBJOUNVJDSQ-UHFFFAOYSA-N	2.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NC4CO2H	3.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_5$	9.6×10^{3}		Wang et al. (2017)	Q	81, 240
ZKTRJZJYWMAEEY-UHFFFAOYSA-N	7.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C65NO3CO2H	8.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	1.1×10^{3}		Wang et al. (2017)	Q	81, 240
JEDGAPUZBUOYQF-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C721PAN	5.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_7$	4.3×10^{6}		Wang et al. (2017)	Q	81, 240
OMUZIQDFMVGNTC-UHFFFAOYSA-N	6.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C811NO3	1.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{13}NO_5$	1.7×10^{4}		Wang et al. (2017)	Q	81, 240
WYXUZPCNBFFDRO-UHFFFAOYSA-N	5.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C823NO3	1.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_{13}NO_5$	2.2×10^{4}		Wang et al. (2017)	Q	81, 240
QAJOXMTYFQHFPC-UHFFFAOYSA-N	4.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C811PAN	4.7×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	3.1×10^{6}		Wang et al. (2017)	Q	81, 240
BOYXRVFXWMBNIT-UHFFFAOYSA-N	3.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C823PAN	4.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	1.3×10^{6}		Wang et al. (2017)	Q	81, 240
GRHNTSHNCZZYLE-UHFFFAOYSA-N	2.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C137NO3	1.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{21}NO_5$	3.8×10^{4}		Wang et al. (2017)	Q	81, 240
CQGOUXQAADNZJX-UHFFFAOYSA-N	2.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C137PAN	4.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{14}H_{21}NO_7$	2.5×10^{6}		Wang et al. (2017)	Q	81, 240
KJDMPVAHMJBAAO-UHFFFAOYSA-N	9.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MACRNBCO2H	1.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	2.6×10^{6}		Wang et al. (2017)	Q	81, 240
WQOIEXBGIWRREH-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:MACRNCO2H	3.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	8.5×10^{5}		Wang et al. (2017)	Q	81, 240
GPIMHHNLFCYMAO-UHFFFAOYSA-N	5.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C57NO3CO2H	2.8×10^{9}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_7$	1.6×10^{8}		Wang et al. (2017)	Q	81, 240
VNPCVOYEGJTTSH-UHFFFAOYSA-N	2.3×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C58NO3CO2H	4.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_7$	5.0×10^{8}		Wang et al. (2017)	Q	81, 240
QOEJXJLKIMUJIJ-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:INAHCO2H	1.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_7$	1.7×10^{9}		Wang et al. (2017)	Q	81, 240
KDGUUBLLRPAORR-UHFFFAOYSA-N	5.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:INAHPCO2H	2.3×10^{11}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_8$	2.5×10^{9}		Wang et al. (2017)	Q	81, 240
CHIYBIMSWIBBRD-UHFFFAOYSA-N	1.6×10^{5}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:INANCO2H	3.6×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_9$	3.6×10^{7}		Wang et al. (2017)	Q	81, 240
QEPBKMYMBRWSSY-UHFFFAOYSA-N	4.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:INB1HPCO2H	2.0×10^{11}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_8$	2.9×10^{8}		Wang et al. (2017)	Q	81, 240
XWZUZABUMCCUCE-UHFFFAOYSA-N	1.8×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:INB1NACO2H	3.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_9$	5.1×10^{6}		Wang et al. (2017)	Q	81, 240
FONBWUWRCYYCPB-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:INB1NBCO2H	3.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_9$	7.3×10^{6}		Wang et al. (2017)	Q	81, 240
YGORAHXKOXOIMV-UHFFFAOYSA-N	2.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:INCNCO2H	3.6×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_8N_2O_9$	2.0×10^{7}		Wang et al. (2017)	Q	81, 240
LXTUVHDUSAOJOD-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C139NO3	6.6×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{21}NO_7$	1.9×10^{8}		Wang et al. (2017)	Q	81, 240
UFNZJLDHNJULFY-UHFFFAOYSA-N	6.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:CONM2CO2H	7.4×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_6$	8.3×10^{4}		Wang et al. (2017)	Q	81, 240
LTGNKSWVEYSUMY-UHFFFAOYSA-N	3.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:MMALNACO2H	1.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_7$	4.5×10^{7}		Wang et al. (2017)	Q	81, 240
REHIBMNEJUPYOU-UHFFFAOYSA-N	6.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:MMALNBCO2H	1.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_7$	1.9×10^{7}		Wang et al. (2017)	Q	81, 240
RAMGTVAYJVLLRG-UHFFFAOYSA-N	5.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:INANCOCO2H	5.8×10^{7}		Wang et al. (2017)	Q	81, 239
$C_5H_6N_2O_9$	8.5×10^{6}		Wang et al. (2017)	Q	81, 240
XEVMEFHPLZUFAK-UHFFFAOYSA-N	6.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C732NO3	4.7×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_{11}NO_6$	3.7×10^{7}		Wang et al. (2017)	Q	81, 240
SXYZBZXZNRYERD-UHFFFAOYSA-N	4.9×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C732PAN	1.7×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_8$	1.7×10^{9}		Wang et al. (2017)	Q	81, 240
WNUKRJOERGBBRT-UHFFFAOYSA-N	2.0×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C1211NO3	5.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{19}NO_6$	5.6×10^{7}		Wang et al. (2017)	Q	81, 240
DQVGSELEPUBBSS-UHFFFAOYSA-N	2.9×10^{5}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:C1211PAN	1.6×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{19}NO_8$	4.2×10^{9}		Wang et al. (2017)	Q	81, 240
IROGWMVYBREROI-UHFFFAOYSA-N	9.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:C813NO3	8.5×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{13}NO_7$	4.6×10^{7}		Wang et al. (2017)	Q	81, 240
GYZVFQOTJWTWBE-UHFFFAOYSA-N	7.1×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C1212NO3	2.3×10^{10}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{19}NO_8$	1.3×10^{10}		Wang et al. (2017)	Q	81, 240
NTNWJSADTNTFHH-UHFFFAOYSA-N	3.0×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C1213NO3	2.6×10^{11}		Wang et al. (2017)	Q	81, 239
$C_{12}H_{19}NO_8$	1.8×10^{11}		Wang et al. (2017)	Q	81, 240
FRAJAIDKFGOMCR-UHFFFAOYSA-N	3.6×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:C1310NO3	7.3×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{13}H_{21}NO_7$	1.4×10^{10}		Wang et al. (2017)	Q	81, 240
YNRLOWIUKIUEHR-UHFFFAOYSA-N	3.0×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:C151NO3	7.4×10^{8}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{25}NO_7$	2.6×10^{10}		Wang et al. (2017)	Q	81, 240
BHPYCCPMXIBJRO-UHFFFAOYSA-N	8.7×10^{8}		Wang et al. (2017)	Q	81, 241
MCM:CHOOCH2NO3	5.8		Wang et al. (2017)	Q	81, 239
$C_2H_3NO_5$	1.4×10^{1}		Wang et al. (2017)	Q	81, 240
OAQKKIQKQLJUJT-UHFFFAOYSA-N	2.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:CHOOMPAN	1.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_3NO_7$	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
XZTQWYQUABOKPG-UHFFFAOYSA-N	1.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:ETHFORMNO3	5.4		Wang et al. (2017)	Q	81, 239
$C_3H_5NO_5$	3.5		Wang et al. (2017)	Q	81, 240
DOXRBPLNMOIQGP-UHFFFAOYSA-N	1.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:METACETNO3	3.9		Wang et al. (2017)	Q	81, 239
$C_3H_5NO_5$	1.9×10^{1}		Wang et al. (2017)	Q	81, 240
HRSAJZJMUADCNM-UHFFFAOYSA-N	3.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:MMCFNO3	1.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_3NO_7$	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
IFMSYUVMGRDEMV-UHFFFAOYSA-N	7.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:ACEC2H4NO3	3.2		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_5$	2.5×10^{1}		Wang et al. (2017)	Q	81, 240
QOXSFWPQUXLCPI-UHFFFAOYSA-N	9.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:ACETMEPAN	1.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_7$	1.8×10^{3}		Wang et al. (2017)	Q	81, 240
QMSGSFOWAUFKPL-UHFFFAOYSA-N	1.7×10^{-2}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:COO2C3PAN	1.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_7$	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
YQMLKDOXYNVTNM-UHFFFAOYSA-N	7.1×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:ETACETNO3	3.6		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_5$	3.5		Wang et al. (2017)	Q	81, 240
KORDSAOMZNGUAL-UHFFFAOYSA-N	2.4×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:IPRFORMNO3	3.0		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_5$	6.9×10^{-1}		Wang et al. (2017)	Q	81, 240
DZSICYNSKFSRMV-UHFFFAOYSA-N	1.8×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:NBZFUOOH	2.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_4H_5NO_7$	3.0×10^{6}		Wang et al. (2017)	Q	81, 240
TXWHLSUKLWEERR-UHFFFAOYSA-N	2.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:ACCOMEPAN	5.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_5NO_8$	5.1×10^{5}		Wang et al. (2017)	Q	81, 240
ZQOVYYMCAFZVPL-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	81, 241
MCM:ACETC2PAN	1.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_7$	2.1×10^{3}		Wang et al. (2017)	Q	81, 240
VMVPPLVFXDAZML-UHFFFAOYSA-N	6.5×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:COO2C4PAN	1.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_7$	1.7×10^{3}		Wang et al. (2017)	Q	81, 240
GBAXNZCSCJEGAE-UHFFFAOYSA-N	1.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:IPRACBNO3	2.8		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	8.1		Wang et al. (2017)	Q	81, 240
ZEVCPCUWRCOHCL-UHFFFAOYSA-N	3.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:IPRACBPAN	1.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_7$	3.9×10^{2}		Wang et al. (2017)	Q	81, 240
UJCZQTHKWBYHPW-UHFFFAOYSA-N	2.2×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:IPRACNO3	2.0		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	8.0×10^{-1}		Wang et al. (2017)	Q	81, 240
JAQKAPGOMZJVBI-UHFFFAOYSA-N	2.2×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:MTBEAALNO3	2.7		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	2.5		Wang et al. (2017)	Q	81, 240
NIMOOIUOXYQIIM-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:MTBEAALPAN	9.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_7$	6.5×10^{1}		Wang et al. (2017)	Q	81, 240
WKTKTTPKCZOXAQ-UHFFFAOYSA-N	1.1×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:NPRACANO3	2.8		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	8.1		Wang et al. (2017)	Q	81, 240
FPQZKAXTSOKJRB-UHFFFAOYSA-N	3.4×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NPRACBNO3	2.8		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	1.9		Wang et al. (2017)	Q	81, 240
HTKMYQNNJMTEJQ-UHFFFAOYSA-N	1.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:NPRACCNO3	2.8		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_5$	1.5×10^{1}		Wang et al. (2017)	Q	81, 240
PSJLJILPBUYXRJ-UHFFFAOYSA-N	3.1		Wang et al. (2017)	Q	81, 241
MCM:NPXYFUOOH	1.2×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_7$	8.9×10^{5}		Wang et al. (2017)	Q	81, 240
ARRSNVVNYKGUFK-UHFFFAOYSA-N	5.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NTLFUOOH	2.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_7$	2.2×10^{6}		Wang et al. (2017)	Q	81, 240
OAXQEILKHMZHNV-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:MCOOTBNO3	1.6		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	2.9		Wang et al. (2017)	Q	81, 240
BCWPDUXSEGSVPT-UHFFFAOYSA-N	1.2×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:NBUACANO3	2.6		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	6.9		Wang et al. (2017)	Q	81, 240
GNPRUWODPALWHJ-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	81, 241
MCM:NBUACBNO3	2.6		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	5.0		Wang et al. (2017)	Q	81, 240
UFOXFUDLAIUTHC-UHFFFAOYSA-N	4.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:NBUACCNO3	2.6		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	1.4		Wang et al. (2017)	Q	81, 240
PYXJHVBEHHCABK-UHFFFAOYSA-N	1.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:NDMMALYOOH	2.2×10^{11}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_8$	9.8×10^{7}		Wang et al. (2017)	Q	81, 240
RZSLUQVSVWAZFJ-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NEBFUOOH	1.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_7$	1.4×10^{6}		Wang et al. (2017)	Q	81, 240
CZSCMTWZZQSKMX-UHFFFAOYSA-N	9.8×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NMXYFUOOH	1.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_7$	4.9×10^{5}		Wang et al. (2017)	Q	81, 240
URYSYTGABCBDCM-UHFFFAOYSA-N	6.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NOXYFUOOH	6.8×10^{7}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_7$	3.2×10^{5}		Wang et al. (2017)	Q	81, 240
CPPAIMSHWPDUBG-UHFFFAOYSA-N	2.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NTMB1FUOOH	1.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_7$	1.7×10^{7}		Wang et al. (2017)	Q	81, 240
WRMOSOIHGVCRMO-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PRCOOMPAN	8.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_7$	5.6×10^{2}		Wang et al. (2017)	Q	81, 240
NSDDFRROKVQLRJ-UHFFFAOYSA-N	1.4×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:SBUACANO3	1.6		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	5.3×10^{-1}		Wang et al. (2017)	Q	81, 240
FWAMAOJLVLFAOA-UHFFFAOYSA-N	1.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:SBUACBNO3	3.0		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_5$	4.0		Wang et al. (2017)	Q	81, 240
FVMFJLQQOIKLHP-UHFFFAOYSA-N	2.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:TBUACPAN	6.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_7$	7.3×10^{1}		Wang et al. (2017)	Q	81, 240
WTCUHXTZKDYOTB-UHFFFAOYSA-N	2.6×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:NIPBFUOOH	1.7×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{11}NO_7$	1.3×10^{6}		Wang et al. (2017)	Q	81, 240
MJSJHBOZYWKETN-UHFFFAOYSA-N	5.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NMEBFUOOH	1.0×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{11}NO_7$	3.2×10^{5}		Wang et al. (2017)	Q	81, 240
LKMBYBKEMVMSAU-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NPBFUOOH	1.5×10^{8}		Wang et al. (2017)	Q	81, 239
$C_7H_{11}NO_7$	1.1×10^{6}		Wang et al. (2017)	Q	81, 240
DGKCEZHRNXTHAZ-UHFFFAOYSA-N	4.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:NTMB2FUOOH	6.3×10^{7}		Wang et al. (2017)	Q	81, 239
$C_7H_{11}NO_7$	1.8×10^{5}		Wang et al. (2017)	Q	81, 240
IRLXCLTZUJZGMJ-UHFFFAOYSA-N	2.4×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C1013NO3	3.1		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_5$	5.4		Wang et al. (2017)	Q	81, 240
TWKDJCLTDHUPBZ-UHFFFAOYSA-N	3.2		Wang et al. (2017)	Q	81, 241
MCM:C1013PAN	9.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{17}NO_7$	4.8×10^{2}		Wang et al. (2017)	Q	81, 240
QVQKWVAIHQGLJY-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	81, 241
MCM:C1014NO3	7.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{17}NO_6$	1.9×10^{3}		Wang et al. (2017)	Q	81, 240
OQZDTLQTCPZSBL-UHFFFAOYSA-N	7.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C152NO3	3.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{25}NO_7$	1.3×10^{7}		Wang et al. (2017)	Q	81, 240
VUWXYQDBWQFZDF-UHFFFAOYSA-N	7.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:NBZFUONE	1.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_3NO_6$	4.3×10^{6}		Wang et al. (2017)	Q	81, 240
LXADUFLCRLLGHU-UHFFFAOYSA-N	8.3×10^{1}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C23O3CPAN	7.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_5NO_8$	2.8×10^{5}		Wang et al. (2017)	Q	81, 240
BCRDXKGRUUAZSU-UHFFFAOYSA-N	3.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:ACBUONANO3	1.7×10^{3}		Wang et al. (2017)	Q	81, 239
$C_6H_9NO_6$	2.2×10^{3}		Wang et al. (2017)	Q	81, 240
PDSBHIWVTCGSAN-UHFFFAOYSA-N	9.1		Wang et al. (2017)	Q	81, 241
MCM:C23O3MCPAN	7.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_8$	6.0×10^{4}		Wang et al. (2017)	Q	81, 240
MJYWDTPJLIMPPV-UHFFFAOYSA-N	2.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:NEBFUONE	1.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_6$	2.3×10^{6}		Wang et al. (2017)	Q	81, 240
LZGWKDALCOZNIJ-UHFFFAOYSA-N	8.1		Wang et al. (2017)	Q	81, 241
MCM:C23O3ECPAN	5.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_8$	3.2×10^{4}		Wang et al. (2017)	Q	81, 240
SOMJWLUSPZTMJM-UHFFFAOYSA-N	1.5×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:NIPBFUONE	1.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_6$	2.0×10^{6}		Wang et al. (2017)	Q	81, 240
OEYHEYBMUYSQHE-UHFFFAOYSA-N	4.8		Wang et al. (2017)	Q	81, 241
MCM:NPBFUONE	1.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_6$	1.7×10^{6}		Wang et al. (2017)	Q	81, 240
WTNUMEKWPLLNDJ-UHFFFAOYSA-N	6.6		Wang et al. (2017)	Q	81, 241
MCM:CH3OCH2NO3	3.4×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_2H_5NO_4$	3.4×10^{-1}		Wang et al. (2017)	Q	81, 240
VHAYDBAVTGOZLW-UHFFFAOYSA-N	4.5×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:DMMANO3	8.1		Wang et al. (2017)	Q	81, 239
$C_3H_7NO_5$	5.5		Wang et al. (2017)	Q	81, 240
ZKGVKOFAVUIIEY-UHFFFAOYSA-N	3.0×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:DMMBNO3	9.3		Wang et al. (2017)	Q	81, 239
$C_3H_7NO_5$	1.0×10^{-1}		Wang et al. (2017)	Q	81, 240
ADJOFNYUECRONI-UHFFFAOYSA-N	1.7×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:ETOMENO3	5.8×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_3H_7NO_3$	6.6×10^{-1}		Wang et al. (2017)	Q	81, 240
ZMUPMMOTQUHRHQ-UHFFFAOYSA-N	3.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:MEMOXYPAN	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_3H_5NO_6$	2.2×10^{2}		Wang et al. (2017)	Q	81, 240
JBHGAGLULWBGCW-UHFFFAOYSA-N	1.0×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:DIETETNO3	2.8×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_4$	4.2×10^{-2}		Wang et al. (2017)	Q	81, 240
CAMRTYJYAQGENN-UHFFFAOYSA-N	7.3×10^{-3}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:ETOC2NO3	2.5×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_4$	2.5		Wang et al. (2017)	Q	81, 240
GDNQXPDYGNUKII-UHFFFAOYSA-N	4.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:ETOMEPAN	9.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_4H_7NO_6$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
CCYZAMBLJVQHMC-UHFFFAOYSA-N	1.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:IPROC21NO3	2.6×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	2.0×10^{-2}		Wang et al. (2017)	Q	81, 240
YQGFTPNVRZNXAP-UHFFFAOYSA-N	8.0×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:MTBEANO3	1.5×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	2.7×10^{-2}		Wang et al. (2017)	Q	81, 240
NXHUJDLNRCHXIE-UHFFFAOYSA-N	8.3×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:MTBEBNO3	1.5×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_5H_{11}NO_4$	6.2×10^{-1}		Wang et al. (2017)	Q	81, 240
HWZCMFJGZXOLOM-UHFFFAOYSA-N	4.1×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:MTBEBPAN	5.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_5H_9NO_6$	1.4×10^{1}		Wang et al. (2017)	Q	81, 240
PQCDPGWYIKXNFH-UHFFFAOYSA-N	5.5×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:BOXMPAN	6.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	5.1×10^{1}		Wang et al. (2017)	Q	81, 240
CPESEOWHBGRFRT-UHFFFAOYSA-N	3.2×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:DIIPRETNO3	1.4×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	4.9×10^{-3}		Wang et al. (2017)	Q	81, 240
RYKOUPKPIPKSCM-UHFFFAOYSA-N	1.5×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:ETBEANO3	1.2×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	3.2×10^{-1}		Wang et al. (2017)	Q	81, 240
WGHLTNOFPVNDHK-UHFFFAOYSA-N	4.1×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:ETBEAPAN	4.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	9.1		Wang et al. (2017)	Q	81, 240
ZFJPSAIQYMAFAB-UHFFFAOYSA-N	3.6×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:ETBEBNO3	1.4×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	7.1×10^{-3}		Wang et al. (2017)	Q	81, 240
BIDDBAQEKWTVIC-UHFFFAOYSA-N	1.1×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:ETBECNO3	1.2×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	4.0×10^{-1}		Wang et al. (2017)	Q	81, 240
MGOGEALWXAMIEO-UHFFFAOYSA-N	5.0×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:ETBECPAN	4.8×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	2.3×10^{1}		Wang et al. (2017)	Q	81, 240
JICVHVAZXJWJCM-UHFFFAOYSA-N	2.1×10^{-2}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:IPROMC2NO3	2.0×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_4$	4.6×10^{-1}		Wang et al. (2017)	Q	81, 240
XJQWDDGHWZGMDK-UHFFFAOYSA-N	2.9×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:IPROMCPAN	8.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_6H_{11}NO_6$	2.0×10^{1}		Wang et al. (2017)	Q	81, 240
SFYHCJJQTXJNNN-UHFFFAOYSA-N	3.9×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:MO2EOLANO3	1.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_7NO_5$	5.6×10^{2}		Wang et al. (2017)	Q	81, 240
FJVLHDUAJQRZPG-UHFFFAOYSA-N	3.2		Wang et al. (2017)	Q	81, 241
MCM:MO2EOLBNO3	1.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_7NO_5$	1.3×10^{3}		Wang et al. (2017)	Q	81, 240
QPXHYMSZINTGRC-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:EOX2OLANO3	1.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_5$	3.6×10^{2}		Wang et al. (2017)	Q	81, 240
UVLBVBPSPHSYND-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	81, 241
MCM:EOX2OLBNO3	9.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_5$	3.2×10^{2}		Wang et al. (2017)	Q	81, 240
DLOZDRFLLIHYBD-UHFFFAOYSA-N	8.9		Wang et al. (2017)	Q	81, 241
MCM:H2C3OCNO3	9.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_5$	9.1×10^{2}		Wang et al. (2017)	Q	81, 240
VJBSYBJCULHXOZ-UHFFFAOYSA-N	3.0		Wang et al. (2017)	Q	81, 241
MCM:PR2OHMONO3	1.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_4H_9NO_5$	3.8×10^{2}		Wang et al. (2017)	Q	81, 240
YOBYTHKQRGEURN-UHFFFAOYSA-N	8.5×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:IEAPAN	3.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_7$	2.3×10^{5}		Wang et al. (2017)	Q	81, 240
NFJKKZSQGXUZSI-UHFFFAOYSA-N	9.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:IECPAN	3.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_5H_7NO_7$	9.1×10^{4}		Wang et al. (2017)	Q	81, 240
UMKIAKGFUATPHT-UHFFFAOYSA-N	8.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:BOXEOHANO3	6.2×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_5$	1.4×10^{2}		Wang et al. (2017)	Q	81, 240
NBMGDPHUZJHVTA-UHFFFAOYSA-N	3.6		Wang et al. (2017)	Q	81, 241
MCM:BOXEOHBNO3	6.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_6H_{13}NO_5$	1.4×10^{2}		Wang et al. (2017)	Q	81, 240
YIIBDLSBOAJITL-UHFFFAOYSA-N	3.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:BOXPOLANO3	5.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_7H_{15}NO_5$	8.3×10^{1}		Wang et al. (2017)	Q	81, 240
QDPFCROPCZKQGS-UHFFFAOYSA-N	1.6		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:BOXPOLBNO3	6.5×10^{2}		Wang et al. (2017)	Q	81, 239
$C_7H_{15}NO_5$	9.1×10^{1}		Wang et al. (2017)	Q	81, 240
UNWFJVCQCSAFHA-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:BCSOZNO3	1.3×10^{6}		Wang et al. (2017)	Q	81, 239
$C_{15}H_{25}NO_7$	5.3×10^{3}		Wang et al. (2017)	Q	81, 240
HGUJSQZJFHDFKY-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:EPXDLPAN	3.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_4H_3NO_7$	1.2×10^{5}		Wang et al. (2017)	Q	81, 240
VASNFLPKLUXZKF-UHFFFAOYSA-N	8.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:EPXMDLPAN	1.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_5H_5NO_7$	2.3×10^{4}		Wang et al. (2017)	Q	81, 240
KZASOTCYMWAOFE-UHFFFAOYSA-N	3.5×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:BZEMUCPAN	9.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_5NO_7$	1.0×10^{5}		Wang et al. (2017)	Q	81, 240
RFFCGVCNFANFMQ-UHFFFAOYSA-N	7.1		Wang et al. (2017)	Q	81, 241
MCM:EPXM2DLPAN	9.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_7$	6.3×10^{3}		Wang et al. (2017)	Q	81, 240
KYBHJMDXHJGYTK-UHFFFAOYSA-N	4.2×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:EPXMEDLPAN	8.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_7$	3.5×10^{3}		Wang et al. (2017)	Q	81, 240
XUUSESMFYTYXHU-UHFFFAOYSA-N	4.4×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:OXYMUCPAN	2.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_7$	7.1×10^{3}		Wang et al. (2017)	Q	81, 240
VIRSPYOLFRMIKR-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:OETLMUCPAN	2.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_7$	4.3×10^{3}		Wang et al. (2017)	Q	81, 240
PYAKBDFKVOPHPS-UHFFFAOYSA-N	2.8		Wang et al. (2017)	Q	81, 241
MCM:BZEMUCNO3	1.1×10^{8}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_7$	1.7×10^{8}		Wang et al. (2017)	Q	81, 240
UGJSRYKPNYMSMJ-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:OXYMUCNO3	7.8×10^{8}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_7$	3.2×10^{7}		Wang et al. (2017)	Q	81, 240
PMXJWIAVDRSVOJ-UHFFFAOYSA-N	2.6×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:OETLMUCNO3	6.3×10^{8}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	1.9×10^{7}		Wang et al. (2017)	Q	81, 240
KUQUSIKCNRTUGT-UHFFFAOYSA-N	7.6×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:EPXKTMPAN	1.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_7$	2.6×10^{4}		Wang et al. (2017)	Q	81, 240
DBXZZDVADSLSOS-UHFFFAOYSA-N	1.0×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:EPXMKTPAN	1.1×10^{5}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_7$	2.6×10^{4}		Wang et al. (2017)	Q	81, 240
UTKXQAWEMGMHOV-UHFFFAOYSA-N	4.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:BOXPROANO3	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_7H_{13}NO_5$	3.3×10^{1}		Wang et al. (2017)	Q	81, 240
FWQXAWHLSYKKGA-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	81, 241
MCM:EPXEKTPAN	9.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_7$	1.6×10^{4}		Wang et al. (2017)	Q	81, 240
ZMAMXAXJQIDKIS-UHFFFAOYSA-N	3.1×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:TLEMUCPAN	5.5×10^{5}		Wang et al. (2017)	Q	81, 239
$C_7H_7NO_7$	2.0×10^{5}		Wang et al. (2017)	Q	81, 240
AUCFXVOKAUAJMN-UHFFFAOYSA-N	2.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:EBZMUCPAN	4.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_7$	1.0×10^{5}		Wang et al. (2017)	Q	81, 240
IJCUBYYAOSTAFY-UHFFFAOYSA-N	9.8		Wang et al. (2017)	Q	81, 241
MCM:MXYMUCPAN	3.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_7$	4.0×10^{4}		Wang et al. (2017)	Q	81, 240
FZEVZMXGRRYMCK-UHFFFAOYSA-N	1.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:PXYMUCPAN	3.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_7$	5.9×10^{4}		Wang et al. (2017)	Q	81, 240
JEHOQLADMHJYMP-UHFFFAOYSA-N	8.1		Wang et al. (2017)	Q	81, 241
MCM:IPBZMUCPAN	4.6×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_7$	6.2×10^{4}		Wang et al. (2017)	Q	81, 240
JAYKUYZEOSXCLM-UHFFFAOYSA-N	3.4		Wang et al. (2017)	Q	81, 241
MCM:METLMUCPAN	2.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_7$	1.9×10^{4}		Wang et al. (2017)	Q	81, 240
ZBESLNAUTTYMKY-UHFFFAOYSA-N	5.1		Wang et al. (2017)	Q	81, 241
MCM:PBZMUCPAN	4.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_7$	6.0×10^{4}		Wang et al. (2017)	Q	81, 240
BNKFVONIJIEPHK-UHFFFAOYSA-N	6.3		Wang et al. (2017)	Q	81, 241
MCM:PETLMUCPAN	2.8×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_7$	2.8×10^{4}		Wang et al. (2017)	Q	81, 240
ZDDBRQJYUBFFIJ-UHFFFAOYSA-N	8.1		Wang et al. (2017)	Q	81, 241
MCM:TM124MUPAN	1.7×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_7$	1.3×10^{4}		Wang et al. (2017)	Q	81, 240
TXJRVENADFPPLH-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:TM135MUPAN	2.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_7$	3.7×10^{4}		Wang et al. (2017)	Q	81, 240
APWJKVMWYCHHEO-UHFFFAOYSA-N	2.9		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DMEBMUPAN	1.9×10^5		Wang et al. (2017)	Q	81, 239
$C_{10}H_{13}NO_7$	1.9×10^4		Wang et al. (2017)	Q	81, 240
OJIPANRKTQADST-UHFFFAOYSA-N	2.1		Wang et al. (2017)	Q	81, 241
MCM:DETLMUPAN	1.5×10^5		Wang et al. (2017)	Q	81, 239
$C_{11}H_{15}NO_7$	1.3×10^4		Wang et al. (2017)	Q	81, 240
WGGPAZKPQBFIGY-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	81, 241
MCM:TM123MUNO3	2.8×10^7		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	3.0×10^7		Wang et al. (2017)	Q	81, 240
CNKHLWZBBXJTJR-UHFFFAOYSA-N	5.0×10^2		Wang et al. (2017)	Q	81, 241
MCM:TLEMUCNO3	1.5×10^9		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_7$	3.5×10^8		Wang et al. (2017)	Q	81, 240
KLAQKLFQZHHGRD-UHFFFAOYSA-N	8.3×10^3		Wang et al. (2017)	Q	81, 241
MCM:EBZMUCNO3	1.4×10^9		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_7$	2.0×10^8		Wang et al. (2017)	Q	81, 240
ZZJNOSBMORNYPY-UHFFFAOYSA-N	1.7×10^4		Wang et al. (2017)	Q	81, 241
MCM:MXYMUCNO3	8.5×10^8		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_7$	7.8×10^7		Wang et al. (2017)	Q	81, 240
YZJRXCREGHPQLR-UHFFFAOYSA-N	6.5×10^3		Wang et al. (2017)	Q	81, 241
MCM:PXYMUCNO3	8.5×10^8		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_7$	9.3×10^7		Wang et al. (2017)	Q	81, 240
GICKPQRZPMBHKH-UHFFFAOYSA-N	1.6×10^3		Wang et al. (2017)	Q	81, 241
MCM:IPBZMUCNO3	1.3×10^9		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	1.5×10^8		Wang et al. (2017)	Q	81, 240
UHFJHZLCDDVXBJ-UHFFFAOYSA-N	1.1×10^4		Wang et al. (2017)	Q	81, 241
MCM:METLMUCNO3	7.6×10^8		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	4.6×10^7		Wang et al. (2017)	Q	81, 240
WWNOXWKNSLKIMY-UHFFFAOYSA-N	9.8×10^2		Wang et al. (2017)	Q	81, 241
MCM:PBZMUCNO3	1.1×10^9		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	1.4×10^8		Wang et al. (2017)	Q	81, 240
QLDJRFHCOXXYTH-UHFFFAOYSA-N	9.3×10^3		Wang et al. (2017)	Q	81, 241
MCM:PETLMUCNO3	7.6×10^8		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	5.8×10^7		Wang et al. (2017)	Q	81, 240
PIVPLJYVWKBKLM-UHFFFAOYSA-N	1.0×10^3		Wang et al. (2017)	Q	81, 241
MCM:TM124MUNO3	2.2×10^7		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	7.8×10^6		Wang et al. (2017)	Q	81, 240
NIRISDMZVMYRLC-UHFFFAOYSA-N	5.0×10^1		Wang et al. (2017)	Q	81, 241
MCM:TM135MUNO3	2.2×10^7		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_7$	1.4×10^7		Wang et al. (2017)	Q	81, 240
WYJKGTDXAIWZNI-UHFFFAOYSA-N	7.3×10^1		Wang et al. (2017)	Q	81, 241

Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DMEBMUNO3	1.9×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{10}H_{15}NO_7$	7.1×10^{6}		Wang et al. (2017)	Q	81, 240
KKQBKVQGVIRRAG-UHFFFAOYSA-N	2.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DETLMUNO3	1.4×10^{7}		Wang et al. (2017)	Q	81, 239
$C_{11}H_{17}NO_7$	4.6×10^{6}		Wang et al. (2017)	Q	81, 240
YPPYKYPDSBIFHG-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DMCNO3	2.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_3H_5NO_6$	3.6×10^{1}		Wang et al. (2017)	Q	81, 240
XNSIPMZBSRCICM-UHFFFAOYSA-N	5.4×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:MMFNO3	1.5×10^{2}		Wang et al. (2017)	Q	81, 239
$C_3H_5NO_6$	4.5		Wang et al. (2017)	Q	81, 240
KROMLYNKDFILIM-UHFFFAOYSA-N	4.5×10^{-2}		Wang et al. (2017)	Q	81, 241
ISOP1N5OOH $C_5H_9NO_6$ LLNBZHMZWYQLAS-UHFFFAOYSA-N	2.3×10^{7}	14000	Wieser et al. (2023)	Q	439
C520ONO2 $C_5H_9NO_8$ ZSADVAXZKGJKSG-UHFFFAOYSA-N	2.9×10^{9}	21000	Wieser et al. (2023)	Q	439
ROO6R6ONO2 $C_6H_{11}NO_6$ CRECMHNOVVIMCR-UHFFFAOYSA-N	6.1×10^{5}	12000	Wieser et al. (2023)	Q	439
C624ONO2 $C_6H_{11}NO_7$ XYBUKFJLXVIRLY-UHFFFAOYSA-N	2.0×10^{10}	19000	Wieser et al. (2023)	Q	439
ROO6R5ONO2 $C_7H_{11}NO_7$ LNWOWXJMUJHMJJ-UHFFFAOYSA-N	1.7×10^{5}	15000	Wieser et al. (2023)	Q	439
ROO6R1ONO2 $C_{10}H_{17}NO_6$ JOFCABYMPNXMIS-UHFFFAOYSA-N	1.4×10^{2}	15000	Wieser et al. (2023)	Q	439
LIMAB15ONO2OOH $C_{10}H_{19}NO_7$ JBKULLYZCMWERK-UHFFFAOYSA-N	5.0×10^{9}	19000	Wieser et al. (2023)	Q	439

A4.7 Nitriles with oxygen (C, H, O, N)

Table A4.7: Nitriles with oxygen (C, H, O, N)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
isocyanic acid HNCO [75-13-8] OWIKHYCFFJSOEH-UHFFFAOYSA-N	2.0×10^{-1} 2.6×10^{-1} 2.1×10^{-1}	4700 4100	Roberts and Liu (2019) Borduas et al. (2016) Roberts et al. (2011) Burkholder et al. (2019)	M M M W	592 593 594
methyl isocyanate CH_3NCO [624-83-9] HAMGRBXTJNITHG-UHFFFAOYSA-N	1.3×10^{-2}		Roberts and Liu (2019)	M	
hydroxyacetonitrile C_2H_3NO (glycolonitrile) [107-16-4] LTYRAPJYLUPLCI-UHFFFAOYSA-N	1.3		HSDB (2015)	Q	100
2-hydroxypropanenitrile C_3H_5NO [78-97-7] WOFDVDFSGLBFAC-UHFFFAOYSA-N	1.0		HSDB (2015)	Q	100
3-hydroxypropanenitrile C_3H_5NO (ethylene cyanohydrin) [109-78-4] WSGYTJNNHPZFKR-UHFFFAOYSA-N	1.3×10^{3} 2.3×10^{4} 3.2×10^{2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
methyl cyanoacetate $C_4H_5NO_2$ [105-34-0] ANGDWNBGPBMQHW-UHFFFAOYSA-N	3.5×10^{1}		Ebert et al. (2023)	?	317
cyanoethanoic acid, ethyl ester $C_5H_7NO_2$ (ethyl cyanoacetate) [105-56-6] ZIUSEGSNTOUIPT-UHFFFAOYSA-N	3.4×10^{1} 3.4×10^{1} 1.3×10^{1} 7.7×10^{1} 4.9 7.7 3.5×10^{1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Yao et al. (2002) Yaws (1999)	V V Q Q Q Q ?	187 68 230 21
2-hydroxybenzoic acid nitrile C_7H_5NO (2-cyanophenol) [611-20-1] CHZCERSEMVWNHL-UHFFFAOYSA-N	2.8×10^{1}		Hilal et al. (2008)	Q	

Table A4.7: Nitriles with oxygen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-hydroxybenzoic acid nitrile	4.0×10^{4}		Hilal et al. (2008)	Q	
C_7H_5NO	1.6×10^{3}		Modarresi et al. (2007)	Q	68
(3-cyanophenol)	3.6×10^{3}		English and Carroll (2001)	Q	231, 232
[873-62-1]	3.3×10^{5}		Nirmalakhandan et al. (1997)	Q	
SGHBRHKBCLLVCI-UHFFFAOYSA-N	3.8×10^{3}		Abraham et al. (1990)	?	
4-hydroxybenzoic acid nitrile	1.4×10^{4}		Hilal et al. (2008)	Q	
C_7H_5NO	2.0×10^{3}		Modarresi et al. (2007)	Q	68
(4-cyanophenol)	3.3×10^{5}		Nirmalakhandan et al. (1997)	Q	
[767-00-0]	1.2×10^{4}		Abraham et al. (1990)	?	
CVNOWLNNPYYEOH-UHFFFAOYSA-N					
phenyl isocyanate	2.5×10^{-5}		Yaws (2003)	X	238, 12
C_7H_5NO	2.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
[103-71-9]	1.8×10^{-5}		Yaws (1999)	?	21, 12
DGTNSSLYPYDJGL-UHFFFAOYSA-N					
1,1',1"-nitrilotris-2-propanol	1.0×10^{6}		HSDB (2015)	Q	449
$C_9H_{21}NO_3$					
(triisopropanolamine)					
[122-20-3]					
SLINHMUFWFWBMU-UHFFFAOYSA-N					
cyometrinil	1.1×10^{4}		MacBean (2012a)	?	
$C_{10}H_7N_3O$					
[78370-21-5]					
PYKLUAIDKVVEOS-JLHYYAGUSA-N					
fenpropathrin	5.5×10^{-2}		HSDB (2015)	V	
$C_{22}H_{23}NO_3$	1.7×10^{1}		Siebers and Mattusch (1996)	V	12
[39515-41-8]					
XQUXKZZNEFRCAW-UHFFFAOYSA-N					

A4.8 Nitro compounds (RNO_2)

Table A4.8: Nitro compounds (RNO_2)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
nitromethane	3.4×10^{-1}	4000	Burkholder et al. (2019)	L	
CH_3NO_2	3.4×10^{-1}	4000	Burkholder et al. (2015)	L	
[75-52-5]	3.6×10^{-1}	3900	Brockbank (2013)	L	1
LYGJENNIWJXYER-UHFFFAOYSA-N	3.4×10^{-1}	4000	Sander et al. (2011)	L	
	3.4×10^{-1}	4000	Sander et al. (2006)	L	
	3.5×10^{-1}	4000	Beneš and Dohnal (1999)	M	
	3.6×10^{-1}		Park et al. (1987)	M	
	4.5×10^{-1}		Rohrschneider (1973)	M	
	3.4×10^{-2}		Yaws (2003)	X	238
	3.5×10^{-1}		Gaffney and Senum (1984)	X	391
	4.4×10^{-1}		Hayer et al. (2022)	Q	20
	2.5×10^{-1}		Keshavarz et al. (2022)	Q	
	6.2×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
	3.4×10^{-1}		Hilal et al. (2008)	Q	
	3.3×10^{-2}		Modarresi et al. (2007)	Q	68
		3700	Kühne et al. (2005)	Q	
	2.3×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	6.2×10^{-1}		English and Carroll (2001)	Q	231, 232
	2.8×10^{-2}		Katritzky et al. (1998)	Q	
	7.3×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	3.5×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		3500	Kühne et al. (2005)	?	
	3.4×10^{-2}		Yaws (1999)	?	21
	1.8×10^{-1}		Abraham and Weathersby (1994)	?	21
	3.6×10^{-2}		Yaws and Yang (1992)	?	21
	3.6×10^{-1}		Abraham et al. (1990)	?	
nitromethane-13C CH_3NO_2 [32480-00-5] LYGJENNIWJXYER-OUBTZVSYSA-N	4.8×10^{-1}	5000	Hiatt (2013)	M	
nitroethane	2.1×10^{-1}	4400	Burkholder et al. (2019)	L	
$C_2H_5NO_2$	2.1×10^{-1}	4400	Burkholder et al. (2015)	L	
[79-24-3]	2.1×10^{-1}	4700	Brockbank (2013)	L	1
MCSAJNNLRCFZED-UHFFFAOYSA-N	2.1×10^{-1}	4400	Sander et al. (2011)	L	
	2.1×10^{-1}	4400	Sander et al. (2006)	L	
	2.2×10^{-1}	4400	Beneš and Dohnal (1999)	M	
	1.4×10^{-1}		Friant and Suffet (1979)	M	38, 595
	1.9×10^{-1}		Hwang et al. (1992)	V	
	2.1×10^{-1}		Hine and Mookerjee (1975)	V	

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	2.1×10^{-1}		Gaffney and Senum (1984)	X	391
	3.4×10^{-1}		Keshavarz et al. (2022)	Q	
	3.7×10^{-1}		Duchowicz et al. (2020)	Q	185
	2.1×10^{-1}		Li et al. (2014)	Q	242
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	3.0×10^{-2}		Modarresi et al. (2007)	Q	68
		4100	Kühne et al. (2005)	Q	
	2.3×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	3.1×10^{-1}		English and Carroll (2001)	Q	231, 261
	2.6×10^{-2}		Katritzky et al. (1998)	Q	
	6.1×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	1.5×10^{-1}		Suzuki et al. (1992)	Q	233
	2.1×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		4200	Kühne et al. (2005)	?	
	2.5×10^{-1}		Yaws (1999)	?	21
	2.1×10^{-1}		Abraham et al. (1990)	?	
1-nitropropane	1.3×10^{-1}	4700	Burkholder et al. (2019)	L	
$C_3H_7NO_2$	1.3×10^{-1}	4700	Burkholder et al. (2015)	L	
[108-03-2]	1.4×10^{-1}	5100	Brockbank (2013)	L	1
JSZOAYXJRCEYSX-UHFFFAOYSA-N	1.3×10^{-1}	4700	Sander et al. (2011)	L	
	1.3×10^{-1}	4700	Sander et al. (2006)	L	
	1.3×10^{-1}	4700	Beneš and Dohnal (1999)	M	
	1.6×10^{-1}		Welke et al. (1998)	M	
	1.1×10^{-1}		Hine and Mookerjee (1975)	V	
	9.2×10^{-2}		Keshavarz et al. (2022)	Q	
	4.8×10^{-1}		Duchowicz et al. (2020)	Q	300
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	1.5×10^{-1}		Hilal et al. (2008)	Q	
	2.3×10^{-2}		Modarresi et al. (2007)	Q	68
		4400	Kühne et al. (2005)	Q	
	1.2×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	1.2×10^{-1}		English and Carroll (2001)	Q	231, 232
	3.1×10^{-2}		Katritzky et al. (1998)	Q	
	4.7×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	7.2×10^{-3}		Suzuki et al. (1992)	Q	233
	1.1×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		4400	Kühne et al. (2005)	?	
	1.2×10^{-1}		Yaws (1999)	?	21, 12
	1.6×10^{-1}		Yaws and Yang (1992)	?	21, 12
	1.1×10^{-1}		Abraham et al. (1990)	?	

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
2-nitropropane	8.3×10^{-2}	4500	Burkholder et al. (2019)	L	
$CH_3CH(NO_2)CH_3$	8.3×10^{-2}	4500	Burkholder et al. (2015)	L	
[79-46-9]	8.6×10^{-2}	4800	Brockbank (2013)	L	1
FGLBSLMDCBOPQK-UHFFFAOYSA-N	8.3×10^{-2}	4500	Sander et al. (2011)	L	
	8.3×10^{-2}	4500	Sander et al. (2006)	L	
	8.4×10^{-2}	4500	Beneš and Dohnal (1999)	M	
	8.3×10^{-2}		Duchowicz et al. (2020)	V	187
	8.3×10^{-2}		HSDB (2015)	V	
	8.0×10^{-2}		Hine and Mookerjee (1975)	V	
	2.2×10^{-1}		Duchowicz et al. (2020)	Q	
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	7.2×10^{-2}		Hilal et al. (2008)	Q	
	2.7×10^{-2}		Modarresi et al. (2007)	Q	68
		4400	Kühne et al. (2005)	Q	
	8.6×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	7.2×10^{-2}		English and Carroll (2001)	Q	231, 275
	2.1×10^{-2}		Katritzky et al. (1998)	Q	
	4.1×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	8.4×10^{-3}		Suzuki et al. (1992)	Q	233
		4400	Kühne et al. (2005)	?	
	8.2×10^{-2}		Yaws (1999)	?	21, 12
	1.1×10^{-1}		Yaws and Yang (1992)	?	21, 12
	8.0×10^{-2}		Abraham et al. (1990)	?	
1-nitrobutane	7.6×10^{-2}		Brockbank (2013)	L	
$C_4H_9NO_2$	8.3×10^{-2}		Duchowicz et al. (2020)	V	187
[627-05-4]	5.6×10^{-1}		Duchowicz et al. (2020)	Q	
NALZTFARIYUCBY-UHFFFAOYSA-N	9.7×10^{-2}		Hilal et al. (2008)	Q	
	1.8×10^{-2}		Modarresi et al. (2007)	Q	68
	3.7×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	7.5×10^{-2}		Abraham et al. (1990)	?	
tert-butylnitrite	7.9×10^{-3}		Hilal et al. (2008)	Q	
C_4H_9ONO					
[540-80-7]					
IOGXOCVLYRDXLW-UHFFFAOYSA-N					
1-nitropentane	4.7×10^{-2}		Amoore and Buttery (1978)	V	
$C_5H_{11}NO_2$	6.0×10^{-2}		Hilal et al. (2008)	Q	
[628-05-7]	1.4×10^{-2}		Modarresi et al. (2007)	Q	68
BVALZCVRLDMXOQ-UHFFFAOYSA-N	2.9×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	4.7×10^{-2}		Abraham et al. (1990)	?	

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tris(hydroxymethyl)ethane trinitrate	2.2×10^{3}		Zhang et al. (2010)	Q	288, 289
$C_5H_9N_3O_9$	1.4×10^{2}		Zhang et al. (2010)	Q	288, 290
[3032-55-1]	2.4×10^{3}		Zhang et al. (2010)	Q	288, 291
IPPYBNCEPZCLNI-UHFFFAOYSA-N	3.4×10^{1}		Zhang et al. (2010)	Q	288, 292
1-nitrohexane	4.5×10^{-2}		Hilal et al. (2008)	Q	
$C_6H_{13}NO_2$					
[646-14-0]					
FEYJIFXFOHFGCC-UHFFFAOYSA-N					
nitrocyclohexane	2.4×10^{-1}		Hilal et al. (2008)	Q	
$C_6H_{11}NO_2$					
[1122-60-7]					
NJNQUTDUIPVROZ-UHFFFAOYSA-N					
2-nitroethanol	2.0×10^{2}		Raventos-Duran et al. (2010)	Q	243, 244
$C_2H_5NO_3$	3.1×10^{2}		Raventos-Duran et al. (2010)	Q	245
[625-48-9]	4.9×10^{3}		Raventos-Duran et al. (2010)	Q	246
KIPMDPDAFINLIV-UHFFFAOYSA-N	1.6×10^{2}		Hilal et al. (2008)	Q	
1-nitro-2-propanol	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	243, 244
$C_3H_7NO_3$	2.5×10^{2}		Raventos-Duran et al. (2010)	Q	245
[3156-73-8]	3.9×10^{3}		Raventos-Duran et al. (2010)	Q	246
PFNCKQIYLAVYJF-UHFFFAOYSA-N	7.9×10^{1}		Hilal et al. (2008)	Q	
2-nitro-1-propanol	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	243, 244
$C_3H_7NO_3$	2.5×10^{2}		Raventos-Duran et al. (2010)	Q	245
[2902-96-7]	3.9×10^{3}		Raventos-Duran et al. (2010)	Q	246
PCNWBUOSTLGPMI-UHFFFAOYSA-N	9.9×10^{1}		Hilal et al. (2008)	Q	
1-nitro-2-butanol	7.3×10^{1}		Hilal et al. (2008)	Q	
$C_4H_9NO_3$					
[3156-74-9]					
FMEFHKJRIGHSLB-UHFFFAOYSA-N					
2-nitro-1-butanol	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	272, 244
$C_4H_9NO_3$	2.0×10^{2}		Raventos-Duran et al. (2010)	Q	245
[609-31-4]	2.5×10^{3}		Raventos-Duran et al. (2010)	Q	246
MHIHRIPETCJEMQ-UHFFFAOYSA-N	7.5×10^{1}		Hilal et al. (2008)	Q	
3-nitro-2-butanol	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
$C_4H_9NO_3$	2.0×10^{2}		Raventos-Duran et al. (2010)	Q	245
[6270-16-2]	2.5×10^{3}		Raventos-Duran et al. (2010)	Q	246
OJVOGABFNZDOOZ-UHFFFAOYSA-N	5.7×10^{1}		Hilal et al. (2008)	Q	
nitroguanidine	2.2×10^{10}		HSDB (2015)	V	
$CH_4N_4O_2$					
[556-88-7]					
IDCPFAYURAQKDZ-UHFFFAOYSA-N					

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tetranitromethane CN_4O_8 [509-14-8] NYTOUQBROMCLBJ-UHFFFAOYSA-N	4.1×10^{-3}		HSDB (2015)	V	
N-methyl-N'-nitro-N-nitrosoguanidine $C_2H_5N_5O_3$ [70-25-7] VZUNGTLZRAYYDE-UHFFFAOYSA-N	8.2×10^{6}		HSDB (2015)	Q	100
2-(hydroxymethyl)-2-nitro-1,3-propanediol $C_4H_9NO_5$ [126-11-4] OLQJQHSAWMFDJE-UHFFFAOYSA-N	2.1×10^{6}		HSDB (2015)	Q	100
MCM:NC4DCO2H	6.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_4H_3NO_5$	3.5×10^{6}		Wang et al. (2017)	Q	81, 240
ODFCIXRXNCCVGH-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NC4MDCO2H	4.2×10^{6}		Wang et al. (2017)	Q	81, 239
$C_5H_5NO_5$	4.7×10^{6}		Wang et al. (2017)	Q	81, 240
LXEJKNKBIPISQO-UHFFFAOYSA-N	6.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NC4EDCO2H	3.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_5$	6.9×10^{6}		Wang et al. (2017)	Q	81, 240
GVSLZEQKUBDLJE-UHFFFAOYSA-N	3.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:DNPHENOOH	7.3×10^{16}		Wang et al. (2017)	Q	81, 239
$C_6H_6N_2O_{10}$	8.0×10^{10}		Wang et al. (2017)	Q	81, 240
AKJGOKAIBHUAAE-UHFFFAOYSA-N	5.4×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:NCATECOOH	8.1×10^{17}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_9$	1.6×10^{10}		Wang et al. (2017)	Q	81, 240
UERHMILVGXASDJ-UHFFFAOYSA-N	4.4×10^{9}		Wang et al. (2017)	Q	81, 241
MCM:NC5MDCO2H	2.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_6H_7NO_5$	1.1×10^{7}		Wang et al. (2017)	Q	81, 240
VRGZGZRSZACGSZ-UHFFFAOYSA-N	2.5×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NC4IPDCO2H	3.5×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_5$	3.5×10^{6}		Wang et al. (2017)	Q	81, 240
VOBLVGUNJWYRHD-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:NC4PDCO2H	3.0×10^{6}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_5$	4.2×10^{6}		Wang et al. (2017)	Q	81, 240
MSTRQTMGALLSFO-UHFFFAOYSA-N	2.2×10^{3}		Wang et al. (2017)	Q	81, 241

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DNCRESOOH	4.0×10^{16}		Wang et al. (2017)	Q	81, 239
$C_7H_8N_2O_{10}$	3.6×10^{10}		Wang et al. (2017)	Q	81, 240
FHWDGQSKNURQKZ-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:MNCATECOOH	3.0×10^{17}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_9$	1.7×10^{11}		Wang et al. (2017)	Q	81, 240
OCHAAZKMUDWIOE-UHFFFAOYSA-N	4.4×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:TL4ONO2OOH	1.4×10^{14}		Wang et al. (2017)	Q	81, 239
$C_7H_9NO_8$	2.8×10^{9}		Wang et al. (2017)	Q	81, 240
MEXRHSIIQRTIBR-UHFFFAOYSA-N	3.5×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:DNEBNZLOOH	3.6×10^{16}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}N_2O_{10}$	2.3×10^{10}		Wang et al. (2017)	Q	81, 240
FNCRENCSRXRIPJ-UHFFFAOYSA-N	3.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:DNMXYOLOOH	2.7×10^{16}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}N_2O_{10}$	2.2×10^{11}		Wang et al. (2017)	Q	81, 240
KSAVSEUSLRIGAB-UHFFFAOYSA-N	5.9×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:DNOXYOLOOH	3.2×10^{16}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}N_2O_{10}$	5.9×10^{10}		Wang et al. (2017)	Q	81, 240
PBZRLTNSSYSOGL-UHFFFAOYSA-N	7.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:DNPXYOLOOH	2.7×10^{16}		Wang et al. (2017)	Q	81, 239
$C_8H_{10}N_2O_{10}$	3.1×10^{10}		Wang et al. (2017)	Q	81, 240
AYHFAKIJCOHXBG-UHFFFAOYSA-N	1.5×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:ENCATECOOH	2.6×10^{17}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_9$	8.9×10^{10}		Wang et al. (2017)	Q	81, 240
QJBJEZDKVLRDGQ-UHFFFAOYSA-N	1.8×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:MXNCATCOOH	1.6×10^{17}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_9$	6.2×10^{10}		Wang et al. (2017)	Q	81, 240
QYJOURKZCRGVGB-UHFFFAOYSA-N	3.4×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:MXOHNO2OOH	1.8×10^{14}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_8$	1.2×10^{9}		Wang et al. (2017)	Q	81, 240
RRWTXIWIABDEOZ-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:OXNCATCOOH	3.9×10^{17}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_9$	1.2×10^{10}		Wang et al. (2017)	Q	81, 240
GWPIPVPJLOZVKC-UHFFFAOYSA-N	3.7×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PXNCATCOOH	3.0×10^{17}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_9$	5.5×10^{9}		Wang et al. (2017)	Q	81, 240
RMUFWTRDQQMPCD-UHFFFAOYSA-N	1.4×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:TM124NOOH	1.8×10^{14}		Wang et al. (2017)	Q	81, 239
$C_8H_{11}NO_8$	1.3×10^{9}		Wang et al. (2017)	Q	81, 240
LGMZUZOZZXWRQX-UHFFFAOYSA-N	5.1×10^{4}		Wang et al. (2017)	Q	81, 241

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DNIPBZLOOH	3.2×10^{16}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}N_2O_{10}$	2.3×10^{10}		Wang et al. (2017)	Q	81, 240
YKBFACRSJWRBHR-UHFFFAOYSA-N	3.7×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:DNMETOLOOH	2.1×10^{16}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}N_2O_{10}$	1.4×10^{11}		Wang et al. (2017)	Q	81, 240
LAMZNFDUTXWEFA-UHFFFAOYSA-N	1.5×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:DNOETOLOOH	2.5×10^{16}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}N_2O_{10}$	3.9×10^{10}		Wang et al. (2017)	Q	81, 240
KMVIJWGCTFHDMC-UHFFFAOYSA-N	7.6×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:DNPBNZLOOH	2.9×10^{16}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}N_2O_{10}$	1.9×10^{10}		Wang et al. (2017)	Q	81, 240
YOHJWFCUZUQBMA-UHFFFAOYSA-N	2.8×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:DNPETOLOOH	2.1×10^{16}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}N_2O_{10}$	1.9×10^{10}		Wang et al. (2017)	Q	81, 240
IOZSITWJVFMIBH-UHFFFAOYSA-N	2.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:DNT123LOOH	1.7×10^{16}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}N_2O_{10}$	3.9×10^{10}		Wang et al. (2017)	Q	81, 240
GBPJMJLXQYJDMC-UHFFFAOYSA-N	4.5×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:DNT124LOOH	1.4×10^{16}		Wang et al. (2017)	Q	81, 239
$C_9H_{12}N_2O_{10}$	2.0×10^{10}		Wang et al. (2017)	Q	81, 240
INCIWBVFUFSSNB-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:EMPONO2OOH	1.4×10^{14}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_8$	1.5×10^{9}		Wang et al. (2017)	Q	81, 240
FZXCIHOWKZKJRK-UHFFFAOYSA-N	6.3×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:IPNCATCOOH	2.5×10^{17}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_9$	8.3×10^{10}		Wang et al. (2017)	Q	81, 240
NYRKVILWQFQUNU-UHFFFAOYSA-N	9.3×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:MTNCATCOOH	1.5×10^{17}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_9$	3.6×10^{10}		Wang et al. (2017)	Q	81, 240
MCLPDHQAEZEULP-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:OTNCATCOOH	3.6×10^{17}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_9$	7.1×10^{9}		Wang et al. (2017)	Q	81, 240
MVMRAYXEOTUUSG-UHFFFAOYSA-N	2.5×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:PNCATECOOH	2.1×10^{17}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_9$	6.6×10^{10}		Wang et al. (2017)	Q	81, 240
AWPUGBPLGLTYEJ-UHFFFAOYSA-N	5.9×10^{7}		Wang et al. (2017)	Q	81, 241
MCM:PTNCATCOOH	2.8×10^{17}		Wang et al. (2017)	Q	81, 239
$C_9H_{13}NO_9$	3.5×10^{9}		Wang et al. (2017)	Q	81, 240
IJEUJFHQTRRKRP-UHFFFAOYSA-N	9.6×10^{6}		Wang et al. (2017)	Q	81, 241

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
nitrobenzene	4.7×10^{-1}	6100	Brockbank (2013)	L	1
$C_6H_5NO_2$	6.7×10^{-1}		Chao et al. (2017)	M	
[98-95-3]	6.4×10^{-1}	7500	Hiatt (2013)	M	
LQNUZADURLCDLV-UHFFFAOYSA-N	1.4×10^{-1}		Zhang et al. (2013)	M	327
	2.3×10^{-2}	11000	Dewulf et al. (1999)	M	596
	1.2		Altschuh et al. (1999)	M	
	1.4×10^{-1}		Hellmann (1987)	M	88
	4.1×10^{-1}		Warner et al. (1980)	M	
	4.7×10^{-1}		Chao et al. (2017)	V	
	4.8×10^{-1}	6400	Bernauer et al. (2006)	V	1
	7.7×10^{-1}		Mackay et al. (2006d)	V	
	4.2×10^{-1}		Lide and Frederikse (1995)	V	
	7.7×10^{-1}		Mackay et al. (1995)	V	
	4.6×10^{-1}		Hwang et al. (1992)	V	
	7.8×10^{-1}		Yoshida et al. (1983)	V	
	4.3×10^{-1}		Warner et al. (1980)	V	
	4.2×10^{-1}		Hine and Mookerjee (1975)	V	
	4.7×10^{-1}	4500	Goldstein (1982)	X	299
	4.2×10^{-1}		Hilal et al. (2008)	C	
	4.1×10^{-1}		Schüürmann (2000)	C	21
	7.5×10^{-1}		Mackay et al. (1995)	C	
	7.5×10^{-1}		Ryan et al. (1988)	C	
	4.1×10^{-1}		Shen (1982)	C	
	1.1		Keshavarz et al. (2022)	Q	
	2.1		Duchowicz et al. (2020)	Q	300
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	2.7×10^{-1}		Modarresi et al. (2007)	Q	68
		4600	Kühne et al. (2005)	Q	
	4.2×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	5.1×10^{-1}		Yao et al. (2002)	Q	230
	2.9×10^{-1}		Katritzky et al. (1998)	Q	
	3.3		Nirmalakhandan et al. (1997)	Q	
	2.0×10^{-1}		Russell et al. (1992)	Q	280
	7.0×10^{-1}		Suzuki et al. (1992)	Q	233
	4.1×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		5600	Kühne et al. (2005)	?	
	4.7×10^{-1}		Yaws (1999)	?	21
	4.2×10^{-1}		Abraham et al. (1990)	?	
nitrobenzene-d5	8.5×10^{-1}	7500	Hiatt (2013)	M	
$C_6D_5NO_2$					
[4165-60-0]					
LQNUZADURLCDLV-RALIUCGRSA-N					

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
2-nitrotoluene	2.4×10^{-1}	5800	Brockbank (2013)	L	
$C_6H_4(NO_2)CH_3$	9.6×10^{-1}		Chao et al. (2017)	M	
[88-72-2]	7.9×10^{-1}		Altschuh et al. (1999)	M	
PLAZTCDQAHEYBI-UHFFFAOYSA-N	2.7×10^{-1}		Mackay et al. (2006d)	V	
	1.9×10^{-1}		Schüürmann (2000)	V	
	1.8×10^{-1}		Lide and Frederikse (1995)	V	
	2.7×10^{-1}		Mackay et al. (1995)	V	
	1.7×10^{-1}		Hine and Mookerjee (1975)	V	
	7.7×10^{-2}	2900	Goldstein (1982)	X	299
	1.5		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	300
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	4.2×10^{-1}		Zhang et al. (2010)	Q	288, 289
	2.4×10^{-1}		Zhang et al. (2010)	Q	288, 290
	2.5×10^{-1}		Zhang et al. (2010)	Q	288, 291
	1.8×10^{-1}		Zhang et al. (2010)	Q	288, 292
	4.2×10^{-1}		Zhang et al. (2010)	Q	288, 289
	2.4×10^{-1}		Zhang et al. (2010)	Q	288, 290
	2.2×10^{-1}		Zhang et al. (2010)	Q	288, 291
	1.8×10^{-1}		Zhang et al. (2010)	Q	288, 292
	1.4×10^{-1}		Hilal et al. (2008)	Q	
	2.3×10^{-1}		Modarresi et al. (2007)	Q	68
		4900	Kühne et al. (2005)	Q	
	1.4×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	2.3		Nirmalakhandan et al. (1997)	Q	
	5.7×10^{-1}		Suzuki et al. (1992)	Q	233
	7.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		5900	Kühne et al. (2005)	?	
	1.7×10^{-1}		Abraham et al. (1990)	?	
3-nitrotoluene	2.7×10^{-1}	7000	Brockbank (2013)	L	
$C_6H_4(NO_2)CH_3$	1.3		Chao et al. (2017)	M	
[99-08-1]	1.1		Altschuh et al. (1999)	M	
QZYHIOPPLUPUJF-UHFFFAOYSA-N	2.8×10^{-1}		Li and Carr (1993)	M	
	1.3×10^{-1}		Mackay et al. (2006d)	V	
	1.3×10^{-1}		Mackay et al. (1995)	V	
	1.4×10^{-1}		Hine and Mookerjee (1975)	V	
	1.4×10^{-1}	3200	Goldstein (1982)	X	299
	1.5		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	300
	4.2×10^{-1}		Zhang et al. (2010)	Q	288, 289
	2.5×10^{-1}		Zhang et al. (2010)	Q	288, 290
	4.1×10^{-1}		Zhang et al. (2010)	Q	288, 291
	1.8×10^{-1}		Zhang et al. (2010)	Q	288, 292
	1.8×10^{-1}		Hilal et al. (2008)	Q	

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{-1}		Modarresi et al. (2007)	Q	68
		4900	Kühne et al. (2005)	Q	
	1.4×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.3		Nirmalakhandan et al. (1997)	Q	
	5.7×10^{-1}		Suzuki et al. (1992)	Q	233
	1.1		Duchowicz et al. (2020)	?	186, 21
		4900	Kühne et al. (2005)	?	
	1.3×10^{-1}		Yaws (1999)	?	21, 38
	1.4×10^{-1}		Abraham et al. (1990)	?	
4-nitrotoluene	8.9×10^{-1}	7100	Brockbank (2013)	L	
$C_6H_4(NO_2)CH_3$	1.8		Altschuh et al. (1999)	M	
[99-99-0]	2.8		Mackay et al. (2006d)	V	
ZPTVNYMJQHSSEA-UHFFFAOYSA-N	2.0×10^{-1}		Lide and Frederikse (1995)	V	
	2.8		Mackay et al. (1995)	V	
	1.6×10^{-1}	3100	Goldstein (1982)	X	299
	1.5		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	185
	1.4×10^{-1}		Li et al. (2014)	Q	242
	4.2×10^{-1}		Zhang et al. (2010)	Q	288, 289
	2.8×10^{-1}		Zhang et al. (2010)	Q	288, 290
	9.0×10^{-1}		Zhang et al. (2010)	Q	288, 291
	1.8×10^{-1}		Zhang et al. (2010)	Q	288, 292
	2.0×10^{-1}		Hilal et al. (2008)	Q	
	2.4×10^{-1}		Modarresi et al. (2007)	Q	68
		4900	Kühne et al. (2005)	Q	
	1.8		Duchowicz et al. (2020)	?	186, 21
		3800	Kühne et al. (2005)	?	
1,2-dinitrobenzene	1.9×10^{2}		Duchowicz et al. (2020)	V	187
$C_6H_4N_2O_4$	1.9×10^{2}		HSDB (2015)	V	
[528-29-0]	3.5×10^{2}		Duchowicz et al. (2020)	Q	
IZUKQUVSCNEFMJ-UHFFFAOYSA-N	1.2×10^{2}		Zhang et al. (2010)	Q	288, 289
	3.2×10^{1}		Zhang et al. (2010)	Q	288, 290
	2.6×10^{1}		Zhang et al. (2010)	Q	288, 291
	2.7×10^{1}		Zhang et al. (2010)	Q	288, 292
1,3-dinitrobenzene	1.8×10^{2}		Chao et al. (2017)	M	
$C_6H_4N_2O_4$	2.0×10^{2}		Altschuh et al. (1999)	M	
[99-65-0]			Mackay et al. (2006d)	V	560
WDCYWAQPCXBPJA-UHFFFAOYSA-N	5.0×10^{2}		Mackay et al. (1995)	V	
	3.9×10^{1}		Smith et al. (1981a)	V	
	2.5×10^{2}		Keshavarz et al. (2022)	Q	
	2.1×10^{2}		Duchowicz et al. (2020)	Q	
	2.0×10^{2}		Gharagheizi et al. (2012)	Q	
	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	246

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\ Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	2.0×10^{2}		Duchowicz et al. (2020)	?	186, 21
1,4-dinitrobenzene	2.0×10^{-1}		Mackay et al. (2006d)	V	
$C_6H_4N_2O_4$	2.0×10^{-1}		Mackay et al. (1995)	V	
[100-25-4]	1.2×10^{2}		HSDB (2015)	Q	100
FYFDQJRXFWGIBS-UHFFFAOYSA-N					
1,3,5-trinitrobenzene	1.5×10^{3}		HSDB (2015)	V	
$C_6H_3N_3O_6$	2.7×10^{2}		Yaws (2003)	X	238, 81
[99-35-4]	2.8×10^{2}		Gharagheizi et al. (2010)	Q	247
UATJOMSPNYCXIX-UHFFFAOYSA-N					
2,4,6-trinitrophenol	3.0×10^{5}		Ebert et al. (2023)	?	317
$C_6H_3N_3O_7$					
(picric acid)					
[88-89-1]					
OXNIZHLAWKMVMX-UHFFFAOYSA-N					
2-nitrobenzenamine	7.1×10^{1}	6800	Brockbank (2013)	L	
$C_6H_6N_2O_2$	1.7×10^{2}		Altschuh et al. (1999)	M	
(2-nitroaniline)	1.0×10^{2}		Abraham et al. (1994a)	R	
[88-74-4]	2.0×10^{2}		Keshavarz et al. (2022)	Q	
DPJCXCZTLWNFOH-UHFFFAOYSA-N	2.5×10^{2}		Duchowicz et al. (2020)	Q	185
	3.1×10^{1}		Hilal et al. (2008)	Q	
	2.1×10^{2}		Modarresi et al. (2007)	Q	68
	4.5×10^{2}		Nirmalakhandan et al. (1997)	Q	
	1.7×10^{2}		Duchowicz et al. (2020)	?	186, 21
3-nitrobenzenamine	6.9×10^{2}		Meylan and Howard (1991)	V	
$C_6H_6N_2O_2$	1.2×10^{3}		Abraham et al. (1994a)	R	
(3-nitroaniline)	4.2×10^{3}		Keshavarz et al. (2022)	Q	
[99-09-2]	1.5×10^{3}		Duchowicz et al. (2020)	Q	
XJCVRTZCHMZPBD-UHFFFAOYSA-N	2.7×10^{3}		Hilal et al. (2008)	Q	
	4.0×10^{2}		Modarresi et al. (2007)	Q	68
	6.0×10^{2}		English and Carroll (2001)	Q	231, 232
	4.4×10^{2}		Nirmalakhandan et al. (1997)	Q	
	1.3×10^{3}		Meylan and Howard (1991)	Q	
	1.2×10^{3}		Duchowicz et al. (2020)	?	186, 21
	1.2×10^{3}		HSDB (2015)	?	421
4-nitrobenzenamine	8.7×10^{3}	8200	Brockbank (2013)	L	
$C_6H_6N_2O_2$	8.6×10^{3}		Altschuh et al. (1999)	M	
(4-nitroaniline)	1.4×10^{4}		Abraham et al. (1994a)	R	
[100-01-6]	1.8×10^{2}		Yaws (2003)	X	238
TYMLOMAKGOJONV-UHFFFAOYSA-N	4.2×10^{3}		Keshavarz et al. (2022)	Q	
	1.5×10^{3}		Duchowicz et al. (2020)	Q	
	8.5×10^{2}		Gharagheizi et al. (2012)	Q	
	1.7×10^{2}		Gharagheizi et al. (2010)	Q	247
	2.2×10^{3}		Hilal et al. (2008)	Q	

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.5×10^{2}		Modarresi et al. (2007)	Q	68
	4.4×10^{2}		Nirmalakhandan et al. (1997)	Q	
	7.8×10^{3}		Duchowicz et al. (2020)	?	186, 21
2,4-dinitrobenzenamine $C_6H_5N_3O_4$ [97-02-9] LXQOQPGNCGEELI-UHFFFAOYSA-N	6.5×10^{4}		HSDB (2015)	Q	547
2-methyl-6-nitroaniline $C_7H_8N_2O_2$ [570-24-1] FCMRHMPITHLLLA-UHFFFAOYSA-N	4.6×10^{1}		Abraham et al. (2019)	Q	
1-methyl-2,3-dinitrobenzene $C_7H_6N_2O_4$ (2,3-dinitrotoluene; 2,3-DNT) [602-01-7] DYSXLQBUUOPLBB-UHFFFAOYSA-N	1.1×10^{2}		HSDB (2015)	Q	449
	1.1×10^{2}		Zhang et al. (2010)	Q	288, 289
	2.2×10^{1}		Zhang et al. (2010)	Q	288, 290
	9.5		Zhang et al. (2010)	Q	288, 291
	1.5×10^{1}		Zhang et al. (2010)	Q	288, 292
	1.1×10^{2}		Zhang et al. (2010)	Q	288, 289
	2.3×10^{1}		Zhang et al. (2010)	Q	288, 290
	1.1×10^{1}		Zhang et al. (2010)	Q	288, 291
	1.5×10^{1}		Zhang et al. (2010)	Q	288, 292
1-methyl-2,4-dinitrobenzene $C_7H_6N_2O_4$ (2,4-dinitrotoluene; 2,4-DNT) [121-14-2] RMBFBMJGBANMMK-UHFFFAOYSA-N	4.0×10^{1}	7900	Brockbank (2013)	L	1
	1.8×10^{2}		Altschuh et al. (1999)	M	
	1.1×10^{1}		Mackay et al. (2006d)	V	
	1.0×10^{2}		Schüürmann (2000)	V	
	1.1×10^{1}		Mackay et al. (1995)	V	
	6.3×10^{1}		Smith et al. (1981a)	V	
	2.1×10^{-1}	2900	Goldstein (1982)	X	299
	2.2		Mackay et al. (1995)	C	
	3.1×10^{-2}		Ryan et al. (1988)	C	
	3.4×10^{2}		Keshavarz et al. (2022)	Q	
	1.6×10^{2}		Duchowicz et al. (2020)	Q	
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	246
	1.1×10^{2}		Zhang et al. (2010)	Q	288, 289
	1.6×10^{1}		Zhang et al. (2010)	Q	288, 290
	5.0		Zhang et al. (2010)	Q	288, 291
	1.5×10^{1}		Zhang et al. (2010)	Q	288, 292
	1.8×10^{2}		Duchowicz et al. (2020)	?	186, 21

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-1,4-dinitrobenzene	1.8×10^{1}		HSDB (2015)	V	
$C_7H_6N_2O_4$	1.1×10^{2}		Zhang et al. (2010)	Q	288, 289
(2,5-dinitrotoluene; 2,5-DNT)	1.8×10^{1}		Zhang et al. (2010)	Q	288, 290
[619-15-8]	1.4		Zhang et al. (2010)	Q	288, 291
KZBOXYKTSUUBTO-UHFFFAOYSA-N	1.5×10^{1}		Zhang et al. (2010)	Q	288, 292
2-methyl-1,3-dinitrobenzene	4.8	7600	Brockbank (2013)	L	
$C_7H_6N_2O_4$	1.3×10^{1}		Duchowicz et al. (2020)	V	187
(2,6-dinitrotoluene; 2,6-DNT)	1.5×10^{1}		HSDB (2015)	V	
[606-20-2]	1.4×10^{1}		Mackay et al. (2006d)	V	
XTRDKALNCIHHNI-UHFFFAOYSA-N	1.4×10^{1}		Mackay et al. (1995)	V	
	1.2		Mackay et al. (1995)	C	
	3.1×10^{-2}		Ryan et al. (1988)	C	
	1.6×10^{2}		Duchowicz et al. (2020)	Q	
	1.6		Li et al. (2014)	Q	242
	1.1×10^{2}		Zhang et al. (2010)	Q	288, 289
	2.1×10^{1}		Zhang et al. (2010)	Q	288, 290
	4.3		Zhang et al. (2010)	Q	288, 291
	1.5×10^{1}		Zhang et al. (2010)	Q	288, 292
4-methyl-1,2-dinitrobenzene	3.3×10^{1}	9600	Brockbank (2013)	L	
$C_7H_6N_2O_4$	1.1×10^{2}		HSDB (2015)	Q	449
(3,4-dinitrotoluene; 3,4-DNT)	1.1×10^{2}		Zhang et al. (2010)	Q	288, 289
[610-39-9]	3.9×10^{1}		Zhang et al. (2010)	Q	288, 290
INYDMNPNDHRJQJ-UHFFFAOYSA-N	3.1×10^{1}		Zhang et al. (2010)	Q	288, 291
	1.5×10^{1}		Zhang et al. (2010)	Q	288, 292
1-methyl-2,4,6-trinitrobenzene	4.7×10^{2}	7700	Brockbank (2013)	L	1
$C_7H_5N_3O_6$	4.7×10^{2}		HSDB (2015)	V	
(2,4,6-trinitrotoluene; TNT)	5.4×10^{2}		Schüürmann (2000)	V	
[118-96-7]		6200	Kühne et al. (2005)	Q	
SPSSULHKWOKEEL-UHFFFAOYSA-N		6400	Kühne et al. (2005)	?	
2,4,6-trinitro-1,3-dimethyl-5-*tert*-butylbenzene	3.2×10^{-1}		Lee et al. (2012)	M	
$C_{12}H_{15}N_3O_6$	1.7×10^{-2}		Amoore and Buttery (1978)	V	
(musk xylene)	1.3×10^{3}		HSDB (2015)	Q	100
[81-15-2]	9.5×10^{3}		Zhang et al. (2010)	Q	288, 289
XMWRWTSZNLOZFN-UHFFFAOYSA-N	5.6		Zhang et al. (2010)	Q	288, 290
	4.8×10^{-2}		Zhang et al. (2010)	Q	288, 291
	1.5×10^{2}		Zhang et al. (2010)	Q	288, 292
2-nitrophenol	9.9		Chao et al. (2017)	M	
$HOC_6H_4(NO_2)$	1.4	5700	Guo and Brimblecombe (2007)	M	
[88-75-5]	8.3×10^{-1}	6300	Harrison et al. (2002)	M	
IQUPABOKLQSFBK-UHFFFAOYSA-N	8.9×10^{-1}	6300	Müller and Heal (2001)	M	
	7.7×10^{-1}		Tremp et al. (1993)	M	12
	6.1×10^{-1}		Mackay et al. (2006c)	V	
	2.9		Lide and Frederikse (1995)	V	

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	7.9×10^{-1}		Riederer (1990)	V	
	7.3×10^{-1}		Schwarzenbach et al. (1988)	V	12
	2.8		Leuenberger et al. (1985)	V	418
	9.2×10^{-1}		Abraham et al. (1994a)	R	
	6.9×10^{-1}	4600	Goldstein (1982)	X	299
	1.3		Ryan et al. (1988)	C	
	1.1		Abraham et al. (2019)	Q	
	6.6		Wang et al. (2017)	Q	81, 239
	2.0		Wang et al. (2017)	Q	81, 240
	2.1×10^{-1}		Wang et al. (2017)	Q	81, 241
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.6		Raventos-Duran et al. (2010)	Q	246
	5.3		Hilal et al. (2008)	Q	
		4400	Kühne et al. (2005)	Q	
	3.5×10^{1}		Katritzky et al. (1998)	Q	
	1.5×10^{4}		Nirmalakhandan et al. (1997)	Q	
		6300	Kühne et al. (2005)	?	
	7.0×10^{-1}		Abraham et al. (1990)	?	
3-nitrophenol	1.6×10^{2}		Guo and Brimblecombe (2007)	M	557
$HOC_6H_4(NO_2)$	1.0		Lide and Frederikse (1995)	V	
[554-84-7]	4.9×10^{3}		Gaffney and Senum (1984)	X	391
RTZZCYNQPHTPPL-UHFFFAOYSA-N	2.1×10^{4}		Keshavarz et al. (2022)	Q	
	1.4×10^{4}		Duchowicz et al. (2020)	Q	300
	2.2×10^{3}		Abraham et al. (2019)	Q	
	2.0×10^{3}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{4}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{3}		Raventos-Duran et al. (2010)	Q	246
	9.5×10^{3}		Hilal et al. (2008)	Q	
	2.1×10^{2}		Modarresi et al. (2007)	Q	68
	4.8×10^{3}		English and Carroll (2001)	Q	231, 232
	1.5×10^{4}		Nirmalakhandan et al. (1997)	Q	
	4.9×10^{3}		Duchowicz et al. (2020)	?	186, 21
	4.6×10^{3}		Abraham et al. (1990)	?	
4-nitrophenol	1.4×10^{1}		Chao et al. (2017)	M	
$HOC_6H_4(NO_2)$	2.1×10^{2}		Guo and Brimblecombe (2007)	M	557
[100-02-7]	7.7×10^{2}		Tremp et al. (1993)	M	12
BTJIUGUIPKRLHP-UHFFFAOYSA-N	3.0×10^{2}		Lide and Frederikse (1995)	V	
	2.0×10^{4}		Riederer (1990)	V	
	3.0×10^{2}		Schwarzenbach et al. (1988)	V	12
	9.4×10^{4}		Yoshida et al. (1983)	V	
	2.6×10^{4}	9100	Parsons et al. (1971)	T	419
	9.8	6000	Goldstein (1982)	X	299
	1.6		Ryan et al. (1988)	C	
	2.1×10^{4}		Keshavarz et al. (2022)	Q	

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	2.2×10^4		Duchowicz et al. (2020)	Q	185
	1.4×10^4		Abraham et al. (2019)	Q	
	2.4×10^4		Li et al. (2014)	Q	242
	2.0×10^3		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^3		Raventos-Duran et al. (2010)	Q	245
	4.9×10^3		Raventos-Duran et al. (2010)	Q	246
	6.1×10^3		Hilal et al. (2008)	Q	
	2.3×10^2		Modarresi et al. (2007)	Q	68
	1.5×10^4		Nirmalakhandan et al. (1997)	Q	
	2.4×10^4		Duchowicz et al. (2020)	?	186, 21
	2.6×10^4		Abraham et al. (1990)	?	
4-nitroanisole $C_7H_7NO_3$ [100-17-4] BNUHAJGCKIQFGE-UHFFFAOYSA-N	5.0		Ebert et al. (2023)	?	367
3-methyl-2-nitrophenol $C_7H_7NO_3$ [4920-77-8] QIORDSKCCHRSSD-UHFFFAOYSA-N	3.2		Tremp et al. (1993)	M	12
	2.4		Schwarzenbach et al. (1988)	V	12
	1.9×10^2		Modarresi et al. (2007)	Q	68
		4700	Kühne et al. (2005)	Q	
		4200	Kühne et al. (2005)	?	
4-methyl-2-nitrophenol $C_7H_7NO_3$ [119-33-5] SYDNSSSQVSOXTN-UHFFFAOYSA-N	6.7×10^{-1}		Tremp et al. (1993)	M	12
	6.1×10^{-1}		Schwarzenbach et al. (1988)	V	12
	3.9		Wang et al. (2017)	Q	81, 239
	1.9		Wang et al. (2017)	Q	81, 240
	2.5×10^{-1}		Wang et al. (2017)	Q	81, 241
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.2		Raventos-Duran et al. (2010)	Q	246
		4700	Kühne et al. (2005)	Q	
		6800	Kühne et al. (2005)	?	
5-methyl-2-nitrophenol $C_7H_7NO_3$ [700-38-9] NQXUSSVLFOBRSE-UHFFFAOYSA-N	7.7×10^{-1}		Tremp et al. (1993)	M	12
	6.7×10^{-1}		Schwarzenbach et al. (1988)	V	12
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	272, 244
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.2		Raventos-Duran et al. (2010)	Q	246
		4700	Kühne et al. (2005)	Q	
		5600	Kühne et al. (2005)	?	
6-methyl-2-nitrophenol $C_7H_7NO_3$ [13073-29-5] AQDKZPFDOWHRDZ-UHFFFAOYSA-N	2.9×10^{-1}		Tremp et al. (1993)	M	12
	3.9		Wang et al. (2017)	Q	81, 239
	2.0×10^1		Wang et al. (2017)	Q	81, 240
	1.2×10^{-1}		Wang et al. (2017)	Q	81, 241
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9		Raventos-Duran et al. (2010)	Q	245
	1.2		Raventos-Duran et al. (2010)	Q	246

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		4700	Kühne et al. (2005)	Q	
		5200	Kühne et al. (2005)	?	
3-methyl-4-nitrophenol	6.2×10^{2}		Tremp et al. (1993)	M	12
$C_7H_7NO_3$	1.6×10^{3}		Raventos-Duran et al. (2010)	Q	272, 244
[2581-34-2]	3.9×10^{3}		Raventos-Duran et al. (2010)	Q	245
PIIZYNQECPTVEO-UHFFFAOYSA-N	3.9×10^{3}		Raventos-Duran et al. (2010)	Q	246
	2.1×10^{2}		Modarresi et al. (2007)	Q	68
4-methoxy-2-nitrophenol	5.3		Tremp et al. (1993)	M	12
$C_7H_7NO_4$	2.3×10^{-1}		Schwarzenbach et al. (1988)	V	12
[1568-70-3]	6.2		Raventos-Duran et al. (2010)	Q	243, 244
YBUGOACXDPDUIR-UHFFFAOYSA-N	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	246
	9.4×10^{1}		Modarresi et al. (2007)	Q	68
		4900	Kühne et al. (2005)	Q	
		6600	Kühne et al. (2005)	?	
4-amino-2,6-dinitrotoluene $C_7H_7N_3O_4$ [19406-51-0] KQRJATLINVYHEZ-UHFFFAOYSA-N	7.3×10^{3}		Ebert et al. (2023)	?	367
4-hydroxy-3-nitro-benzaldehyde	9.4		Schwarzenbach et al. (1988)	V	12
$C_7H_5NO_4$	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
[3011-34-5]	2.0×10^{2}		Raventos-Duran et al. (2010)	Q	245
YTHJCZRFJGXPTL-UHFFFAOYSA-N	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	246
2,4-dinitrophenol	9.7×10^{2}		Chao et al. (2017)	M	
$C_6H_4N_2O_5$	1.1×10^{2}		Tremp et al. (1993)	M	12
[51-28-5]	3.5×10^{1}		Schwarzenbach et al. (1988)	V	12
UFBJCMHMOXMLKC-UHFFFAOYSA-N	1.5×10^{4}		Ryan et al. (1988)	C	
	2.0×10^{2}		Abraham et al. (2019)	Q	
	2.6×10^{3}		Wang et al. (2017)	Q	81, 239
	2.1×10^{3}		Wang et al. (2017)	Q	81, 240
	3.0		Wang et al. (2017)	Q	81, 241
	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{2}		Raventos-Duran et al. (2010)	Q	246
	3.6×10^{2}		Zhang et al. (2010)	Q	288, 289
	6.2×10^{2}		Zhang et al. (2010)	Q	288, 290
	4.7		Zhang et al. (2010)	Q	288, 291
	1.3×10^{3}		Zhang et al. (2010)	Q	288, 292
	4.7×10^{1}		Modarresi et al. (2007)	Q	68
		5000	Kühne et al. (2005)	Q	
		3300	Kühne et al. (2005)	?	

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,5-dinitrophenol	1.5×10^{1}		Schwarzenbach et al. (1988)	V	12
$C_6H_4N_2O_5$	1.1×10^{2}		Abraham et al. (2019)	Q	
[329-71-5]	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	272, 244
UWEZBKLLMKVIPI-UHFFFAOYSA-N	4.9×10^{2}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{2}		Raventos-Duran et al. (2010)	Q	246
picramic acid	1.0×10^{6}		HSDB (2015)	Q	100
$C_6H_5N_3O_5$					
(4,6-dinitro-2-aminophenol)					
[96-91-3]					
QXYMVUZOGFVPGH-UHFFFAOYSA-N					
4-amino-2-nitrophenol	4.5×10^{6}		HSDB (2015)	Q	100
$C_6H_6N_2O_3$					
[119-34-6]					
WHODQVWERNSQEO-UHFFFAOYSA-N					
2-amino-5-nitrophenol	1.3×10^{7}		HSDB (2015)	Q	100
$C_6H_6N_2O_3$					
[121-88-0]					
DOPJTDJKZNWLRB-UHFFFAOYSA-N					
2-amino-4-nitrophenol	4.5×10^{6}		HSDB (2015)	Q	100
$C_6H_6N_2O_3$					
[99-57-0]					
VLZVIIYRNMWPSN-UHFFFAOYSA-N					
4-nitro-*o*-phenylenediamine	1.3×10^{6}		HSDB (2015)	Q	100
$C_6H_7N_3O_2$					
(4-nitro-1,2-diaminobenzene)					
[99-56-9]					
RAUWPNXIALNKQM-UHFFFAOYSA-N					
4-nitrobenzene-1,3-diamine	1.7×10^{5}		HSDB (2015)	Q	100
$C_6H_7N_3O_2$					
[5131-58-8]					
DPIZKMGPXNXSGL-UHFFFAOYSA-N					
2-nitro-1,4-benzenediamine	1.7×10^{5}		HSDB (2015)	Q	100
$C_6H_7N_3O_2$					
[5307-14-2]					
HVHNMNGARPCGGD-UHFFFAOYSA-N					
4-methyl-2,6-dinitrophenol	1.9×10^{2}		Tremp et al. (1993)	M	12
$C_7H_6N_2O_5$	3.2×10^{2}		Zhang et al. (2010)	Q	288, 289
(2,6-dinitro-*p*-cresol)	3.4×10^{3}		Zhang et al. (2010)	Q	288, 290
[609-93-8]	8.8×10^{1}		Zhang et al. (2010)	Q	288, 291
HOYRZHJJAHRMLL-UHFFFAOYSA-N	8.0		Zhang et al. (2010)	Q	288, 292
	4.0×10^{1}		Modarresi et al. (2007)	Q	68
		3000	Kühne et al. (2005)	Q	
		3400	Kühne et al. (2005)	?	

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-4,6-dinitrophenol	4.3×10^{1}		Tremp et al. (1993)	M	12
$C_7H_6N_2O_5$	7.0		Warner et al. (1980)	M	
(6-methyl-2,4-dinitrophenol;	9.2×10^{1}		Mackay et al. (2006d)	V	
4,6-dinitro-*o*-cresol; DNOC)					
[534-52-1]	2.3×10^{1}		Schwarzenbach et al. (1988)	V	12
ZXVONLUNISGICL-UHFFFAOYSA-N	9.1×10^{1}		Suntio et al. (1988)	V	12
	9.0×10^{-1}		Barcelo and Hennion (1997)	X	569
	7.0		Shen (1982)	C	
	1.7		Keshavarz et al. (2022)	Q	
	1.3×10^{3}		Duchowicz et al. (2020)	Q	
	1.5×10^{3}		Wang et al. (2017)	Q	81, 239
	1.7×10^{4}		Wang et al. (2017)	Q	81, 240
	3.4		Wang et al. (2017)	Q	81, 241
	3.2×10^{2}		Zhang et al. (2010)	Q	288, 289
	2.3×10^{3}		Zhang et al. (2010)	Q	288, 290
	1.9×10^{1}		Zhang et al. (2010)	Q	288, 291
	7.2×10^{2}		Zhang et al. (2010)	Q	288, 292
	4.1		Goodarzi et al. (2010)	Q	570
	3.4×10^{1}		Modarresi et al. (2007)	Q	68
		5400	Kühne et al. (2005)	Q	
	7.0		Duchowicz et al. (2020)	?	186, 21
		4200	Kühne et al. (2005)	?	
5-nitrobenzimidazole	2.7×10^{1}		HSDB (2015)	Q	100
$C_7H_5N_3O_2$					
[94-52-0]					
XPAZGLFMMUODDK-UHFFFAOYSA-N					
3-nitrobenzoic acid	3.4×10^{3}		Abraham et al. (2019)	Q	
$C_7H_5NO_4$					
[121-92-6]					
AFPHTEQTJZKQAQ-UHFFFAOYSA-N					
4-nitrobenzoic acid	3.2×10^{3}		Abraham et al. (2019)	Q	
$C_7H_5NO_4$	2.6×10^{4}		HSDB (2015)	Q	100
[62-23-7]					
OTLNPYWUJOZPPA-UHFFFAOYSA-N					
3,5-dinitrobenzoic acid	8.0×10^{4}		Abraham et al. (2019)	Q	
$C_7H_4N_2O_6$					
[99-34-3]					
VYWYYJYRVSBHJQ-UHFFFAOYSA-N					
2,4,6-trinitrobenzoic acid	3.8×10^{8}		HSDB (2015)	Q	100
$C_7H_3N_3O_8$					
[129-66-8]					
KAQBNBSMMVTKRN-UHFFFAOYSA-N					

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dinitrotoluene $C_7H_6N_2O_4$ [25321-14-6] MOSFIJXAXDLOML-UHFFFAOYSA-N	1.1×10^{2}		HSDB (2015)	Q	449
1-methyl-3,5-dinitrobenzene $C_7H_6N_2O_4$ [618-85-9] RUIFULUFLANOCI-UHFFFAOYSA-N	1.1×10^{2}		HSDB (2015)	Q	449
1-methoxy-2-nitrobenzene $C_7H_7NO_3$ [91-23-6] CFBYEGUGFPZCNF-UHFFFAOYSA-N	2.3×10^{1}		Duchowicz et al. (2020)	V	187
	2.3×10^{1}		HSDB (2015)	V	
	3.3×10^{1}		Duchowicz et al. (2020)	Q	
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	7.8		Raventos-Duran et al. (2010)	Q	246
	1.6×10^{2}		Katritzky et al. (1998)	Q	
2-methyl-5-nitrobenzenamine $C_7H_8N_2O_2$ (5-nitro-*o*-toluidine) [99-55-8] DSBIJCMXAIKKKI-UHFFFAOYSA-N	1.2×10^{3}		HSDB (2015)	Q	100
2-methoxy-5-nitrobenzenamine $C_7H_8N_2O_3$ (5-nitro-*o*-anisidine) [99-59-2] NIPDVSLAMPAWTP-UHFFFAOYSA-N	7.6×10^{2}		HSDB (2015)	Q	547
(2-nitroethenyl)benzene $C_8H_7NO_2$ [102-96-5] PIAOLBVUVDXHHL-UHFFFAOYSA-N	2.8		HSDB (2015)	Q	449
1,2-dimethyl-3-nitrobenzene $C_8H_9NO_2$ [83-41-0] FVHAWXWFPBPFOS-UHFFFAOYSA-N	1.9×10^{-1}		HSDB (2015)	Q	449
	3.9×10^{-1}		Zhang et al. (2010)	Q	288, 289
	2.9×10^{-1}		Zhang et al. (2010)	Q	288, 290
	2.6×10^{-1}		Zhang et al. (2010)	Q	288, 291
	1.0×10^{-1}		Zhang et al. (2010)	Q	288, 292
1,2-dimethyl-4-nitrobenzene $C_8H_9NO_2$ [99-51-4] HFZKOYWDLDYELC-UHFFFAOYSA-N	3.9×10^{-1}		Zhang et al. (2010)	Q	288, 289
	3.1×10^{-1}		Zhang et al. (2010)	Q	288, 290
	8.0×10^{-1}		Zhang et al. (2010)	Q	288, 291
	1.0×10^{-1}		Zhang et al. (2010)	Q	288, 292
1,4-dimethyl-2-nitrobenzene $C_8H_9NO_2$ [89-58-7] BSFHJMGROOFSRA-UHFFFAOYSA-N	3.9×10^{-1}		Zhang et al. (2010)	Q	288, 289
	2.5×10^{-1}		Zhang et al. (2010)	Q	288, 290
	2.2×10^{-1}		Zhang et al. (2010)	Q	288, 291
	1.0×10^{-1}		Zhang et al. (2010)	Q	288, 292

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4-dimethyl-1-nitrobenzene	3.9×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_8H_9NO_2$	3.1×10^{-1}		Zhang et al. (2010)	Q	288, 290
[89-87-2]	4.3×10^{-1}		Zhang et al. (2010)	Q	288, 291
BBUPBICWUURTNP-UHFFFAOYSA-N	1.0×10^{-1}		Zhang et al. (2010)	Q	288, 292
4-methyl-2-nitroanisole	7.2		Zhang et al. (2010)	Q	288, 289
$C_8H_9NO_3$	1.6		Zhang et al. (2010)	Q	288, 290
[119-10-8]	6.0×10^{1}		Zhang et al. (2010)	Q	288, 291
LGNMURXRPLMVJI-UHFFFAOYSA-N	2.7		Zhang et al. (2010)	Q	288, 292
2-methyl-3-nitrobenzoic acid $C_8H_7NO_4$ [1975-50-4] YPQAFWHSMWWPLX-UHFFFAOYSA-N	2.2×10^{3}		Abraham et al. (2019)	Q	
3-methyl-4-nitrobenzoic acid $C_8H_7NO_4$ [3113-71-1] XDTTUTIFWDAMIX-UHFFFAOYSA-N	9.2×10^{2}		Abraham et al. (2019)	Q	
2-methyl-3,5-dinitrobenzoic acid $C_8H_6N_2O_6$ [28169-46-2] CDVNZMKTJIBBBV-UHFFFAOYSA-N	3.7×10^{6}		Abraham et al. (2019)	Q	
1-(1-methylethyl)-4-nitrobenzene	2.4×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_9H_{11}NO_2$	1.3×10^{-1}		Zhang et al. (2010)	Q	288, 290
[1817-47-6]	3.9×10^{-1}		Zhang et al. (2010)	Q	288, 291
JXMYUMNAEKRMIP-UHFFFAOYSA-N	1.4×10^{-1}		Zhang et al. (2010)	Q	288, 292
5-nitro-8-hydroxyquinoline $C_9H_6N_2O_3$ (nitroxoline) [4008-48-4] RJIWZDNTCBHXAL-UHFFFAOYSA-N	2.7×10^{3}		Abraham et al. (2019)	Q	
2-(1-methylpropyl)-4,6-dinitrophenol	2.2		Tremp et al. (1993)	M	12
$C_{10}H_{12}N_2O_5$	2.0×10^{-2}		Suntio et al. (1988)	V	12
(dinoseb)	1.9×10^{-4}		Barcelo and Hennion (1997)	X	569
[88-85-7]	1.4×10^{2}		Zhang et al. (2010)	Q	288, 289
OWZPCEFYPSAJFR-UHFFFAOYSA-N	5.2×10^{2}		Zhang et al. (2010)	Q	288, 290
	1.3×10^{2}		Zhang et al. (2010)	Q	288, 291
	4.3×10^{2}		Zhang et al. (2010)	Q	288, 292
	6.2×10^{-3}		Goodarzi et al. (2010)	Q	570, 573
		6400	Kühne et al. (2005)	Q	
	1.7×10^{3}		MacBean (2012a)	?	12
		7200	Kühne et al. (2005)	?	
			Mackay et al. (2006d)	W	597

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1-nitronaphthalene	4.6		Chao et al. (2017)	M	
$C_{10}H_7NO_2$	5.6		Altschuh et al. (1999)	M	
[86-57-7]			Mackay et al. (2006d)	V	560
RJKGJBPXVHTNJL-UHFFFAOYSA-N	2.9×10^{-1}		Mackay et al. (1995)	V	
	3.8		Keshavarz et al. (2022)	Q	
	9.8		Duchowicz et al. (2020)	Q	
	6.4		Abraham et al. (2019)	Q	
	3.5		Parnis et al. (2015)	Q	371
	4.7		Zhang et al. (2010)	Q	288, 289
	4.2		Zhang et al. (2010)	Q	288, 290
	1.6		Zhang et al. (2010)	Q	288, 291
	4.7		Zhang et al. (2010)	Q	288, 292
	2.1		Modarresi et al. (2007)	Q	68
	5.6		Duchowicz et al. (2020)	?	186, 21
2-nitronaphthalene	6.8		Parnis et al. (2015)	Q	371
$C_{10}H_7NO_2$					
[581-89-5]					
ZJYJZEAJZXVAMF-UHFFFAOYSA-N					
1,3-dinitronaphthalene	1.2×10^{2}		Parnis et al. (2015)	Q	371
$C_{10}H_6N_2O_4$					
[606-37-1]					
ULALSFRIGPMWRS-UHFFFAOYSA-N					
1,5-dinitronaphthalene	1.1×10^{2}		Parnis et al. (2015)	Q	371
$C_{10}H_6N_2O_4$					
[605-71-0]					
ZUTCJXFCHHDFJS-UHFFFAOYSA-N					
1,8-dinitronaphthalene	5.2×10^{3}		Parnis et al. (2015)	Q	371
$C_{10}H_6N_2O_4$					
[602-38-0]					
AVCSMMMOCOTIHF-UHFFFAOYSA-N					
dinoterb	1.7		Barcelo and Hennion (1997)	X	569
$C_{10}H_{12}N_2O_5$	9.1×10^{-1}		Goodarzi et al. (2010)	Q	570, 571
[1420-07-1]	9.3×10^{-1}		MacBean (2012a)	?	
IIPZYDQGBIWLBU-UHFFFAOYSA-N					
4-(1-methylpropyl)-2-nitrophenol	1.0×10^{-1}		Tremp et al. (1993)	M	12
$C_{10}H_{13}NO_3$	2.4×10^{-1}		Schwarzenbach et al. (1988)	V	12
(4-*sec*-butyl-2-nitrophenol)	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
[3555-18-8]	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
GCDCKEORRIGZKI-UHFFFAOYSA-N	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	246
		5800	Kühne et al. (2005)	Q	
		4300	Kühne et al. (2005)	?	

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methyl-4-nitronaphthalene $C_{11}H_9NO_2$ [880-93-3] FRLVKAJKOYFHKQ-UHFFFAOYSA-N	7.7		Parnis et al. (2015)	Q	371
1-methyl-5-nitronaphthalene $C_{11}H_9NO_2$ [91137-27-8] AOSRALZFDNFXFZ-UHFFFAOYSA-N	5.0		Parnis et al. (2015)	Q	371
1-methyl-6-nitronaphthalene $C_{11}H_9NO_2$ [105752-67-8] SOXBGESONWKYDX-UHFFFAOYSA-N	5.0		Parnis et al. (2015)	Q	371
2-methyl-1-nitronaphthalene $C_{11}H_9NO_2$ [881-03-8] IZNWACYOILBFEG-UHFFFAOYSA-N	1.5		Parnis et al. (2015)	Q	371
3-methyl-1-nitronaphthalene $C_{11}H_9NO_2$ [13615-38-8] HKMFJWNUOWBRGF-UHFFFAOYSA-N	3.9		Parnis et al. (2015)	Q	371
3-nitrodibenzofuran $C_{12}H_7NO_3$ [5410-97-9] UVFAHDAUVZRVCC-UHFFFAOYSA-N	2.6×10^{1}		Parnis et al. (2015)	Q	371
musk ambrette (artificial) $C_{12}H_{16}N_2O_5$ [83-66-9] SUAUILGSCPYJCS-UHFFFAOYSA-N	1.4×10^{1} 7.0×10^{2} 2.4 2.2×10^{-1} 4.6×10^{1}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	100 288, 289 288, 290 288, 291 288, 292
bis(*p*-nitrophenyl) ether $C_{12}H_8N_2O_5$ [101-63-3] MWAGUKZCDDRDCS-UHFFFAOYSA-N	5.4×10^{3} 2.3×10^{2} 3.0×10^{3} 1.1×10^{4}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
4-nitroazobenzene $C_{12}H_9N_3O_2$ [2491-52-3] TZTDJBMGPQLSLI-UHFFFAOYSA-N	1.8×10^{1}		Ebert et al. (2023)	?	317
4-nitro-N-phenylbenzenamine $C_{12}H_{10}N_2O_2$ [836-30-6] XXYMSQQCBUKFHE-UHFFFAOYSA-N	2.4×10^{3} 1.7×10^{2} 2.9×10^{4} 2.5×10^{3}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-cyclohexyl-4,6-dinitrophenol $C_{12}H_{14}N_2O_5$ [131-89-5] QJYHUJAGJUHXJN-UHFFFAOYSA-N	1.8×10^{2}		HSDB (2015)	Q	100
dinoseb acetate $C_{12}H_{14}N_2O_6$ [2813-95-8] RDJTWDKSYLLHRW-UHFFFAOYSA-N	1.5×10^{3}		Ebert et al. (2023)	?	317
dipicrylamine $C_{12}H_5N_7O_{12}$ (2,2',4,4',6,6'-hexanitrodiphenylamine) [131-73-7] CBCIHIVRDWLAME-UHFFFAOYSA-N	4.3×10^{11}		HSDB (2015)	Q	100
1,2-dihydro-5-nitroacenaphthylene $C_{12}H_9NO_2$ (5-nitroacenaphthene) [602-87-9] CUARLQDWYSRQDF-UHFFFAOYSA-N	9.0 9.2		HSDB (2015) Parnis et al. (2015)	Q Q	100 371
2-nitro-1,1'-biphenyl $C_{12}H_9NO_2$ [86-00-0] YOJKKXRJMXIKSR-UHFFFAOYSA-N	1.6×10^{1}		Parnis et al. (2015)	Q	371
3-nitro-1,1'-biphenyl $C_{12}H_9NO_2$ [2113-58-8] FYRPEHRWMVMHQM-UHFFFAOYSA-N	9.9		Parnis et al. (2015)	Q	371
4-nitro-1,1'-biphenyl $C_{12}H_9NO_2$ [92-93-3] BAJQRLZAPXASRD-UHFFFAOYSA-N	2.8 2.5×10^{1}		HSDB (2015) Parnis et al. (2015)	Q Q	547 371
2-nitro-9H-fluorene $C_{13}H_9NO_2$ [607-57-8] XFOHWECQTFIEIX-UHFFFAOYSA-N	3.4×10^{1} 9.5×10^{1}		HSDB (2015) Parnis et al. (2015)	Q Q	547 371
5-*tert*-butyl-4,6-dinitro-1,2,3-trimethylbenzene $C_{13}H_{18}N_2O_4$ [145-39-1] MINYPECWDZURGR-UHFFFAOYSA-N	3.4×10^{1} 2.1 4.6×10^{-2} 1.1		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
penoxaline	1.2×10^{1}		Fendinger and Glotfelty (1990)	M	
$C_{13}H_{19}N_3O_4$	2.7×10^{-1}		Glotfelty et al. (1987)	V	
(pendimethalin)	2.6×10^{-3}		Barcelo and Hennion (1997)	X	569
[40487-42-1]	4.8×10^{-3}		Goodarzi et al. (2010)	Q	570
CHIFOSRWCNZCFN-UHFFFAOYSA-N	4.8		Hilal et al. (2008)	Q	
	3.4×10^{1}		Modarresi et al. (2007)	Q	68
	7.9×10^{-1}		Maniere et al. (2011)	?	166
2,6-dinitro-4-octylphenol	1.6×10^{4}		HSDB (2015)	Q	100
$C_{14}H_{20}N_2O_5$					
[4097-33-0]					
NYGISSDEOKKXOE-UHFFFAOYSA-N					
musk ketone	3.0		Lee et al. (2012)	M	
$C_{14}H_{18}N_2O_5$	5.2×10^{3}		HSDB (2015)	Q	100
[81-14-1]	2.1×10^{4}		Zhang et al. (2010)	Q	288, 289
WXCMHFPAUCOJIG-UHFFFAOYSA-N	2.6×10^{2}		Zhang et al. (2010)	Q	288, 290
	8.4		Zhang et al. (2010)	Q	288, 291
	5.0×10^{2}		Zhang et al. (2010)	Q	288, 292
moskene	4.8×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_{18}N_2O_4$	1.4×10^{1}		Zhang et al. (2010)	Q	288, 290
[116-66-5]	7.5×10^{-1}		Zhang et al. (2010)	Q	288, 291
UHWURQRPEIFIAK-UHFFFAOYSA-N	2.5		Zhang et al. (2010)	Q	288, 292
nitrothal-isopropyl	5.7×10^{2}		Ebert et al. (2023)	?	317
$C_{14}H_{17}NO_6$					
[10552-74-6]					
VJAWBEFMCIINFU-UHFFFAOYSA-N					
9-ethyl-3-nitrocarbazole	3.3×10^{2}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_{12}N_2O_2$	6.9×10^{2}		Zhang et al. (2010)	Q	288, 290
[86-20-4]	1.1×10^{3}		Zhang et al. (2010)	Q	288, 291
WONHLSYSHMRRGO-UHFFFAOYSA-N	2.5×10^{2}		Zhang et al. (2010)	Q	288, 292
2-nitroanthracene	1.0×10^{2}		Parnis et al. (2015)	Q	371
$C_{14}H_9NO_2$					
[3586-69-4]					
NZWGQBVOKHEKLD-UHFFFAOYSA-N					
9-nitroanthracene	1.6×10^{1}		Parnis et al. (2015)	Q	371
$C_{14}H_9NO_2$					
[602-60-8]					
LSIKFJXEYJIZNB-UHFFFAOYSA-N					
3-nitrophenanthrene	5.4×10^{1}		Parnis et al. (2015)	Q	371
$C_{14}H_9NO_2$					
[17024-19-0]					
CPRHWWUDRYJODK-UHFFFAOYSA-N					

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
9-nitrophenanthrene $C_{14}H_9NO_2$ [954-46-1] QTTCNQHPKFAYEZ-UHFFFAOYSA-N	3.2×10^{1}		Parnis et al. (2015)	Q	371
binapacryl $C_{15}H_{18}N_2O_6$ [485-31-4] ZRDUSMYWDRPZRM-UHFFFAOYSA-N	2.2×10^{2}		Ebert et al. (2023)	?	317
2-nitrofluoranthene $C_{16}H_9NO_2$ [13177-29-2] VBCBFNMZBHKVQN-UHFFFAOYSA-N	8.2×10^{1}		Parnis et al. (2015)	Q	371
3-nitrofluoranthene $C_{16}H_9NO_2$ [892-21-7] PIHGQKMEAMSUNA-UHFFFAOYSA-N	1.1×10^{2}		Parnis et al. (2015)	Q	371
1-[(2,4-dinitrophenyl)azo]-2-naphthol $C_{16}H_{10}N_4O_5$ (C.I. pigment orange 5) [3468-63-1] HBHZKFOUIUMKHV-UHFFFAOYSA-N	1.1×10^{9}		HSDB (2015)	Q	100
3,7-dinitrofluoranthene $C_{16}H_8N_2O_4$ [105735-71-5] WAAHHGKGQYVTNS-UHFFFAOYSA-N	4.9×10^{4}		HSDB (2015)	Q	100
1,3-dinitropyrene $C_{16}H_8N_2O_4$ [75321-20-9] UJIPQBOHUQDIAA-UHFFFAOYSA-N	6.3×10^{3}		Parnis et al. (2015)	Q	371
1,6-dinitropyrene $C_{16}H_8N_2O_4$ [42397-64-8] GUXACCKTQWVTLG-UHFFFAOYSA-N	7.6×10^{4} 7.3×10^{3}		HSDB (2015) Parnis et al. (2015)	Q Q	100 371
1,8-dinitropyrene $C_{16}H_8N_2O_4$ [42397-65-9] BLYXNIHKOMELAP-UHFFFAOYSA-N	7.6×10^{4} 2.3×10^{4}		HSDB (2015) Parnis et al. (2015)	Q Q	100 371
1-nitropyrene $C_{16}H_9NO_2$ [5522-43-0] ALRLPDGCPYIVHP-UHFFFAOYSA-N	3.9×10^{2} 2.0×10^{2}		HSDB (2015) Parnis et al. (2015)	Q Q	100 371

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
2-nitropyrene $C_{16}H_9NO_2$ [789-07-1] MAZCGYFIOOIVHE-UHFFFAOYSA-N	9.0×10^{1}		Parnis et al. (2015)	Q	371
4-nitropyrene $C_{16}H_9NO_2$ [57835-92-4] UISKIUIWPSPSAV-UHFFFAOYSA-N	3.9×10^{2}		HSDB (2015)	Q	100
N,N-diethyl-4-[(4-nitrophenyl)azo]aniline	3.7		Duchowicz et al. (2020)	V	187
$C_{16}H_{18}N_4O_2$ [3025-52-3] LVQIWDUSUJTZJF-ISLYRVAYSA-N	1.5×10^{3}		Duchowicz et al. (2020)	Q	
disperse red 1 $C_{16}H_{18}N_4O_3$ [2872-52-8] FOQABOMYTOFLPZ-ZCXUNETKSA-N	1.2×10^{8} 1.1×10^{6}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
1-[(4-methyl-2-nitrophenyl)azo]-2-naphthalenol $C_{17}H_{13}N_3O_3$ (C.I. Pigment Red 3) [2425-85-6] ZLFVRXUOSPRRKQ-UHFFFAOYSA-N	8.2×10^{6}		HSDB (2015)	Q	100
phenyl 1-hydroxy-4-nitro-2-naphthoate	1.5×10^{4}		Zhang et al. (2010)	Q	288, 289
$C_{17}H_{11}NO_5$	6.7×10^{5}		Zhang et al. (2010)	Q	288, 290
[65208-34-6]	1.1×10^{2}		Zhang et al. (2010)	Q	288, 291
DMPUGHYNLCGVPX-UHFFFAOYSA-N	2.7×10^{5}		Zhang et al. (2010)	Q	288, 292
7-nitrobenz[*a*]anthracene $C_{18}H_{11}NO_2$ [20268-51-3] KOPVBVBUIYTJBG-UHFFFAOYSA-N	9.9×10^{1}		Parnis et al. (2015)	Q	371
6-nitrochrysene $C_{18}H_{11}NO_2$ [7496-02-8] UAWLTQJFZUYROA-UHFFFAOYSA-N	6.6×10^{2}		HSDB (2015)	Q	100
meptyldinocap $C_{18}H_{24}N_2O_6$ [131-72-6] NIOPZPCMRQGZCE-WEVVVXLNSA-N	8.6×10^{1}		Maniere et al. (2011)	?	242, 166

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-nitrobenzo[*a*]pyrene $C_{20}H_{11}NO_2$ [70021-99-7] ICKISBPYFVBVQG-UHFFFAOYSA-N	3.1×10^{3}		HSDB (2015)	Q	449
3-nitrobenzo[*a*]pyrene $C_{20}H_{11}NO_2$ [70021-98-6] CQIJHYPCKYZMIV-UHFFFAOYSA-N	3.1×10^{3}		HSDB (2015)	Q	449
6-nitrobenzo[*a*]pyrene $C_{20}H_{11}NO_2$ [63041-90-7] NMMAFYSZGOFZCM-UHFFFAOYSA-N	3.1×10^{3} 3.3×10^{2}		HSDB (2015) Parnis et al. (2015)	Q Q	449 371
MCM:NPHEN1OOH $C_6H_5NO_4$ QKMAXSKQIHICGE-UHFFFAOYSA-N	2.8×10^{4} 3.0×10^{4} 3.3×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:NCATECHOL $C_6H_5NO_4$ XJNPNXSISMKQEX-UHFFFAOYSA-N	3.2×10^{7} 8.0×10^{7} 6.0×10^{6}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:NCRES1OOH $C_7H_7NO_4$ PUXUHFKGXFXGAC-UHFFFAOYSA-N	1.7×10^{4} 8.9×10^{3} 4.7		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:MNCATECH $C_7H_7NO_4$ DPKDSDOOIONLAG-UHFFFAOYSA-N	5.6×10^{3} 8.5×10^{5} 3.6		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:NEBNZ1OOH $C_8H_9NO_4$ WELXCAQABDDCET-UHFFFAOYSA-N	1.3×10^{4} 4.9×10^{3} 1.7		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:NMXYOL1OOH $C_8H_9NO_4$ WHVCHTZZXIECJY-UHFFFAOYSA-N	9.6×10^{3} 2.2×10^{4} 2.7		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:NOXYOL1OOH $C_8H_9NO_4$ WTJTXPQAQHBAPV-UHFFFAOYSA-N	9.6×10^{3} 1.2×10^{4} 8.9		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:NPXYOL1OOH $C_8H_9NO_4$ MKCNKDVBVLGUFV-UHFFFAOYSA-N	9.6×10^{3} 1.2×10^{4} 2.7		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:DM124OHNO2 $C_8H_9NO_3$ KGDIYDUZVHFMHQ-UHFFFAOYSA-N	2.3 2.4 5.6×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DMPHOHNO2	2.3		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_3$	1.2×10^{1}		Wang et al. (2017)	Q	81, 240
YXNYMZXPUWOUJT-UHFFFAOYSA-N	3.5×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:DNEBNZOL	1.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_8N_2O_5$	9.6×10^{3}		Wang et al. (2017)	Q	81, 240
SYWMIOFIFBKHTK-UHFFFAOYSA-N	2.1		Wang et al. (2017)	Q	81, 241
MCM:DNMXYOL	1.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_8N_2O_5$	2.1×10^{4}		Wang et al. (2017)	Q	81, 240
MHXAYMPVZDCVJX-UHFFFAOYSA-N	1.9×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:DNOXYOL	8.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_8N_2O_5$	1.6×10^{4}		Wang et al. (2017)	Q	81, 240
JCTQXQRGEDMCSI-UHFFFAOYSA-N	2.6		Wang et al. (2017)	Q	81, 241
MCM:DNPXYOL	8.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_8H_8N_2O_5$	6.5×10^{3}		Wang et al. (2017)	Q	81, 240
RROXWBBJMPCPHD-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	81, 241
MCM:EBNZOHNO2	3.5		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_3$	1.3×10^{1}		Wang et al. (2017)	Q	81, 240
RSETVJMGQZKFCF-UHFFFAOYSA-N	7.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:ENCATECH	4.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_4$	5.1×10^{5}		Wang et al. (2017)	Q	81, 240
CGDBCFCRALNPBR-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	81, 241
MCM:MXNCATECH	3.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_4$	4.1×10^{5}		Wang et al. (2017)	Q	81, 240
DNJZITGVNONOFW-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	81, 241
MCM:MXY1OHNO2	2.3		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_3$	1.7×10^{1}		Wang et al. (2017)	Q	81, 240
KJRCHILWKQLEBC-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:OXNCATECH	3.3×10^{3}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_4$	8.0×10^{5}		Wang et al. (2017)	Q	81, 240
BBBHATWMUPCFKG-UHFFFAOYSA-N	3.1		Wang et al. (2017)	Q	81, 241
MCM:OXY1OHNO2	2.3		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_3$	2.6×10^{1}		Wang et al. (2017)	Q	81, 240
KXWOAPZXQJGYPU-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:PXNCATECH	1.1×10^{7}		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_4$	2.5×10^{8}		Wang et al. (2017)	Q	81, 240
MAHUOFZDOBGDSU-UHFFFAOYSA-N	4.7×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:PXY1OHNO2	2.3		Wang et al. (2017)	Q	81, 239
$C_8H_9NO_3$	8.7		Wang et al. (2017)	Q	81, 240
VIQHHRZADKSPIM-UHFFFAOYSA-N	1.0×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NIPBNZ1OOH	1.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_4$	3.6×10^{3}		Wang et al. (2017)	Q	81, 240
IXEXRYHUTBEDFT-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	81, 241
MCM:NMETOL1OOH	8.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_4$	4.4×10^{3}		Wang et al. (2017)	Q	81, 240
OTBVEKBEKVMFBF-UHFFFAOYSA-N	2.1		Wang et al. (2017)	Q	81, 241
MCM:NOETOL1OOH	8.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_4$	6.5×10^{3}		Wang et al. (2017)	Q	81, 240
ZYYASKSQLLYACE-UHFFFAOYSA-N	3.2		Wang et al. (2017)	Q	81, 241
MCM:NPBNZ1OOH	1.2×10^{4}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_4$	3.6×10^{3}		Wang et al. (2017)	Q	81, 240
CVKCTJQZVRPANA-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	81, 241
MCM:NPETOL1OOH	8.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_4$	3.2×10^{3}		Wang et al. (2017)	Q	81, 240
PGRGKKYGDUKVIK-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	81, 241
MCM:NT123L1OOH	5.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_4$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
QUQYRHULCDEZAA-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:NT124L1OOH	5.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_4$	4.6×10^{4}		Wang et al. (2017)	Q	81, 240
DLQITMPSPXAOFG-UHFFFAOYSA-N	2.9×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:DNIPBNZOL	1.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}N_2O_5$	3.6×10^{3}		Wang et al. (2017)	Q	81, 240
[29385-11-3]	1.4		Wang et al. (2017)	Q	81, 241
HBYHYLBZPLCIEE-UHFFFAOYSA-N	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	272, 244
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	246
MCM:DNMETOL	8.7×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}N_2O_5$	2.4×10^{4}		Wang et al. (2017)	Q	81, 240
NLLBSWNZAUXBGJ-UHFFFAOYSA-N	1.3×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:DNOETOL	7.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}N_2O_5$	1.0×10^{4}		Wang et al. (2017)	Q	81, 240
AGMONASRVOHMRW-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	81, 241
MCM:DNPBNZOL	1.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}N_2O_5$	5.8×10^{3}		Wang et al. (2017)	Q	81, 240
FCIYPWNHZQHVEQ-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	81, 241
MCM:DNPETOL	7.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}N_2O_5$	3.9×10^{3}		Wang et al. (2017)	Q	81, 240
DZWALJMRDDSGJQ-UHFFFAOYSA-N	8.9×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DNT123BOL	6.2×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}N_2O_5$	1.7×10^{4}		Wang et al. (2017)	Q	81, 240
KTYJIHPJHVSEQH-UHFFFAOYSA-N	3.8		Wang et al. (2017)	Q	81, 241
MCM:DNT124BOL	4.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_9H_{10}N_2O_5$	1.4×10^{4}		Wang et al. (2017)	Q	81, 240
HCZZKJMHIZGVJN-UHFFFAOYSA-N	3.9×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:HOEMPHNO2	2.1		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_3$	1.0×10^{1}		Wang et al. (2017)	Q	81, 240
YSPMBFYZTNTHGD-UHFFFAOYSA-N	2.6×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:IPBNZOHNO2	3.2		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_3$	5.6		Wang et al. (2017)	Q	81, 240
RRFSVDKJKYCCEK-UHFFFAOYSA-N	6.5×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:IPNCATECH	4.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_4$	2.0×10^{5}		Wang et al. (2017)	Q	81, 240
MCPZUPZVJHDAPC-UHFFFAOYSA-N	1.6		Wang et al. (2017)	Q	81, 241
MCM:MET1OHNO2	2.1		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_3$	1.0×10^{1}		Wang et al. (2017)	Q	81, 240
QDGFKFKXXCXYOS-UHFFFAOYSA-N	8.7×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:MTNCATECH	2.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_4$	2.6×10^{5}		Wang et al. (2017)	Q	81, 240
CJFAOEWQLMJWBQ-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	81, 241
MCM:OET1OHNO2	2.1		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_3$	1.5×10^{1}		Wang et al. (2017)	Q	81, 240
MEMHWZGPMLWUCR-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:OTNCATECH	2.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_4$	4.6×10^{5}		Wang et al. (2017)	Q	81, 240
JWEUFFGZFSJOFB-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	81, 241
MCM:PBNZOHNO2	2.8		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_3$	8.5		Wang et al. (2017)	Q	81, 240
SNIBPLNVBYUZKZ-UHFFFAOYSA-N	6.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:PET1OHNO2	2.1		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_3$	5.6		Wang et al. (2017)	Q	81, 240
DXOFURYTWRHSOS-UHFFFAOYSA-N	6.3×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:PNCATECH	3.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_4$	2.9×10^{5}		Wang et al. (2017)	Q	81, 240
UWDKGIAMIWLDOZ-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	81, 241
MCM:PTNCATECH	8.9×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_4$	1.8×10^{8}		Wang et al. (2017)	Q	81, 240
POSTUROPYARVPT-UHFFFAOYSA-N	3.7×10^{4}		Wang et al. (2017)	Q	81, 241

Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:T123NCATEC	2.0×10^{3}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_4$	6.0×10^{5}		Wang et al. (2017)	Q	81, 240
NRIGBHNXEXAXSY-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	81, 241
MCM:T124NCATEC	6.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_4$	4.8×10^{8}		Wang et al. (2017)	Q	81, 240
XNILZTOSMSXQOP-UHFFFAOYSA-N	8.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:TM123OHNO2	1.5		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_3$	3.3×10^{1}		Wang et al. (2017)	Q	81, 240
GRYTUHBAWMNFLK-UHFFFAOYSA-N	3.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:TM124OHNO2	9.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_9H_{11}NO_3$	2.4×10^{4}		Wang et al. (2017)	Q	81, 240
NKOCMNXLDSIDQC-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	81, 241

A5 Organic species with fluorine (F)

A5.1 Organic fluorine

Table A5.1: Organic fluorine

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
fluoromethane	6.1×10^{-4}	2100	Burkholder et al. (2019)	L	1
CH_3F	6.1×10^{-4}	2000	Burkholder et al. (2015)	L	
[593-53-3]	6.2×10^{-4}	2200	Brockbank (2013)	L	1, 598
NBVXSUQYWXRMNV-UHFFFAOYSA-N	6.1×10^{-4}	2000	Sander et al. (2011)	L	
	6.1×10^{-4}	2000	Sander et al. (2006)	L	
	5.8×10^{-4}	2200	Wilhelm et al. (1977)	L	
	5.8×10^{-4}	2100	Swain and Thornton (1962)	M	
	5.8×10^{-4}	2200	Glew and Moelwyn-Hughes (1953)	M	599
	5.8×10^{-4}		Duchowicz et al. (2020)	V	187
	5.1×10^{-4}		Mackay and Shiu (1981)	V	
	5.8×10^{-4}		Hine and Mookerjee (1975)	V	
	7.1×10^{-4}		Yaws (2003)	X	238, 81
	1.0×10^{-7}		Hayer et al. (2022)	Q	20
	2.6×10^{-3}		Duchowicz et al. (2020)	Q	
	8.7×10^{-5}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	6.7×10^{-4}		Gharagheizi et al. (2010)	Q	247
	9.2×10^{-5}		Hilal et al. (2008)	Q	
		2200	Kühne et al. (2005)	Q	
	5.1×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	7.7×10^{-4}		English and Carroll (2001)	Q	231, 232
	6.5×10^{-4}		Russell et al. (1992)	Q	280
	5.8×10^{-4}		Suzuki et al. (1992)	Q	233
	1.9×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	5.9×10^{-4}		Irmann (1965)	Q	
		2200	Kühne et al. (2005)	?	
	7.1×10^{-4}		Yaws (1999)	?	21, 81
	4.7×10^{-4}		Abraham and Weathersby (1994)	?	21
	7.0×10^{-4}		Yaws and Yang (1992)	?	21, 81
difluoromethane	6.4×10^{-4}	2100	Kutsuna (2017)	M	1
CH_2F_2	6.8×10^{-4}	2500	Anderson (2011)	M	
(R32)	3.0×10^{-4}	3500	Miguel et al. (2000)	M	
[75-10-5]	6.9×10^{-4}	2400	Maaßen (1995)	M	600
RWRIWBAIICGTTQ-UHFFFAOYSA-N	6.9×10^{-4}	2300	Reichl (1995)	M	601
	7.9×10^{-4}		Hayer et al. (2022)	Q	20
	1.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	8.4×10^{-4}		Hilal et al. (2008)	Q	
		2200	Kühne et al. (2005)	Q	
	3.1×10^{-2}		Yaffe et al. (2003)	Q	249, 250
		2400	Kühne et al. (2005)	?	

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.6×10^{-4}		Yaws (1999)	?	21
	8.6×10^{-4}		Yaws and Yang (1992)	?	21
trifluoromethane	1.3×10^{-4}	2500	Burkholder et al. (2019)	L	
CHF_3	1.2×10^{-4}	2200	Burkholder et al. (2019)	L	71
(R23)	1.3×10^{-4}	2500	Burkholder et al. (2015)	L	
[75-46-7]	1.2×10^{-4}	2200	Burkholder et al. (2015)	L	71
XPDWGBQVDMORPB-UHFFFAOYSA-N	1.3×10^{-4}	3300	Sander et al. (2011)	L	
	1.3×10^{-4}	3200	Wilhelm et al. (1977)	L	
	2.1×10^{-4}	2500	Miguel et al. (2000)	M	
	1.3×10^{-4}	2400	Zheng et al. (1997)	M	602
	1.2×10^{-4}	2400	Maaßen (1995)	M	603
	1.0×10^{-4}		Hine and Mookerjee (1975)	V	
	1.3×10^{-4}		Yaws (2003)	X	238
	1.0×10^{-4}		Irmann (1965)	C	
	1.3×10^{-4}		Hayer et al. (2022)	Q	20
	1.0×10^{-4}		Keshavarz et al. (2022)	Q	
	8.8×10^{-4}		Duchowicz et al. (2020)	Q	185
	1.3×10^{-4}	2700	Li et al. (2019)	Q	1
	4.0×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	1.3×10^{-4}		Gharagheizi et al. (2010)	Q	247
	2.0×10^{-4}		Hilal et al. (2008)	Q	
	4.0×10^{-5}		Modarresi et al. (2007)	Q	68
		2200	Kühne et al. (2005)	Q	
	1.2×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	1.1×10^{-4}		Irmann (1965)	Q	
	1.0×10^{-4}		Duchowicz et al. (2020)	?	186, 21
		3000	Kühne et al. (2005)	?	
	1.3×10^{-4}		Yaws (1999)	?	21
	1.3×10^{-4}		Yaws and Yang (1992)	?	21
tetrafluoromethane	2.1×10^{-6}	1800	Burkholder et al. (2019)	L	1
CF_4	1.7×10^{-6}	2300	Burkholder et al. (2019)	L	71
(carbontetrafluoride)	2.1×10^{-6}	1800	Burkholder et al. (2015)	L	1
[75-73-0]	1.7×10^{-6}	2300	Burkholder et al. (2015)	L	71
TXEYQDLBPFQVAA-UHFFFAOYSA-N	2.1×10^{-6}	2300	Warneck and Williams (2012)	L	
	2.1×10^{-6}	1800	Sander et al. (2011)	L	1
	2.1×10^{-6}	1800	Wilhelm et al. (1977)	L	
	2.0×10^{-6}	2000	Reichl (1995)	M	604
	2.1×10^{-6}	1800	Scharlin and Battino (1995)	M	605
	2.1×10^{-6}	1800	Scharlin and Battino (1994)	M	606
	2.1×10^{-6}		Park et al. (1982)	M	
	2.1×10^{-6}	1600	Cosgrove and Walkley (1981)	M	11
	2.0×10^{-6}	1900	Wen and Muccitelli (1979)	M	607

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.1×10^{-6}	1800	Ashton et al. (1968)	M	608
	2.0×10^{-6}	1500	Morrison and Johnstone (1954)	M	609
	1.9×10^{-6}		Hine and Mookerjee (1975)	V	
	3.3×10^{-6}		Pierotti (1965)	T	
	1.8×10^{-6}		Yaws (2003)	X	238
	1.9×10^{-6}		Irmann (1965)	C	
	2.8×10^{-6}		Hayer et al. (2022)	Q	20
	6.9×10^{-7}		Keshavarz et al. (2022)	Q	
	1.4×10^{-5}		Duchowicz et al. (2020)	Q	
	2.1×10^{-6}	1800	Li et al. (2019)	Q	1
	5.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
	9.2×10^{-6}		Hilal et al. (2008)	Q	
	3.2×10^{-6}		Modarresi et al. (2007)	Q	68
		2200	Kühne et al. (2005)	Q	
	2.9×10^{-6}		Goss (2005)	Q	
	2.0×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	1.0×10^{-6}	-840	Bonifácio et al. (2001)	Q	
	1.2×10^{-8}		Katritzky et al. (1998)	Q	
	5.4×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
	1.6×10^{-6}		Irmann (1965)	Q	
	1.9×10^{-6}		Duchowicz et al. (2020)	?	186, 21
		1900	Kühne et al. (2005)	?	
	1.9×10^{-6}		Yaws (1999)	?	21
	2.1×10^{-6}	1700	Yaws et al. (1999)	?	21
	1.8×10^{-6}		Yaws and Yang (1992)	?	21
fluoroethane	4.6×10^{-4}		Yaws (2003)	X	238
C_2H_5F	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[353-36-6]	3.1×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
UHCBBWUQDAVSMS-UHFFFAOYSA-N	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	4.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
	4.8×10^{-4}		Hilal et al. (2008)	Q	
	3.2×10^{-4}		Modarresi et al. (2007)	Q	68
	4.6×10^{-4}		Yaws (1999)	?	21
	5.0×10^{-4}		Abraham and Weathersby (1994)	?	21
	4.4×10^{-4}		Yaws and Yang (1992)	?	21
1,1-difluoroethane	4.9×10^{-4}	2600	Burkholder et al. (2019)	L	610, 71
$C_2H_4F_2$	4.9×10^{-4}	2600	Burkholder et al. (2015)	L	611, 71
(R152a)	4.9×10^{-4}	2800	Zheng et al. (1997)	M	612
[75-37-6]	5.0×10^{-4}	2800	Maaßen (1995)	M	613
NPNPZTNLOVBDOC-UHFFFAOYSA-N	4.9×10^{-4}	2700	Reichl (1995)	M	614
	4.2×10^{-4}	2300	McLinden (1989)	V	
	4.8×10^{-4}		Hine and Mookerjee (1975)	V	
	4.8×10^{-4}		Irmann (1965)	C	295

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.7×10^{-4}		Hayer et al. (2022)	Q	20
	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	2.9×10^{-4}		Hilal et al. (2008)	Q	
	1.4×10^{-4}		Modarresi et al. (2007)	Q	68
		2600	Kühne et al. (2005)	Q	
	9.0×10^{-4}		English and Carroll (2001)	Q	231, 232
	1.4×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	4.3×10^{-4}		Irmann (1965)	Q	
	4.9×10^{-4}		Duchowicz et al. (2020)	?	186, 21
		2800	Kühne et al. (2005)	?	
	3.9×10^{-4}		Yaws (1999)	?	21, 298
	3.7×10^{-4}		Yaws and Yang (1992)	?	21, 298
1,2-difluoroethane $C_2H_4F_2$ [624-72-6] AHFMSNDOYCFEPH-UHFFFAOYSA-N	2.5×10^{-5}		HSDB (2015)	Q	100
1,1,1,2-tetrafluoroethane $C_2H_2F_4$ (R134a) [811-97-2] LVGUZGTVOIAKKC-UHFFFAOYSA-N	1.6×10^{-4}	2700	Burkholder et al. (2019)	L	71
	1.6×10^{-4}	2700	Burkholder et al. (2015)	L	71
	1.5×10^{-4}	3100	Ooki and Yokouchi (2011)	M	71
	1.6×10^{-4}	2900	Zheng et al. (1997)	M	615
	1.6×10^{-4}	3000	Maaßen (1995)	M	616
	1.6×10^{-4}	2900	Reichl (1995)	M	617
	1.9×10^{-4}	1400	Chang and Criddle (1995)	M	618
	1.4×10^{-4}	2600	McLinden (1989)	V	
	2.5×10^{-4}		Hayer et al. (2022)	Q	20
	1.5×10^{-4}	3100	Li et al. (2019)	Q	1
	6.5×10^{-6}		HSDB (2015)	Q	100
	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	1.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	246
	9.7×10^{-5}		Hilal et al. (2008)	Q	
	5.5×10^{-5}		Modarresi et al. (2007)	Q	68
1,1,2,2-tetrafluoroethane $C_2H_2F_4$ [359-35-3] WXGNWUVNYMJENI-UHFFFAOYSA-N	2.9×10^{-4}		Ebert et al. (2023)	?	319

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pentafluoroethane	3.1×10^{-4}	3300	Miguel et al. (2000)	M	
C_2HF_5	3.5×10^{-5}	3000	Reichl (1995)	M	619
(R125)	8.0×10^{-5}	4800	McLinden (1989)	V	
[354-33-6]	1.3×10^{-4}		Hayer et al. (2022)	Q	20
GTLACDSXYULKMZ-UHFFFAOYSA-N	3.5×10^{-5}	3000	Li et al. (2019)	Q	1
	2.0×10^{-4}		HSDB (2015)	Q	100
	3.2×10^{-6}		Zhang et al. (2010)	Q	288, 289
	2.0×10^{-5}		Zhang et al. (2010)	Q	288, 290
	5.7×10^{-5}		Zhang et al. (2010)	Q	288, 291
	2.1×10^{-5}		Zhang et al. (2010)	Q	288, 292
		2600	Kühne et al. (2005)	Q	
		2900	Kühne et al. (2005)	?	
hexafluoroethane	6.5×10^{-7}	2100	Bonifácio et al. (2001)	M	
C_2F_6	5.3×10^{-7}		Park et al. (1982)	M	
[76-16-4]	5.6×10^{-7}	2300	Wen and Muccitelli (1979)	M	620
WMIYKQLTONQJES-UHFFFAOYSA-N	5.8×10^{-7}		Yaws (2003)	X	238
	7.1×10^{-7}		Hayer et al. (2022)	Q	20
	9.3×10^{-7}		Keshavarz et al. (2022)	Q	
	2.2×10^{-5}		Duchowicz et al. (2020)	Q	
	5.8×10^{-7}	2600	Li et al. (2019)	Q	1
	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
	4.1×10^{-7}		Zhang et al. (2010)	Q	288, 289
	1.1×10^{-5}		Zhang et al. (2010)	Q	288, 290
	8.4×10^{-7}		Zhang et al. (2010)	Q	288, 291
	1.9×10^{-6}		Zhang et al. (2010)	Q	288, 292
	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	247
	1.2×10^{-5}		Hilal et al. (2008)	Q	
	1.8×10^{-6}		Modarresi et al. (2007)	Q	68
		2600	Kühne et al. (2005)	Q	
	1.2×10^{-6}	1700	Bonifácio et al. (2001)	Q	
	4.9×10^{-7}		Duchowicz et al. (2020)	?	186, 21
		2900	Kühne et al. (2005)	?	
	5.8×10^{-7}		Yaws (1999)	?	21
	5.8×10^{-7}		Yaws and Yang (1992)	?	21
1-fluoropropane	6.3×10^{-4}		Yaws (2003)	X	238, 621
C_3H_7F	7.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[460-13-9]	5.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
JRHNUZCXXOTJCA-UHFFFAOYSA-N	5.7×10^{-4}		Hilal et al. (2008)	Q	
	6.2×10^{-4}		Yaws (1999)	?	21, 621
	3.6×10^{-4}		Abraham and Weathersby (1994)	?	21
	6.1×10^{-4}		Yaws and Yang (1992)	?	21, 621

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-fluoropropane	6.0×10^{-4}		Yaws (2003)	X	238, 81
C_3H_7F	2.2×10^{-4}		Gharagheizi et al. (2012)	Q	
[420-26-8]	6.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
PRNZBCYBKGCOFI-UHFFFAOYSA-N	2.5×10^{-4}		Hilal et al. (2008)	Q	
	5.9×10^{-4}		Yaws (1999)	?	21, 81
	3.8×10^{-4}		Abraham and Weathersby (1994)	?	21
	5.8×10^{-4}		Yaws and Yang (1992)	?	21, 81
1,1,1,2,2-pentafluoropropane	3.0×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
$C_3H_3F_5$					
[1814-88-6]					
FDOPVENYMZRARC-UHFFFAOYSA-N					
1,1,1,3,3,3-hexafluoropropane	1.2×10^{-6}		Zhang et al. (2010)	Q	288, 289
$C_3H_2F_6$	3.9×10^{-5}		Zhang et al. (2010)	Q	288, 290
[690-39-1]	1.8×10^{-4}		Zhang et al. (2010)	Q	288, 291
NSGXIBWMJZWTPY-UHFFFAOYSA-N	2.7×10^{-6}		Zhang et al. (2010)	Q	288, 292
1,1,1,2,3,3,3-heptafluoropropane	1.4×10^{-5}	3300	Reichl (1995)	M	622
C_3HF_7	2.2×10^{-4}		Hayer et al. (2022)	Q	20
(R227)	6.2×10^{-7}		HSDB (2015)	Q	100
[431-89-0]		2900	Kühne et al. (2005)	Q	
YFMFNYKEUDLDTL-UHFFFAOYSA-N		3300	Kühne et al. (2005)	?	
octafluoropropane	1.2×10^{-7}	6900	Wen and Muccitelli (1979)	M	
C_3F_8	3.0×10^{-7}		Duchowicz et al. (2020)	V	187
(R218)	3.0×10^{-7}		HSDB (2015)	V	
[76-19-7]	3.2×10^{-7}		Yaws (2003)	X	238, 81
QYSGYZVSCZSLHT-UHFFFAOYSA-N	1.1×10^{-3}		Hayer et al. (2022)	Q	20
	5.1×10^{-5}		Duchowicz et al. (2020)	Q	
	4.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	7.7×10^{-8}		Zhang et al. (2010)	Q	288, 289
	1.0×10^{-5}		Zhang et al. (2010)	Q	288, 290
	3.8×10^{-7}		Zhang et al. (2010)	Q	288, 291
	4.5×10^{-7}		Zhang et al. (2010)	Q	288, 292
	3.0×10^{-7}		Gharagheizi et al. (2010)	Q	247
	1.1×10^{-5}		Hilal et al. (2008)	Q	
	3.1×10^{-7}		Yaws (1999)	?	21, 81
decafluorobutane	1.5×10^{-8}		HSDB (2015)	Q	100
C_4F_{10}					
[355-25-9]					
KAVGMUDTWQVPDF-UHFFFAOYSA-N					

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
octafluorocyclobutane	1.2×10^{-6}	3000	Clever et al. (2005)	L	623, 624
C_4F_8	1.3×10^{-6}	3300	Scharlin and Battino (1994)	M	625
[115-25-3]	1.2×10^{-6}		Park et al. (1982)	M	
BCCOBQSFUDVTJQ-UHFFFAOYSA-N	1.2×10^{-6}	3000	Wen and Muccitelli (1979)	M	626
	1.2×10^{-6}		Duchowicz et al. (2020)	V	187
	2.5×10^{-6}		Yaws (2003)	X	238, 374
	1.6×10^{-6}		Hayer et al. (2022)	Q	20
	3.9×10^{-3}		Duchowicz et al. (2020)	Q	
	1.0×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-7}		Zhang et al. (2010)	Q	288, 289
	1.6×10^{-6}		Zhang et al. (2010)	Q	288, 290
	2.2×10^{-6}		Zhang et al. (2010)	Q	288, 291
	1.0×10^{-6}		Zhang et al. (2010)	Q	288, 292
	2.6×10^{-6}		Gharagheizi et al. (2010)	Q	247
	9.2×10^{-6}		Hilal et al. (2008)	Q	
		4500	Kühne et al. (2005)	Q	
		3800	Kühne et al. (2005)	?	
	2.6×10^{-6}		Yaws (1999)	?	21, 374
	2.5×10^{-6}		Yaws and Yang (1992)	?	21, 374
1,1,1,2,2,3,4,5,5,5-decafluoropentane	4.4×10^{-8}		Zhang et al. (2010)	Q	288, 289
$C_5H_2F_{10}$	3.2×10^{-5}		Zhang et al. (2010)	Q	288, 290
[138495-42-8]	1.8×10^{-4}		Zhang et al. (2010)	Q	288, 291
RIQRGMUSBYGDBL-UHFFFAOYSA-N	9.0×10^{-7}		Zhang et al. (2010)	Q	288, 292
dodecafluoropentane	4.6×10^{-8}		Brockbank (2013)	L	
C_5F_{12}	6.1×10^{-6}		Hilal et al. (2008)	Q	
[678-26-2]					
NJCBUSHGCBERSK-UHFFFAOYSA-N					
tetradecafluorohexane	9.3×10^{-9}		Brockbank (2013)	L	
C_6F_{14}	5.4×10^{-10}		HSDB (2015)	Q	100
(perflexane)					
[355-42-0]					
ZJIJAJXFLBMLCK-UHFFFAOYSA-N					
fluorocyclohexane	1.3×10^{-3}		Hilal et al. (2008)	Q	
$C_6H_{11}F$					
[372-46-3]					
GOBGVVAHHOUMDK-UHFFFAOYSA-N					
1-fluoroheptane	2.7×10^{-4}		Hilal et al. (2008)	Q	
$C_7H_{15}F$					
[661-11-0]					
BITLXSQYFZTQGC-UHFFFAOYSA-N					

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexadecafluoroheptane C_7F_{16} [335-57-9] LGUZHRODIJCVOC-UHFFFAOYSA-N	3.0×10^{-9} 1.9×10^{-7}		Brockbank (2013) Hilal et al. (2008)	L Q	
1-fluorooctane $C_8H_{17}F$ [463-11-6] DHIVLKMGKIZOHF-UHFFFAOYSA-N	1.5×10^{-4}		Hilal et al. (2008)	Q	
perfluorooctane C_8F_{18} [307-34-6] YVBBRRALBYAZBM-UHFFFAOYSA-N	8.0×10^{-10}		Brockbank (2013)	L	
eicosafluorononane C_9F_{20} [375-96-2] UVWPNDVAQBNQBG-UHFFFAOYSA-N	4.5×10^{-9}		Hilal et al. (2008)	Q	
perfluoroundecane $C_{11}F_{24}$ [307-49-3] VCIVYCHKSHULON-UHFFFAOYSA-N	1.3×10^{-13} 1.2×10^{-11} 1.2×10^{-9} 6.0×10^{-12}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-henicosafluorododecane $C_{12}H_5F_{21}$ (perfluorodecyl ethane) [154478-87-2] HUPGRQWHZOWFPQ-UHFFFAOYSA-N	5.1×10^{-10}		Plassmann et al. (2010)	Q	
1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluorotetradecane $C_{14}H_{17}F_{13}$ [133331-77-8] WRYIIOKOQSICTB-UHFFFAOYSA-N	6.4×10^{-7}		Plassmann et al. (2010)	Q	
1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoroicosane $C_{20}H_{29}F_{13}$ [154628-00-9] BREOHRVZEZMFOB-UHFFFAOYSA-N	2.5×10^{-7}		Plassmann et al. (2010)	Q	
1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluorodocosane $C_{22}H_{33}F_{13}$ [133310-71-1] ZKYMFADZZFTYJH-UHFFFAOYSA-N	2.0×10^{-7}		Plassmann et al. (2010)	Q	

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluorotetracosane $C_{24}H_{33}F_{17}$ [117146-18-6] FTECWCULPOFDJS-UHFFFAOYSA-N	4.0×10^{-9}		Plassmann et al. (2010)	Q	
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-henicosafluorohexacosane $C_{26}H_{33}F_{21}$ LZENXKBSJNMIKY-UHFFFAOYSA-N	3.2×10^{-11}		Plassmann et al. (2010)	Q	
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosafluorohexacosane $C_{26}H_{29}F_{25}$ [93454-73-0] OUASUHCMZXPMCH-UHFFFAOYSA-N	1.6×10^{-13}		Plassmann et al. (2010)	Q	
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosafluorooctacosane $C_{28}H_{33}F_{25}$ [93454-74-1] CZCMNCOQMXNFTL-UHFFFAOYSA-N	8.0×10^{-14}		Plassmann et al. (2010)	Q	
fluoroethene C_2H_3F (vinyl fluoride) [75-02-5] XUCNUKMRBVNAPB-UHFFFAOYSA-N	8.2×10^{-5}		HSDB (2015)	Q	100
1,1-difluoroethene $C_2H_2F_2$ [75-38-7] BQCIDUSAKPWEOX-UHFFFAOYSA-N	2.5×10^{-5} 2.6×10^{-5} 2.8×10^{-5} 2.8×10^{-5} 5.1×10^{-5} 2.9×10^{-5} 1.6×10^{-5} 2.6×10^{-5} 2.5×10^{-5}		HSDB (2015) Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Hilal et al. (2008) Yaffe et al. (2003) Katritzky et al. (1998) Yaws (1999) Yaws and Yang (1992)	V X Q Q Q Q Q ? ?	 238 247 249, 250 21 21
trifluoroethene C_2HF_3 [359-11-5] MIZLGWKEZAPEFJ-UHFFFAOYSA-N	2.3×10^{-5}		HSDB (2015)	Q	100

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tetrafluoroethene	1.6×10^{-5}	2100	Wilhelm et al. (1977)	L	
C_2F_4	1.6×10^{-5}		HSDB (2015)	V	
[116-14-3]	1.6×10^{-5}		Yaws (2003)	X	238
BFKJFAAPBSQJPD-UHFFFAOYSA-N	9.8×10^{-6}		Irmann (1965)	C	38
	1.4×10^{-5}		Hayer et al. (2022)	Q	20
	2.8×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-5}		Gharagheizi et al. (2010)	Q	247
	1.9×10^{-5}		Hilal et al. (2008)	Q	
		2400	Kühne et al. (2005)	Q	
	2.8×10^{-5}		Yao et al. (2002)	Q	230
		2100	Kühne et al. (2005)	?	
	1.6×10^{-5}		Yaws (1999)	?	21
	1.6×10^{-5}		Yaws and Yang (1992)	?	21
3,3,3-trifluoropropene	1.3×10^{-5}		HSDB (2015)	Q	100
$C_3H_3F_3$					
[677-21-4]					
FDMFUZHCIRHGRG-UHFFFAOYSA-N					
hexafluoropropene	2.9×10^{-6}	2400	Wilhelm et al. (1977)	L	
C_3F_6	6.8×10^{-6}	2600	Maaßen (1995)	M	627
[116-15-4]	7.3×10^{-6}		Hayer et al. (2022)	Q	20
HCDGVLDPFQMKDK-UHFFFAOYSA-N	1.8×10^{-6}		HSDB (2015)	Q	100
	3.6×10^{-5}		Hilal et al. (2008)	Q	
		2800	Kühne et al. (2005)	Q	
		2400	Kühne et al. (2005)	?	
1,1,3,3,3-pentafluoro-2-(trifluoromethyl)-1-propene	2.9×10^{-7}		HSDB (2015)	Q	100
C_4F_8					
(perfluoroisobutylene)					
[382-21-8]					
DAFIBNSJXIGBQB-UHFFFAOYSA-N					
(perfluorobutyl)ethene	9.0×10^{-8}		HSDB (2015)	Q	100
$C_6H_3F_9$	8.8×10^{-8}		Zhang et al. (2010)	Q	288, 289
(4:2 FTO)	3.3×10^{-6}		Zhang et al. (2010)	Q	288, 290
[19430-93-4]	8.6×10^{-6}		Zhang et al. (2010)	Q	288, 291
GVEUEBXMTMZVSD-UHFFFAOYSA-N	3.6×10^{-7}		Zhang et al. (2010)	Q	288, 292
	2.5×10^{-6}	4100	Goss et al. (2006)	Q	
(*E*)-perfluoro(4-methyl-2-pentene)	6.4×10^{-8}		Ebert et al. (2023)	?	367
C_6F_{12}					
[3709-71-5]					
SAPOZTRFWJZUFT-OWOJBTEDSA-N					

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(perfluorohexyl)ethene $C_8H_3F_{13}$ (6:2 FTO) [25291-17-2] FYQFWFHDPNXORA-UHFFFAOYSA-N	1.1×10^{-4}	4900	Abusallout et al. (2022)	M	
	5.3×10^{-7}	4900	Goss et al. (2006)	Q	
(perfluorooctyl)ethene $C_{10}H_3F_{17}$ (8:2 FTO) [21652-58-4] NKAMGQZDVMQEJL-UHFFFAOYSA-N	1.4×10^{-7}	5700	Goss et al. (2006)	Q	
(perfluorodecyl)ethene $C_{12}H_3F_{21}$ (10:2 FTO) [30389-25-4] UCHSAVGOZUCXHC-UHFFFAOYSA-N	3.3×10^{-8}	6500	Goss et al. (2006)	Q	
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosafluorooctacos-13-ene $C_{28}H_{31}F_{25}$ LBVDHZOJOFOXJM-FOCLMDBBSA-N	8.0×10^{-11}		Plassmann et al. (2010)	Q	
fluorobenzene C_6H_5F [462-06-6] PYLWMHQQBFSUBP-UHFFFAOYSA-N	1.5×10^{-3}	4100	Brockbank (2013)	L	1
	1.6×10^{-3}		Mackay and Shiu (1981)	L	
	1.6×10^{-3}	3900	Hiatt (2013)	M	
	1.4×10^{-3}	4300	Dewulf et al. (1999)	M	
	1.1×10^{-3}		Li and Carr (1993)	M	
	1.5×10^{-3}	4400	Hartkopf and Karger (1973)	M	
	1.6×10^{-3}		Schüürmann (2000)	V	
	1.4×10^{-3}		Mackay et al. (1993)	V	
	1.6×10^{-3}		Yaws (2003)	X	238
	1.6×10^{-3}		Sieg et al. (2008)	C	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	8.6×10^{-3}		Duchowicz et al. (2020)	Q	300
	1.6×10^{-3}		Li et al. (2014)	Q	242
	2.2×10^{-3}		Li et al. (2014)	Q	242
	4.1×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.6×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.0×10^{-3}		Hilal et al. (2008)	Q	
	1.4×10^{-3}		Modarresi et al. (2007)	Q	68
		3700	Kühne et al. (2005)	Q	
	1.6×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	2.3×10^{-3}		Yao et al. (2002)	Q	230, 268

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.3×10^{-3}		Katritzky et al. (1998)	Q	
	5.0×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	1.6×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		3800	Kühne et al. (2005)	?	
	1.6×10^{-3}		Yaws (1999)	?	21
	1.2×10^{-3}		Hoff et al. (1993)	?	21
	1.6×10^{-3}		Yaws and Yang (1992)	?	21
	1.5×10^{-3}		Abraham et al. (1990)	?	
1,2-difluorobenzene	1.3×10^{-3}	3700	Brockbank (2013)	L	
$C_6H_4F_2$	1.2×10^{-3}	3500	Brockbank et al. (2013)	M	
(*o*-difluorobenzene)	1.4×10^{-3}		Yaws (2003)	X	238
[367-11-3]	3.6×10^{-3}		Gharagheizi et al. (2012)	Q	
GOYDNIKZWGIXJT-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.2×10^{-3}		Hilal et al. (2008)	Q	
	6.4×10^{-4}		Modarresi et al. (2007)	Q	68
	5.1×10^{-3}		Yao et al. (2002)	Q	230
	1.4×10^{-3}		Yaws (1999)	?	21
	1.4×10^{-3}		Yaws and Yang (1992)	?	21
1,3-difluorobenzene	3.6×10^{-3}		Gharagheizi et al. (2012)	Q	
$C_6H_4F_2$	1.3×10^{-3}		Hilal et al. (2008)	Q	
(*m*-difluorobenzene)	5.2×10^{-4}		Modarresi et al. (2007)	Q	68
[372-18-9]	1.3×10^{-4}		Yaws (1999)	?	21
UEMGWPRHOOEKTA-UHFFFAOYSA-N	1.3×10^{-4}		Yaws and Yang (1992)	?	21
1,4-difluorobenzene	1.6×10^{-3}	3900	Hiatt (2013)	M	
$C_6H_4F_2$	1.3×10^{-3}		Yaws (2003)	X	238
(*p*-difluorobenzene)	4.2×10^{-3}		Gharagheizi et al. (2012)	Q	
[540-36-3]	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
QUGUFLJIAFISSW-UHFFFAOYSA-N	1.8×10^{-3}		Hilal et al. (2008)	Q	
	3.5×10^{-4}		Modarresi et al. (2007)	Q	68
	9.5×10^{-4}		Yao et al. (2002)	Q	230
	1.3×10^{-3}		Yaws (1999)	?	21
	1.3×10^{-3}		Yaws and Yang (1992)	?	21
1,2,3,5-tetrafluorobenzene	5.1×10^{-4}		Duchowicz et al. (2020)	V	187
$C_6H_2F_4$	1.2×10^{-2}		Duchowicz et al. (2020)	Q	
[2367-82-0]	5.0×10^{-4}		Hilal et al. (2008)	Q	
UHHYOKRQTQBKSB-UHFFFAOYSA-N	9.4×10^{-5}		Modarresi et al. (2007)	Q	68
1,2,4,5-tetrafluorobenzene	5.6×10^{-4}		Duchowicz et al. (2020)	V	187
$C_6H_2F_4$	1.1×10^{-2}		Duchowicz et al. (2020)	Q	
[327-54-8]	7.0×10^{-4}		Hilal et al. (2008)	Q	
SDXUIOOHCIQXRP-UHFFFAOYSA-N	1.2×10^{-4}		Modarresi et al. (2007)	Q	68

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pentafluorobenzene C_6HF_5 [363-72-4] WACNXHCZHTVBJM-UHFFFAOYSA-N	7.5×10^{-4}	4800	Hiatt (2013)	M	
hexafluorobenzene C_6F_6 [392-56-3] ZQBFAOFFOQMSGJ-UHFFFAOYSA-N	3.0×10^{-4} 5.5×10^{-4} 2.9×10^{-4} 1.1×10^{-4}	5100 5200	Brockbank (2013) Hiatt (2013) Schröder et al. (2011) Schröder et al. (2011)	L M M Q	1 628
(trifluoromethyl)-benzene $C_6H_5CF_3$ (α,α,α-trifluorotoluene; benzotrifluoride) [98-08-8] GETTZEONDQJALK-UHFFFAOYSA-N	6.0×10^{-4} 5.8×10^{-4} 6.1×10^{-4} 6.2×10^{-4} 5.9×10^{-4} 3.5×10^{-3} 3.2×10^{-3} 7.8×10^{-3} 1.2×10^{-3} 2.0×10^{-4} 5.7×10^{-4} 1.3×10^{-3} 2.7×10^{-4} 6.2×10^{-3} 6.1×10^{-4} 1.9×10^{-2} 6.0×10^{-4} 6.0×10^{-4}		Duchowicz et al. (2020) HSDB (2015) Abraham et al. (1994a) Mackay and Shiu (1981) Yaws (2003) Duchowicz et al. (2020) Gharagheizi et al. (2012) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Gharagheizi et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Yaffe et al. (2003) Yaffe et al. (2003) Nirmalakhandan et al. (1997) Yaws (1999) Yaws and Yang (1992)	V V V V X Q Q Q Q Q Q Q Q Q Q Q ? ?	187 238 243, 244 245 246 247 68 249, 250 249, 250 21 21
decafluorobiphenyl $C_{10}F_{10}$ [434-90-2] ONUFSRWQCKNVSL-UHFFFAOYSA-N	6.7×10^{-3}	3600	Hiatt (2013)	M	
carbonyl fluoride COF_2 [353-50-4] IYRWEQXVUNLMAY-UHFFFAOYSA-N	3.5×10^{-1} 9.9×10^{-3} 2.0×10^{-1}		Mirabel et al. (1996) De Bruyn et al. (1995a) George et al. (1993)	M M X	 451 629
formyl fluoride FCHO [1493-02-3] NHGVZTMBVDFPHJ-UHFFFAOYSA-N	3.0×10^{-2}		Kanakidou et al. (1995)	E	

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-fluoroethanol	4.6×10^{-1}		Burkholder et al. (2019)	L	
C_2H_5FO	4.6×10^{-1}		Burkholder et al. (2015)	L	
[371-62-0]	4.6×10^{-1}		O'Farrell and Waghorne (2010)	M	
GGDYAKVUZMZKRV-UHFFFAOYSA-N	5.5		Duchowicz et al. (2020)	V	187
	1.9		Duchowicz et al. (2020)	Q	
	1.4		HSDB (2015)	Q	100
	2.5		Hilal et al. (2008)	Q	
	5.6		Modarresi et al. (2007)	Q	68
2,2-difluoroethanol	9.3×10^{-1}		Burkholder et al. (2019)	L	
$C_2H_4F_2O$	9.3×10^{-1}		Burkholder et al. (2015)	L	
[359-13-7]	9.2×10^{-1}		O'Farrell and Waghorne (2010)	M	
VOGSDFLJZPNWHY-UHFFFAOYSA-N					
2,2,2-trifluoroethanol	4.7×10^{-1}	6200	Burkholder et al. (2019)	L	
CF_3CH_2OH	4.7×10^{-1}	6200	Burkholder et al. (2015)	L	
[75-89-8]	4.7×10^{-1}	6200	Sander et al. (2011)	L	
RHQDFWAXVIIEBN-UHFFFAOYSA-N	4.7×10^{-1}	6200	Chen et al. (2003)	M	
	4.3×10^{-1}		Eger et al. (1999)	M	14
	5.8×10^{-1}	5900	Rochester and Symonds (1973)	M	
	3.4×10^{-1}		Keshavarz et al. (2022)	Q	
	8.6×10^{-1}		Duchowicz et al. (2020)	Q	
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	3.5×10^{-1}		Zhang et al. (2010)	Q	288, 289
	2.4×10^{-1}		Zhang et al. (2010)	Q	288, 290
	3.8		Zhang et al. (2010)	Q	288, 291
	4.7×10^{-2}		Zhang et al. (2010)	Q	288, 292
	6.1×10^{-1}		Hilal et al. (2008)	Q	
	3.4		Modarresi et al. (2007)	Q	68
		6500	Kühne et al. (2005)	Q	
	7.7×10^{-1}		Goss (2005)	Q	630
	6.1×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	6.9×10^{-1}		English and Carroll (2001)	Q	231, 232
	1.6×10^{-2}		Katritzky et al. (1998)	Q	
	5.0×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	5.7×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		5600	Kühne et al. (2005)	?	
	5.7×10^{-1}		Abraham et al. (1990)	?	
1,1,1-trifluoro-2-propanol	1.3×10^{-1}		Eger et al. (1999)	M	14
$CF_3CHOHCH_3$	4.5×10^{-1}	6300	Rochester and Symonds (1973)	M	
[374-01-6]	4.6×10^{-1}		Keshavarz et al. (2022)	Q	
GILIYJDBJZWGBG-UHFFFAOYSA-N	1.1		Duchowicz et al. (2020)	Q	185
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	246

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	4.9×10^{-1}		Modarresi et al. (2007)	Q	68
		6900	Kühne et al. (2005)	Q	
	5.2×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	4.5×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		6300	Kühne et al. (2005)	?	
2,2,3,3-tetrafluoro-1-propanol	1.4	7000	Burkholder et al. (2019)	L	
$CHF_2CF_2CH_2OH$	1.4	7000	Burkholder et al. (2015)	L	
[76-37-9]	1.4	7000	Sander et al. (2011)	L	
NBUKAOOFKZFCGD-UHFFFAOYSA-N	1.4	7000	Chen et al. (2003)	M	
	7.5×10^{-1}		Eger et al. (1999)	M	14
	1.6	6700	Rochester and Symonds (1973)	M	
	4.6×10^{-1}		Keshavarz et al. (2022)	Q	
	8.3×10^{-1}		Duchowicz et al. (2020)	Q	
	1.2		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	6.0×10^{-1}		Hilal et al. (2008)	Q	
	1.0		Modarresi et al. (2007)	Q	68
		6900	Kühne et al. (2005)	Q	
	3.7×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	1.6		Duchowicz et al. (2020)	?	186, 21
		6600	Kühne et al. (2005)	?	
2,2,3,3,3-pentafluoro-1-propanol	1.4×10^{-1}	4300	Burkholder et al. (2019)	L	
$CF_3CF_2CH_2OH$	1.4×10^{-1}	4300	Burkholder et al. (2015)	L	
[422-05-9]	1.4×10^{-1}	4300	Sander et al. (2011)	L	
PSQZJKGXDGNDFP-UHFFFAOYSA-N	1.4×10^{-1}	4300	Chen et al. (2003)	M	
	6.9×10^{-2}		Eger et al. (1999)	M	14
	4.5×10^{-1}	6000	Rochester and Symonds (1973)	M	
	4.6×10^{-1}		Keshavarz et al. (2022)	Q	
	1.8×10^{-1}		Duchowicz et al. (2020)	Q	185
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.3×10^{-1}		Hilal et al. (2008)	Q	
	4.8×10^{-1}		Modarresi et al. (2007)	Q	68
		6800	Kühne et al. (2005)	Q	
	4.4×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		6000	Kühne et al. (2005)	?	

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1,1,3,3,3-hexafluoro-2-propanol	1.0×10^{-1}		Eger et al. (1999)	M	14
$CF_3CHOHCF_3$	2.4×10^{-1}	6700	Rochester and Symonds (1973)	M	
[920-66-1]	4.6×10^{-1}		Keshavarz et al. (2022)	Q	
BYEAHWXPCBROCE-UHFFFAOYSA-N	2.2		Duchowicz et al. (2020)	Q	
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	2.5×10^{-2}		Hilal et al. (2008)	Q	
	2.6×10^{-1}		Modarresi et al. (2007)	Q	68
		6800	Kühne et al. (2005)	Q	
	2.4×10^{-1}		Goss (2005)	Q	631
	2.3×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	2.3×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		6700	Kühne et al. (2005)	?	
	2.3×10^{-1}		Abraham et al. (1990)	?	
trifluoroacetylfluoride	3.0×10^{-2}		Mirabel et al. (1996)	M	
CF_3COF	9.5×10^{-3}		De Bruyn et al. (1995a)	M	451
[354-34-7]	3.0×10^{-2}		George et al. (1994b)	M	632
DCEPGADSNJKOJK-UHFFFAOYSA-N	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	4.3×10^{-3}		Duchowicz et al. (2020)	Q	
	3.0×10^{-2}		Duchowicz et al. (2020)	?	186, 21
1-fluoro-2-propanone	4.6×10^{-1}		Burkholder et al. (2019)	L	
CH_2FCOCH_3	4.6×10^{-1}		Burkholder et al. (2015)	L	
(fluoroacetone)	4.6×10^{-1}		O'Farrell and Waghorne (2010)	M	
[430-51-3]					
MSWVMWGCNZQPIA-UHFFFAOYSA-N					
1,1,1-trifluoro-2-propanone	1.4	8900	Burkholder et al. (2019)	L	
CF_3COCH_3	1.4	8900	Burkholder et al. (2015)	L	
(1,1,1-trifluoroacetone)	1.4	8900	Sander et al. (2011)	L	
[421-50-1]	1.4	8900	Betterton (1991)	M	
FHUDAMLDXFJHJE-UHFFFAOYSA-N	1.4		Keshavarz et al. (2022)	Q	
	1.8×10^{-2}		Duchowicz et al. (2020)	Q	
	4.9		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	4.4×10^{-2}		Modarresi et al. (2007)	Q	68
	1.3		Duchowicz et al. (2020)	?	186, 21
1,1-difluoro-2-methoxyethane	1.3×10^{-2}		Duchowicz et al. (2020)	V	187
$C_3H_6F_2O$	2.2×10^{-2}		Duchowicz et al. (2020)	Q	
[461-57-4]					
CRGZRXUKXVTRNO-UHFFFAOYSA-N					

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
fluoroethanoic acid	8.0×10^{2}		Burkholder et al. (2019)	L	
CH_2FCOOH	8.0×10^{2}		Burkholder et al. (2015)	L	
(fluoroacetic acid)	8.0×10^{2}		Sander et al. (2011)	L	
[144-49-0]	8.0×10^{2}		Bowden et al. (1998a)	M	
QEWYKACRFQMRMB-UHFFFAOYSA-N	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	6.7×10^{1}		Duchowicz et al. (2020)	Q	185
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	272, 244
	9.9×10^{2}		Raventos-Duran et al. (2010)	Q	245
	9.9		Raventos-Duran et al. (2010)	Q	246
	5.4×10^{2}		Hilal et al. (2008)	Q	
	8.0×10^{2}		Duchowicz et al. (2020)	?	186, 21
difluoroethanoic acid	3.0×10^{2}	6900	Burkholder et al. (2019)	L	
CHF_2COOH	3.0×10^{2}	6900	Burkholder et al. (2015)	L	
(difluoroacetic acid)	3.0×10^{2}	6900	Sander et al. (2011)	L	
[381-73-7]	3.0×10^{2}	6900	Bowden et al. (1998a)	M	
PBWZKZYHONABLN-UHFFFAOYSA-N	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	8.5×10^{1}		Duchowicz et al. (2020)	Q	300
	4.9×10^{2}		Raventos-Duran et al. (2010)	Q	243, 244
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	4.9		Raventos-Duran et al. (2010)	Q	246
	7.2×10^{1}		Hilal et al. (2008)	Q	
		7700	Kühne et al. (2005)	Q	
	3.0×10^{2}		Duchowicz et al. (2020)	?	186, 21
		6900	Kühne et al. (2005)	?	
trifluoroethanoic acid	5.7×10^{1}	4100	Burkholder et al. (2019)	L	
CF_3COOH	5.7×10^{1}	4100	Burkholder et al. (2015)	L	
(trifluoroacetic acid)	8.9×10^{1}	9300	Sander et al. (2011)	L	
[76-05-1]	5.7×10^{1}	4100	Kutsuna and Hori (2008a)	M	
DTQVDTLACAAQTR-UHFFFAOYSA-N	8.3×10^{1}		Kwan (2001)	M	633
	8.8×10^{1}	9300	Bowden et al. (1996)	M	
	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	2.3		Abusallout et al. (2022)	Q	634
	1.9×10^{1}		Duchowicz et al. (2020)	Q	185
	6.2×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.5		Raventos-Duran et al. (2010)	Q	246
	2.3		Zhang et al. (2010)	Q	288, 289
	1.6×10^{-1}		Zhang et al. (2010)	Q	288, 290
	8.0		Zhang et al. (2010)	Q	288, 291
	3.9		Zhang et al. (2010)	Q	288, 292
	4.0×10^{-1}		Hilal et al. (2008)	Q	
	6.3×10^{1}		Modarresi et al. (2007)	Q	68
		7700	Kühne et al. (2005)	Q	
	8.9×10^{1}		Duchowicz et al. (2020)	?	186, 21
		9400	Kühne et al. (2005)	?	

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
perfluoropropanoic acid	8.8		Kwan (2001)	M	633
$C_3HF_5O_2$	4.3×10^{-1}		Abusallout et al. (2022)	Q	634
[422-64-0]					
LRMSQVBRUNSOJL-UHFFFAOYSA-N					
perfluorobutanoic acid	8.1×10^{-1}		Kwan (2001)	M	633
$C_4HF_7O_2$	8.2×10^{-2}		Abusallout et al. (2022)	Q	634
[375-22-4]	8.2×10^{-2}		Zhang et al. (2010)	Q	288, 289
YPJUNDFVDDCYIH-UHFFFAOYSA-N	7.2×10^{-1}		Zhang et al. (2010)	Q	288, 290
	2.5×10^{-1}		Zhang et al. (2010)	Q	288, 291
	6.4×10^{-1}		Zhang et al. (2010)	Q	288, 292
perfluoropentanoic acid	6.7×10^{-1}		Kwan (2001)	M	633
$C_5HF_9O_2$	1.6×10^{-2}		Abusallout et al. (2022)	Q	634
[2706-90-3]					
CXZGQIAOTKWCDB-UHFFFAOYSA-N					
perfluorohexanoic acid	1.1		Kwan (2001)	M	633
$C_6HF_{11}O_2$	3.0×10^{-3}		Abusallout et al. (2022)	Q	634
[307-24-4]	4.4×10^{-1}		Arp et al. (2006)	Q	635
PXUULQAPEKKVAH-UHFFFAOYSA-N	1.2×10^{-1}		Arp et al. (2006)	Q	636
perfluoroheptanoic acid	1.7		Kwan (2001)	M	633
$C_7HF_{13}O_2$	5.8×10^{-4}		Abusallout et al. (2022)	Q	634
[375-85-9]	5.7×10^{-4}		Zhang et al. (2010)	Q	288, 289
ZWBAMYVPMDSJGQ-UHFFFAOYSA-N	5.0×10^{-2}		Zhang et al. (2010)	Q	288, 290
	2.2×10^{-2}		Zhang et al. (2010)	Q	288, 291
	5.6×10^{-3}		Zhang et al. (2010)	Q	288, 292
	1.8×10^{-1}		Arp et al. (2006)	Q	635
	5.7×10^{-2}		Arp et al. (2006)	Q	636
pentadecafluorooctanoic acid	4.9×10^{-2}		Kutsuna and Hori (2008b)	M	
$C_8HF_{15}O_2$	4.0×10^{-1}		Li et al. (2007)	M	
(perfluorooctanoic acid; PFOA)	2.8		Kwan (2001)	M	633
[335-67-1]	1.1×10^{-4}		Abusallout et al. (2022)	Q	634
SNGREZUHAYWORS-UHFFFAOYSA-N	1.1×10^{-4}		Zhang et al. (2010)	Q	288, 289
	1.0×10^{-2}		Zhang et al. (2010)	Q	288, 290
	1.2×10^{-2}		Zhang et al. (2010)	Q	288, 291
	1.1×10^{-3}		Zhang et al. (2010)	Q	288, 292
	1.1×10^{-4}		Zhang et al. (2010)	Q	288, 289
	1.0×10^{-2}		Zhang et al. (2010)	Q	288, 290
	2.1×10^{-2}		Zhang et al. (2010)	Q	288, 291
	1.1×10^{-3}		Zhang et al. (2010)	Q	288, 292
	9.5×10^{-2}		Arp et al. (2006)	Q	635
	2.0×10^{-2}		Arp et al. (2006)	Q	636

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
perfluorononanoic acid $C_9HF_{17}O_2$ [375-95-1] UZUFPBIDKMEQEQ-UHFFFAOYSA-N	4.3×10^{-2} 5.3×10^{-3}		Arp et al. (2006) Arp et al. (2006)	Q Q	635 636
2H,2H-perfluorodecanoic acid $C_{10}H_3F_{17}O_2$ (8:2 FTCA) [27854-31-5] XTBXSCIWOVSSGB-UHFFFAOYSA-N	5.8×10^{-4}		Abusallout et al. (2022)	M	
perfluorodecanoic acid $C_{10}HF_{19}O_2$ [335-76-2] PCIUEQPBYFRTEM-UHFFFAOYSA-N	2.5×10^{-2} 1.1×10^{-3}		Arp et al. (2006) Arp et al. (2006)	Q Q	635 636
perfluoroundecanoic acid $C_{11}HF_{21}O_2$ [2058-94-8] SIDINRCMMRKXGQ-UHFFFAOYSA-N	1.3×10^{-2} 1.9×10^{-4}		Arp et al. (2006) Arp et al. (2006)	Q Q	635 636
perfluorododecanoic acid $C_{12}HF_{23}O_2$ [307-55-1] CXGONMQFMIYUJR-UHFFFAOYSA-N	6.4×10^{-3}		Plassmann et al. (2011)	E	
perfluorotetradecanoic acid $C_{14}HF_{27}O_2$ [376-06-7] RUDINRUXCKIXAJ-UHFFFAOYSA-N	1.6×10^{-3}		Plassmann et al. (2011)	E	
1,1,1,3,3,3-hexafluoro-2-propanone C_3F_6O [684-16-2] VBZWSGALLODQNC-UHFFFAOYSA-N	3.2×10^{-3}		HSDB (2015)	Q	100
desflurane $C_3H_2F_6O$ [57041-67-5] DPYMFVXJLLWWEU-UHFFFAOYSA-N	1.4×10^{-4} 9.0×10^{-5}		HSDB (2015) Abraham and Weathersby (1994)	Q ?	100 21
sevoflurane $C_4H_3F_7O$ [28523-86-6] DFEYYRMXOJXZRJ-UHFFFAOYSA-N	5.2×10^{-5} 1.5×10^{-4}		HSDB (2015) Abraham and Weathersby (1994)	Q ?	100 21
ethyl 2,2,2-trifluoroethyl ether $C_4H_7F_3O$ [461-24-5] ZKNHDJMXIUOHLX-UHFFFAOYSA-N	7.2×10^{-4}		Hilal et al. (2008)	Q	

Table A5.1: Organic fluorine (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
iso-indoklon $C_4H_4F_6O$ (1,1,1,3,3,3-hexafluoro-2-methoxypropane) [13171-18-1] VNXYDFNVQBICRO-UHFFFAOYSA-N	5.6×10^{-5}		Abraham and Weathersby (1994)	?	21
di(2,2,2-trifluoroethyl) ether $C_4H_4F_6O$ (flurothyl) [333-36-8] KGPPDNUWZNWPSI-UHFFFAOYSA-N	9.2×10^{-3} 3.0×10^{-4}	-390	Fukuchi et al. (2002) Abraham and Weathersby (1994)	V ?	33 21
(2,2,2-trifluoroethoxy)-ethene $CF_3CH_2OCHCH_2$ (fluoroxene; fluroxene) [406-90-6] DLEGDLSLRSOURQ-UHFFFAOYSA-N	5.4×10^{-4} 3.3×10^{-4} 5.5×10^{-4} 5.5×10^{-4} 3.2×10^{-4} 3.3×10^{-4} 9.5×10^{-5} 3.6×10^{-4} 5.1×10^{-4}	4000 4000 4300 	Fogg and Sangster (2003) Steward et al. (1973) Allott et al. (1973) Smith et al. (1981b) Stoelting and Longshore (1972) Munson et al. (1964) Hilal et al. (2008) Abraham and Weathersby (1994) Abraham et al. (1990)	L L L M M M Q ? ?	 14 14 14 21
2,2,2-trifluoroethyl methanoate $HCOOCH_2CF_3$ [32042-38-9] CAFROQYMUICGNO-UHFFFAOYSA-N	5.4×10^{-3} 5.4×10^{-3} 5.4×10^{-3} 5.4×10^{-3}	4700 4700 4700 4700	Burkholder et al. (2019) Burkholder et al. (2015) Sander et al. (2011) Kutsuna et al. (2005)	L L L M	
2,2,2-trifluoroethyl ethanoate $CH_3COOCH_2CF_3$ [406-95-1] ZOWSJJBOQDKOHI-UHFFFAOYSA-N	5.5×10^{-3} 5.5×10^{-3} 5.5×10^{-3} 5.7×10^{-3}	5200 5200 5200 5300 6400 5500	Burkholder et al. (2019) Burkholder et al. (2015) Sander et al. (2011) Kutsuna et al. (2004) Kühne et al. (2005) Kühne et al. (2005)	L L L M Q ?	637 638
trifluoroethanoic acid, methyl ester CF_3COOCH_3 (methyl trifluoroacetate) [431-47-0] VMVNZNXAVJHNDJ-UHFFFAOYSA-N	1.1×10^{-3} 1.1×10^{-3} 1.1×10^{-3} 1.2×10^{-3}	5300 5300 5300 4900 6100 5800	Burkholder et al. (2019) Burkholder et al. (2015) Sander et al. (2011) Kutsuna et al. (2004) Kühne et al. (2005) Kühne et al. (2005)	L L L M Q ?	639, 640 641, 642 643
trifluoroethanoic acid, ethyl ester $CF_3COOC_2H_5$ (ethyl trifluoroacetate) [383-63-1] STSCVKRWJPWALQ-UHFFFAOYSA-N	8.9×10^{-4} 8.9×10^{-4} 8.9×10^{-4} 7.1×10^{-4} 8.9×10^{-4}	4900 4900 4900 4900 4900	Burkholder et al. (2019) Burkholder et al. (2015) Sander et al. (2011) Kutsuna and Kaneyasu (2021) Kutsuna et al. (2005)	L L L M M	

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
trifluoro(trifluoromethyl)-oxirane C_3F_6O [428-59-1] PGFXOWRDDHCDTE-UHFFFAOYSA-N	9.3×10^{-6}	2400	Clever et al. (2005)	C	644, 645
3,3,4,4,4-pentafluorobutan-1-ol $C_4H_5OF_5$ [54949-74-5] JPMHUDBOKDBBLG-UHFFFAOYSA-N	5.1×10^{-2} 3.7×10^{-1} 4.0×10^{-2} 1.5×10^{-3}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
1,1,1,3,3,3-hexafluoro-2-methyl-2-propanol $C_4H_4F_6O$ [1515-14-6] FQDXJYBXPOMIBX-UHFFFAOYSA-N	1.8×10^{-2}		Eger et al. (1999)	M	14
2,2,3,4,4,4-hexafluoro-1-butanol $C_4H_4F_6O$ [382-31-0] LVFXLZRISXUAIL-UHFFFAOYSA-N	3.2×10^{-1}		Eger et al. (1999)	M	14
2,2,3,3,4,4,4-heptafluoro-1-butanol $C_4H_3F_7O$ [375-01-9] WXJFKAZDSQLPBX-UHFFFAOYSA-N	2.1×10^{-2}		Eger et al. (1999)	M	14
3,3,4,4,5,5,5-heptafluoro-2-pentanol $C_5H_5F_7O$ [375-14-4] RBPHBIMHZSTIDT-UHFFFAOYSA-N	9.0×10^{-3}		Eger et al. (1999)	M	14
2,2,3,3,4,4,5,5-octafluoro-1-pentanol $C_5H_4F_8O$ [355-80-6] JUGSKHLZINSXPQ-UHFFFAOYSA-N	2.5×10^{-1}		Eger et al. (1999)	M	14
1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxybutane $C_5H_3F_9O$ [163702-07-6] OKIYQFLILPKULA-UHFFFAOYSA-N	9.9×10^{-6} 1.3×10^{-5} 8.4×10^{-6} 3.9×10^{-6}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
1-ethoxy-1,1,2,3,3,3-hexafluoro-2-(trifluoromethyl)propane $C_6H_5F_9O$ [163702-06-5] SQEGLLMNIBLLNQ-UHFFFAOYSA-N	7.5×10^{-6} 4.7×10^{-5} 8.0×10^{-6} 3.3×10^{-6}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1H,1H,2H,2H-perfluorohexan-1-ol	1.3×10^{-3}		Abusallout et al. (2022)	M	
$C_6H_5F_9O$	6.6×10^{-3}	4500	Wu and Chang (2011)	M	11
(4:2 FTOH)	1.3×10^{-2}		Goss et al. (2006)	M	
[2043-47-2]	6.1×10^{-5}	5400	Lei et al. (2004)	M	329
JCMNMOBHVPONLD-UHFFFAOYSA-N	5.6×10^{-1}		Wu and Chang (2011)	V	
	1.8×10^{-3}		Abusallout et al. (2022)	Q	634
	1.8×10^{-3}		Zhang et al. (2010)	Q	288, 289
	1.3×10^{-1}		Zhang et al. (2010)	Q	288, 290
	8.2×10^{-3}		Zhang et al. (2010)	Q	288, 291
	2.4×10^{-4}		Zhang et al. (2010)	Q	288, 292
	4.3×10^{-4}		Arp et al. (2006)	Q	635
	3.1×10^{-5}		Arp et al. (2006)	Q	636
	7.2×10^{-3}	7200	Goss et al. (2006)	Q	
2,2,3,3,4,4,5,5,6,6,6-undecafluoro-1-hexanol $C_6H_3F_{11}O$ [423-46-1] QZFZPVVDBGXQTB-UHFFFAOYSA-N	1.7×10^{-3}		Eger et al. (1999)	M	14
1-ethoxy-1,1,2,2,3,3,4,4,4-nonafluorobutane	7.5×10^{-6}		Zhang et al. (2010)	Q	288, 289
$C_6H_5F_9O$	1.2×10^{-5}		Zhang et al. (2010)	Q	288, 290
[163702-05-4]	7.5×10^{-6}		Zhang et al. (2010)	Q	288, 291
DFUYAWQUODQGFF-UHFFFAOYSA-N	3.0×10^{-6}		Zhang et al. (2010)	Q	288, 292
2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro-1-heptanol $C_7H_4F_{12}O$ [335-99-9] BYKNGMLDSIEFFG-UHFFFAOYSA-N	6.4×10^{-2}		Eger et al. (1999)	M	14
2,2,3,3,4,4,5,5,6,6,7,7,7-tridecafluoro-1-heptanol $C_7H_3F_{13}O$ [375-82-6] STLNAVFVCIRZLL-UHFFFAOYSA-N	6.0×10^{-4}		Eger et al. (1999)	M	14
1H,1H,2H,2H-perfluoro-1-octanol	3.3×10^{-4}	4700	Abusallout et al. (2022)	M	
$C_8H_5F_{13}O$	1.7×10^{-4}	2600	Wu and Chang (2011)	M	11
(6:2 FTOH)	1.5×10^{-3}		Goss et al. (2006)	M	
[647-42-7]	8.5×10^{-5}	7000	Lei et al. (2004)	M	329
GRJRKPMIRMSBNK-UHFFFAOYSA-N	9.4×10^{-4}		Eger et al. (1999)	M	14
	3.9×10^{-1}		Wu and Chang (2011)	V	
	6.6×10^{-5}		Abusallout et al. (2022)	Q	634
	6.5×10^{-5}		Zhang et al. (2010)	Q	288, 289
	9.5×10^{-3}		Zhang et al. (2010)	Q	288, 290
	3.4×10^{-3}		Zhang et al. (2010)	Q	288, 291
	9.9×10^{-6}		Zhang et al. (2010)	Q	288, 292

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.8×10^{-4}		Arp et al. (2006)	Q	635
	1.8×10^{-5}		Arp et al. (2006)	Q	636
	1.8×10^{-3}	8000	Goss et al. (2006)	Q	
2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-1-octanol $C_8H_3F_{15}O$ [307-30-2] PJDOLCGOTSNFJM-UHFFFAOYSA-N	2.3×10^{-4}		Eger et al. (1999)	M	14
3-ethoxyperfluoro(2-methylhexane) $C_9H_5F_{15}O$ [297730-93-9] HHBBIOLEJRWIGU-UHFFFAOYSA-N	1.9×10^{-8}		Ebert et al. (2023)	?	367
methyl perfluoro(8-(fluoroformyl)-5-methyl-4,7-dioxanonanoate)	5.8×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{10}H_3F_{15}O_5$	5.1×10^{-4}		Zhang et al. (2010)	Q	288, 290
[69116-73-0]	2.6×10^{-4}		Zhang et al. (2010)	Q	288, 291
JOMJXRTUQWIHQD-UHFFFAOYSA-N	1.3×10^{-1}		Zhang et al. (2010)	Q	288, 292
3,3,4,4,5,5,6,6,6-nonafluorohexyl methacrylate	3.4×10^{-5}		Zhang et al. (2010)	Q	288, 289
$C_{10}H_9F_9O_2$	1.6×10^{-3}		Zhang et al. (2010)	Q	288, 290
[1799-84-4]	6.5×10^{-4}		Zhang et al. (2010)	Q	288, 291
TYNRPOFACABVSI-UHFFFAOYSA-N	3.4×10^{-5}		Zhang et al. (2010)	Q	288, 292
1H,1H,2H,2H-perfluorodecan-1-ol	2.0×10^{-4}		Abusallout et al. (2022)	M	
$C_{10}H_5F_{17}O$	2.0×10^{-4}	3100	Wu and Chang (2011)	M	11
(8:2 FTOH)	1.7×10^{-4}	8800	Lei et al. (2004)	M	329
[678-39-7]	2.4×10^{-1}		Wu and Chang (2011)	V	
JJUBFBTUBACDHW-UHFFFAOYSA-N	1.1×10^{-4}		Goss et al. (2006)	V	
	2.4×10^{-6}		Abusallout et al. (2022)	Q	634
	2.4×10^{-6}		Zhang et al. (2010)	Q	288, 289
	2.6×10^{-4}		Zhang et al. (2010)	Q	288, 290
	7.3×10^{-4}		Zhang et al. (2010)	Q	288, 291
	4.3×10^{-7}		Zhang et al. (2010)	Q	288, 292
	5.7×10^{-5}		Arp et al. (2006)	Q	635
	1.6×10^{-5}		Arp et al. (2006)	Q	636
	3.8×10^{-4}	8600	Goss et al. (2006)	Q	
2-methoxyperfluoro(2,5-di(propan-2-yl)oxolane) $C_{11}H_3F_{19}O_2$ [957209-18-6] YRGYOFYTTFLPQM-UHFFFAOYSA-N	1.0×10^{-8}		Ebert et al. (2023)	?	367

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl acrylate	1.9×10^{-6}		Zhang et al. (2010)	Q	288, 289
$C_{11}H_7F_{13}O_2$	1.9×10^{-4}		Zhang et al. (2010)	Q	288, 290
[17527-29-6]	2.9×10^{-4}		Zhang et al. (2010)	Q	288, 291
VPKQPPJQTZJZDB-UHFFFAOYSA-N	2.4×10^{-6}		Zhang et al. (2010)	Q	288, 292
2-(perfluorohexyl)ethyl methacrylate	1.2×10^{-6}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_9F_{13}O_2$	1.8×10^{-4}		Zhang et al. (2010)	Q	288, 290
[2144-53-8]	1.3×10^{-4}		Zhang et al. (2010)	Q	288, 291
CDXFIRXEAJABAZ-UHFFFAOYSA-N	1.5×10^{-6}		Zhang et al. (2010)	Q	288, 292
1,1,2,2-tetrahydroperfluoro dodecanol	1.4×10^{-4}		Abusallout et al. (2022)	M	
$C_{12}H_5F_{21}O$	1.3×10^{-4}	2700	Wu and Chang (2011)	M	11
(10:2 FTOH)	2.5×10^{-1}		Wu and Chang (2011)	V	
[865-86-1]	9.0×10^{-8}		Abusallout et al. (2022)	Q	634
FLXYIZWPNQYPIT-UHFFFAOYSA-N	8.6×10^{-8}		Zhang et al. (2010)	Q	288, 289
	2.7×10^{-6}		Zhang et al. (2010)	Q	288, 290
	1.5×10^{-4}		Zhang et al. (2010)	Q	288, 291
	1.6×10^{-8}		Zhang et al. (2010)	Q	288, 292
	4.6×10^{-5}		Arp et al. (2006)	Q	635
	5.2×10^{-5}		Arp et al. (2006)	Q	636
	1.0×10^{-4}	9600	Goss et al. (2006)	Q	
	1.0×10^{-5}		Arp et al. (2006)	E	646
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl acrylate	1.3×10^{-3}		Abusallout et al. (2022)	M	
$C_{13}H_7F_{17}O_2$	7.0×10^{-8}		Zhang et al. (2010)	Q	288, 289
[27905-45-9]	1.1×10^{-5}		Zhang et al. (2010)	Q	288, 290
QUKRIOLKOHUUBM-UHFFFAOYSA-N	1.1×10^{-4}		Zhang et al. (2010)	Q	288, 291
	9.9×10^{-8}		Zhang et al. (2010)	Q	288, 292
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl methacrylate	4.4×10^{-8}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_9F_{17}O_2$	1.0×10^{-5}		Zhang et al. (2010)	Q	288, 290
[1996-88-9]	5.4×10^{-5}		Zhang et al. (2010)	Q	288, 291
HBZFBSFGXQBQTB-UHFFFAOYSA-N	6.4×10^{-8}		Zhang et al. (2010)	Q	288, 292
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecan-1-ol	3.1×10^{-9}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_5F_{25}O$	1.1×10^{-8}		Zhang et al. (2010)	Q	288, 290
[39239-77-5]	3.1×10^{-5}		Zhang et al. (2010)	Q	288, 291
QBBJBWKVSJWYQK-UHFFFAOYSA-N	6.9×10^{-10}		Zhang et al. (2010)	Q	288, 292

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-(perfluorodecyl)ethyl acrylate	2.5×10^{-9}		Zhang et al. (2010)	Q	288, 289
$C_{15}H_7F_{21}O_2$	3.1×10^{-7}		Zhang et al. (2010)	Q	288, 290
[17741-60-5]	2.4×10^{-5}		Zhang et al. (2010)	Q	288, 291
FIAHOPQKBBASOY-UHFFFAOYSA-N	3.7×10^{-9}		Zhang et al. (2010)	Q	288, 292
1,1,2,2-tetrahydroperfluoro-1-hexadecanol	1.1×10^{-10}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_5OF_{29}$	1.4×10^{-11}		Zhang et al. (2010)	Q	288, 290
[60699-51-6]	6.1×10^{-6}		Zhang et al. (2010)	Q	288, 291
ZDUOTHMDVYXZBS-UHFFFAOYSA-N	2.9×10^{-11}		Zhang et al. (2010)	Q	288, 292
2-(perfluorodecyl)ethyl methacrylate	1.6×10^{-9}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_9F_{21}O_2$	3.1×10^{-7}		Zhang et al. (2010)	Q	288, 290
[2144-54-9]	1.1×10^{-5}		Zhang et al. (2010)	Q	288, 291
FQHLOOOXLDQLPF-UHFFFAOYSA-N	2.4×10^{-9}		Zhang et al. (2010)	Q	288, 292
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecyl prop-2-enoate	9.0×10^{-11}		Zhang et al. (2010)	Q	288, 289
$C_{17}H_7F_{25}O_2$	5.0×10^{-9}		Zhang et al. (2010)	Q	288, 290
[34395-24-9]	2.7×10^{-3}		Zhang et al. (2010)	Q	288, 291
SWTZSHBOMGAQKX-UHFFFAOYSA-N	1.6×10^{-10}		Zhang et al. (2010)	Q	288, 292
profluthrin $C_{17}H_{18}F_4O_2$ [223419-20-3] AGMMRUPNXPWLGF-AATRIKPKSA-N	2.5×10^{-2}		Ebert et al. (2023)	?	319
2-perfluorododecylethyl methacrylate	5.8×10^{-11}		Zhang et al. (2010)	Q	288, 289
$C_{18}H_9F_{25}O_2$	5.0×10^{-9}		Zhang et al. (2010)	Q	288, 290
[6014-75-1]	2.3×10^{-6}		Zhang et al. (2010)	Q	288, 291
LFEGLDRNIDJMKB-UHFFFAOYSA-N	9.9×10^{-11}		Zhang et al. (2010)	Q	288, 292
1,1,2,2-tetrahydroperfluoro-1-octadecanol	4.1×10^{-12}		Zhang et al. (2010)	Q	288, 289
$C_{18}H_5OF_{33}$	6.7×10^{-15}		Zhang et al. (2010)	Q	288, 290
[65104-67-8]	1.2×10^{-6}		Zhang et al. (2010)	Q	288, 291
UYSGWTCETIRUHO-UHFFFAOYSA-N	1.1×10^{-12}		Zhang et al. (2010)	Q	288, 292
metofluthrin $C_{18}H_{20}F_4O_3$ [240494-70-6] KVIZNNVXXNFLMU-AATRIKPKSA-N	1.0		HSDB (2015)	V	

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1,2,2- tetrahydroperfluorohexadecyl acrylate	3.3×10^{-12}		Zhang et al. (2010)	Q	288, 289
$C_{19}H_7F29O_2$	4.1×10^{-11}		Zhang et al. (2010)	Q	288, 290
[34362-49-7]	6.5×10^{-4}		Zhang et al. (2010)	Q	288, 291
KLOHTAIHCCMZIL-UHFFFAOYSA-N	6.9×10^{-12}		Zhang et al. (2010)	Q	288, 292
fluoxymesterone $C_{20}H_{29}FO_3$ [76-43-7] YLRFCQOZQXIBAB-YXVJBPKESA-N	1.6×10^{4}		HSDB (2015)	Q	100
dexamethasone $C_{22}H_{29}FO_5$ [50-02-2] UREBDLICKHMUKA-GCMAGEFQSA-N	1.4×10^{2}		HSDB (2015)	Q	100
1,1,2,2-tetrahydroperfluoroeicosyl alcohol	1.5×10^{-13}		Zhang et al. (2010)	Q	288, 289
$C_{20}H_5OF_{37}$	2.2×10^{-18}		Zhang et al. (2010)	Q	288, 290
[65104-65-6]	2.4×10^{-7}		Zhang et al. (2010)	Q	288, 291
FDCQNVKWWMNRQN-UHFFFAOYSA-N	4.6×10^{-14}		Zhang et al. (2010)	Q	288, 292
2-hydroxyfluorobenzene	3.1		Abraham et al. (1994a)	R	
C_6H_5FO	4.3		Keshavarz et al. (2022)	Q	
(*o*-fluorophenol)	5.1×10^{1}		Duchowicz et al. (2020)	Q	300
[367-12-4]	2.3		Hilal et al. (2008)	Q	
HFHFGHLXUCOHLN-UHFFFAOYSA-N	2.9		Modarresi et al. (2007)	Q	68
	3.1		Yaffe et al. (2003)	Q	249, 250
	2.1×10^{2}		Nirmalakhandan et al. (1997)	Q	
	3.1		Duchowicz et al. (2020)	?	186, 21
4-hydroxyfluorobenzene	1.4×10^{1}		Abraham et al. (1994a)	R	
C_6H_5FO	4.3		Keshavarz et al. (2022)	Q	
(*p*-fluorophenol)	1.3×10^{2}		Duchowicz et al. (2020)	Q	
[371-41-5]	7.9		Hilal et al. (2008)	Q	
RHMPLDJJXGPMEX-UHFFFAOYSA-N	3.3		Modarresi et al. (2007)	Q	68
	1.4×10^{1}		Yaffe et al. (2003)	Q	249, 250
	2.1×10^{1}		English and Carroll (2001)	Q	231, 232
	2.1×10^{2}		Nirmalakhandan et al. (1997)	Q	
	1.4×10^{1}		Duchowicz et al. (2020)	?	186, 21
3-fluorophenol C_6H_5FO [372-20-3] SJTBRFHBXDZMPS-UHFFFAOYSA-N	9.0		Hilal et al. (2008)	Q	

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,6-difluorophenol $C_6H_4F_2O$ [28177-48-2] CKKOVFGIBXCEIJ-UHFFFAOYSA-N	7.0×10^{-1}		Hilal et al. (2008)	Q	
4,4'-(hexafluoroisopropylidene)diphenol $C_{15}H_{10}F_6O_2$ [1478-61-1] ZFVMWEVVKGLCIJ-UHFFFAOYSA-N	1.7×10^{4}		HSDB (2015)	Q	449
	1.7×10^{4}		Zhang et al. (2010)	Q	288, 289
	1.4×10^{6}		Zhang et al. (2010)	Q	288, 290
	2.1×10^{5}		Zhang et al. (2010)	Q	288, 291
	5.3×10^{3}		Zhang et al. (2010)	Q	288, 292
flocoumafen $C_{33}H_{25}F_3O_4$ [90035-08-8] KKBGNYHHEIAGOH-UHFFFAOYSA-N	1.4×10^{7}		HSDB (2015)	Q	100
2,3,3,3-tetrafluoro-2-(trifluoromethyl)propanenitrile C_4F_7N [42532-60-5] AASDJASZOZGYMM-UHFFFAOYSA-N	1.6×10^{-8}		Ebert et al. (2023)	?	367
2-fluoroaniline C_6H_6FN [348-54-9] FTZQXOJYPFINKJ-UHFFFAOYSA-N	1.4		Ebert et al. (2023)	?	319
4-fluoroaniline C_6H_6FN [371-40-4] KRZCOLNOCZKSDF-UHFFFAOYSA-N	1.6		HSDB (2015)	Q	449
3-(trifluoromethyl)aniline $C_7H_6F_3N$ [98-16-8] VIUDTWATMPPKEL-UHFFFAOYSA-N	3.9×10^{-1}		Ebert et al. (2023)	?	317
perfluorotributylamine $C_{12}F_{27}N$ [311-89-7] RVZRBWKZFJCCIB-UHFFFAOYSA-N	1.8×10^{-10}		HSDB (2015)	Q	100
	1.8×10^{-10}		Zhang et al. (2010)	Q	288, 289
	3.4×10^{-10}		Zhang et al. (2010)	Q	288, 290
	1.8×10^{-9}		Zhang et al. (2010)	Q	288, 291
	2.7×10^{-10}		Zhang et al. (2010)	Q	288, 292

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-ethyl-1-[3-(trifluoromethyl)phenyl]-2-propanamine $C_{12}H_{16}F_3N$ (fenfluramine) [458-24-2] DBGIVFWFUFKIQN-UHFFFAOYSA-N	3.7×10^{-1}		HSDB (2015)	Q	100
tris(undecafluoropentyl)amine $C_{15}F_{33}N$ [338-84-1] AQZYBQIAUSKCCS-UHFFFAOYSA-N	1.2×10^{-12} 1.0×10^{-12} 3.4×10^{-10} 2.1×10^{-12}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
indaziflam A $C_{16}H_{20}FN_5$ [730979-19-8] YFONKFDEZLYQDH-OPQQBVKSSA-N	1.8×10^{5}		Ebert et al. (2023)	?	319
indaziflam B $C_{16}H_{20}FN_5$ [730979-32-5] YFONKFDEZLYQDH-OUJBWJOFSA-N	5.3×10^{5}		Ebert et al. (2023)	?	319
cinacalcet $C_{22}H_{22}F_3N$ [226256-56-0] VDHAWDNDOKGFTD-MRXNPFEDSA-N	4.5×10^{1}		HSDB (2015)	Q	100
hydramethylnon $C_{25}H_{24}F_6N_4$ [67485-29-4] IQVNEKKDSLOHHK-FNCQTZNRSA-N	4.5 4.5 2.7×10^{6}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
2-fluoroacetamide C_2H_4FNO [640-19-7] FVTWJXMFYOXOKK-UHFFFAOYSA-N	4.4×10^{2}		HSDB (2015)	Q	100
5-fluorouracil $C_4H_3FN_2O_2$ [51-21-8] GHASVSINZRGABV-UHFFFAOYSA-N	5.8×10^{4}		HSDB (2015)	Q	100
perfluoro-N-methylmorpholine $C_5F_{11}NO$ [382-28-5] PQMAKJUXOOVROI-UHFFFAOYSA-N	6.4×10^{-8}		Ebert et al. (2023)	?	367

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-fluoro-2,4-dinitrobenzene $C_6H_3FN_2O_4$ [70-34-8] LOTKRQAVGJMPNV-UHFFFAOYSA-N	1.0×10^{2}		HSDB (2015)	Q	449
5-fluoro-2-nitrophenol $C_6H_4FNO_3$ [446-36-6] QQURWFRNETXFTN-UHFFFAOYSA-N	5.0×10^{-1} 5.8	 4100 6200	Tremp et al. (1993) Schwarzenbach et al. (1988) Kühne et al. (2005) Kühne et al. (2005)	M V Q ?	12 12
4-nitro-3-(trifluoromethyl)phenol $C_7H_4F_3NO_3$ [88-30-2] ZEFMBAFMCSYJOO-UHFFFAOYSA-N	5.2×10^{2} 5.2×10^{2} 6.7×10^{3} 3.9×10^{4} 1.2×10^{3}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	100 288, 289 288, 290 288, 291 288, 292
1-nitro-3-(trifluoromethyl)benzene $C_7H_4F_3NO_2$ [98-46-4] WHNAMGUAXHGCHH-UHFFFAOYSA-N	5.3×10^{-2} 2.0×10^{-1} 5.7×10^{-2} 8.2×10^{-3}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
1-isocyanato-3-(trifluoromethyl)-benzene $C_8H_4F_3NO$ [329-01-1] SXJYSIBLFGQAND-UHFFFAOYSA-N	4.8×10^{-3} 2.5 1.3×10^{-3} 6.4×10^{-2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
flonicamid $C_9H_6F_3N_3O$ [158062-67-0] RLQJEEJISHYWON-UHFFFAOYSA-N	2.4×10^{7} 2.4×10^{7}		HSDB (2015) Maniere et al. (2011)	V ?	 242, 166
trifluridine $C_{10}H_{11}F_3N_2O_5$ [70-00-8] VSQQQLOSPVPRAZ-RRKCRQDMSA-N	1.0×10^{11}		HSDB (2015)	Q	100
N-(4-amino-2-hydroxyphenyl)-2,2,3,3,4,4,4-heptafluorobutanamide $C_{10}H_7F_7N_2O_2$ [847-51-8] STPOJASQXPXVMS-UHFFFAOYSA-N	2.0×10^{8} 2.3×10^{7} 1.5×10^{5} 5.7×10^{6}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
fluometuron $C_{10}H_{11}F_3N_2O$ [2164-17-2] RZILCCPWPBTYDO-UHFFFAOYSA-N	5.8×10^{3} 3.8×10^{3}		Mackay et al. (2006d) HSDB (2015)	V C	

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dinitramine	7.1		HSDB (2015)	V	
$C_{11}H_{13}F_3N_4O_4$	6.5		Mackay et al. (2006d)	V	
[29091-05-2]	6.2		Suntio et al. (1988)	V	12
OFDYMSKSGFSLLM-UHFFFAOYSA-N					
5-methyl-N-[4-(trifluoromethyl)phenyl]-4-isoxazolecarboxamide	8.0×10^4		HSDB (2015)	Q	100
$C_{12}H_9F_3N_2O_2$					
(leflunomide)					
[75706-12-6]					
VHOGYURTWQBHIL-UHFFFAOYSA-N					
fludioxonil	1.9×10^4		Duchowicz et al. (2020)	V	187
$C_{12}H_6F_2N_2O_2$	1.6×10^4		Duchowicz et al. (2020)	Q	
[131341-86-1]	1.9×10^4		Maniere et al. (2011)	?	242, 166
MUJOIMFVNIBMKC-UHFFFAOYSA-N					
fluconazole	9.9×10^7		HSDB (2015)	Q	100
$C_{13}H_{12}F_2N_6O$					
[86386-73-4]					
RFHAOTPXVQNOHP-UHFFFAOYSA-N					
ethalfluralin	7.6×10^{-2}		HSDB (2015)	V	
$C_{13}H_{14}F_3N_3O_4$					
[55283-68-6]					
PTFJIKYUEPWBMS-UHFFFAOYSA-N					
benfluralin	3.4×10^{-2}		HSDB (2015)	V	
$C_{13}H_{16}F_3N_3O_4$			Mackay et al. (2006d)	V	560
(benefin)	7.5×10^{-1}		Suntio et al. (1988)	V	12
[1861-40-1]	1.1×10^{-1}		Maniere et al. (2011)	?	12, 166
SMDHCQAYESWHAE-UHFFFAOYSA-N					
trifluralin	9.5×10^{-2}		Rice et al. (1997b)	M	12
$C_{13}H_{16}F_3N_3O_4$	9.1×10^{-1}		Watanabe (1993)	M	
[1582-09-8]	1.9×10^{-1}		Fendinger et al. (1989)	M	73
ZSDSQXJSNMTJDA-UHFFFAOYSA-N	1.7×10^{-1}		Fendinger et al. (1989)	M	647
			Mackay et al. (2006d)	V	560
	2.5×10^{-1}		Suntio et al. (1988)	V	12
	3.8		Sanders and Seiber (1983)	V	88
	2.5×10^{-3}		Barcelo and Hennion (1997)	X	569
	9.6×10^{-2}		HSDB (2015)	C	
	8.3×10^{-4}		Goodarzi et al. (2010)	Q	570
	1.7		Hilal et al. (2008)	Q	
	2.6×10^{-1}		Modarresi et al. (2007)	Q	68
		5000	Kühne et al. (2005)	Q	
		2100	Kühne et al. (2005)	?	

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
prodiamine $C_{13}H_{17}F_3N_4O_4$ [29091-21-2] RSVPPPHXAASNOL-UHFFFAOYSA-N	1.3		Ebert et al. (2023)	?	317
fluorodifen $C_{13}H_7F_3N_2O_5$ [15457-05-3] HHMCAJWVGYGUEF-UHFFFAOYSA-N	6.5×10^{2}		Mackay et al. (2006d) MacBean (2012a)	V ?	560
profluralin $C_{14}H_{16}F_3N_3O_4$ [26399-36-0] ITVQAKZNYJEWKS-UHFFFAOYSA-N	3.4×10^{-2} 3.2×10^{-2} 2.6×10^{-2} 3.4×10^{-2}		HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) MacBean (2012a)	V V V ?	 12
flumequine $C_{14}H_{12}FNO_3$ [42835-25-6] DPSPPJIUMHPXMA-UHFFFAOYSA-N	3.7×10^{7}		HSDB (2015)	Q	100
fluazifop $C_{15}H_{12}F_3NO_4$ [69335-91-7] YUVKUEAFAVKILW-UHFFFAOYSA-N	3.4×10^{7}		Ebert et al. (2023)	?	317
fluazifop-p $C_{15}H_{12}F_3NO_4$ [83066-88-0] YUVKUEAFAVKILW-SECBINFHSA-N	1.0×10^{6}		Ebert et al. (2023)	?	317
prosulfuron $C_{15}H_{16}F_3N_5O_4S$ [94125-34-5] LTUNNEGNEKBSEH-UHFFFAOYSA-N	$>3.3\times10^{3}$		Maniere et al. (2011)	?	166
flurprimidol $C_{15}H_{15}N_2O_2F_3$ [56425-91-3] VEVZCONIUDBCDC-UHFFFAOYSA-N	7.5×10^{3} 2.5×10^{4}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
flutriafol $C_{16}H_{13}F_2N_3O$ [76674-21-0] JWUCHKBSVLQQCO-UHFFFAOYSA-N	6.1×10^{7} 7.6×10^{4} 7.9×10^{5}		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	187 12, 166
flunitrazepam $C_{16}H_{12}FN_3O_3$ [1622-62-4] PPTYJKAXVCCBDU-UHFFFAOYSA-N	4.3×10^{5}		HSDB (2015)	Q	100

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyhalofop $C_{16}H_{12}FNO_4$ [122008-78-0] ROBSGBGTWRRYSK-SNVBAGLBSA-N	1.7×10^5		Ebert et al. (2023)	?	319
benzpyrimoxan $C_{16}H_{15}F_3N_2O_3$ [1449021-97-9] ZYXYTGQFPZEUFX-UHFFFAOYSA-N	1.1×10^3		Ebert et al. (2023)	?	319
tolprocarb $C_{16}H_{21}F_3N_2O_3$ [911499-62-2] RSOBJVBYZCMJOS-CYBMUJFWSA-N	6.5×10^4		Ebert et al. (2023)	?	319
flutolanil $C_{17}H_{16}F_3NO_2$ [66332-96-5] PTCGDEVVHUXTMP-UHFFFAOYSA-N	3.1×10^3 2.5 6.1×10^4		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	187 242, 166
beflubutamid $C_{18}H_{17}F_4NO_2$ [113614-08-7] FFQPZWRNXKPNPX-UHFFFAOYSA-N	9.1×10^3		Maniere et al. (2011)	?	242, 166
fluxapyroxad $C_{18}H_{12}F_5N_3O$ [907204-31-3] SXSGXWCSHSVPGB-UHFFFAOYSA-N	3.3×10^6		Maniere et al. (2011)	?	12, 166
flurtamone $C_{18}H_{14}F_3NO_2$ [96525-23-4] NYRMIJKDBAQCHC-UHFFFAOYSA-N	1.6×10^8		Ebert et al. (2023)	?	319
picoxystrobin $C_{18}H_{16}F_3NO_4$ [117428-22-5] IBSNKSODLGJUMQ-SDNWHVSQSA-N	1.4×10^3		Ebert et al. (2023)	?	317
sedaxane $C_{18}H_{19}F_2N_3O$ [874967-67-6] XQJQCBDIXRIYRP-UHFFFAOYSA-N	2.5×10^5		Maniere et al. (2011)	?	166
penflufen $C_{18}H_{24}FN_3O$ [494793-67-8] GOFJDXZZHFNFLV-UHFFFAOYSA-N	3.2×10^4		Ebert et al. (2023)	?	319

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
fluazifop-p-butyl $C_{19}H_{20}F_3NO_4$ [79241-46-6] VAIZTNZGPYBOGF-CYBMUJFWSA-N	2.0×10^{1}		Maniere et al. (2011)	?	12, 166
picolinafen $C_{19}H_{12}F_4N_2O_2$ [137641-05-5] CWKFPEBMTGKLKX-UHFFFAOYSA-N	6.2×10^{2}		Maniere et al. (2011)	?	12, 166
diflufenican $C_{19}H_{11}F_5N_2O_2$ [83164-33-4] WYEHFWKAOXOVJD-UHFFFAOYSA-N	6.4×10^{1} 1.1×10^{3} 3.0×10^{1} $<8.5\times10^{1}$		Keshavarz et al. (2022) Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	Q Q ? ?	 186, 21 242, 166
fluazifop-butyl $C_{19}H_{20}F_3NO_4$ [69806-50-4] VAIZTNZGPYBOGF-UHFFFAOYSA-N	4.7×10^{1}		HSDB (2015)	V	
flumioxazin $C_{19}H_{15}FN_2O_4$ [103361-09-7] FOUWCSDKDDHKQP-UHFFFAOYSA-N	1.6×10^{1} 1.6×10^{1}		HSDB (2015) Maniere et al. (2011)	V ?	 12, 166
fluridone $C_{19}H_{14}F_3NO$ [59756-60-4] YWBVHLJPRPCRSD-UHFFFAOYSA-N	1.2×10^{3} 2.8×10^{3} 1.9×10^{2}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Duchowicz et al. (2020)	V V V Q	187 560
cyhalofop-butyl $C_{20}H_{20}FNO_4$ [122008-85-9] TYIYMOAHACZAMQ-CQSZACIVSA-N	1.0×10^{3} 1.1×10^{3}		MacBean (2012b) Maniere et al. (2011)	X ?	352 242, 166
raltegravir $C_{20}H_{21}FN_6O_5$ [518048-05-0] CZFFBEXEKNGXKS-UHFFFAOYSA-N	1.1×10^{17}		HSDB (2015)	Q	100
fluacrypyrim $C_{20}H_{21}N_2O_5F_3$ [229977-93-9] MXWAGQASUDSFBG-RVDMUPIBSA-N	3.0×10^{2}		MacBean (2012a)	?	12
trifloxystrobin $C_{20}H_{19}F_3N_2O_4$ [141517-21-7] ONCZDRURRATYFI-UHFFFAOYSA-N	4.3×10^{2} 4.3×10^{2}		MacBean (2012b) Maniere et al. (2011)	X ?	352 166

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
isopyrazam $C_{20}H_{23}F_2N_3O$ [881685-58-1] XTDZGXBTXBEZDN-UHFFFAOYSA-N	5.3×10^{3} 2.7×10^{4}		Maniere et al. (2011) Maniere et al. (2011)	? ?	242, 166 242, 166
syn-isopyrazam $C_{20}H_{23}F_2N_3O$ [683777-13-1] XTDZGXBTXBEZDN-HEHGZKQESA-N	5.2×10^{6}		Ebert et al. (2023)	?	319
anti-isopyrazam $C_{20}H_{23}F_2N_3O$ [683777-14-2] XTDZGXBTXBEZDN-XEZPLFJOSA-N	2.6×10^{6}		Ebert et al. (2023)	?	319
etoxazole $C_{21}H_{23}F_2NO_2$ [153233-91-1] IXSZQYVWNJNRAL-UHFFFAOYSA-N	9.6×10^{1} 9.9×10^{1} 1.7×10^{2} 2.8×10^{1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Maniere et al. (2011)	V V Q ?	187 166
droperidol $C_{22}H_{22}FN_3O_2$ [548-73-2] RMEDXOLNCUSCGS-UHFFFAOYSA-N	3.7×10^{11}		HSDB (2015)	Q	100
paliperidone $C_{23}H_{27}FN_4O_3$ [144598-75-4] PMXMIIMHBWHSKN-UHFFFAOYSA-N	1.2×10^{15}		HSDB (2015)	Q	100
risperidone $C_{23}H_{27}FN_4O_2$ [106266-06-2] RAPZEAPATHNIPO-UHFFFAOYSA-N	4.5×10^{10}		HSDB (2015)	Q	100
ezetimibe $C_{24}H_{21}F_2NO_3$ [163222-33-1] OLNTVTPDXPETLC-XPWALMASSA-N	2.2×10^{12}		HSDB (2015)	Q	100
cyflumetofen $C_{24}H_{24}F_3NO_4$ [400882-07-7] AWSZRJQNBMEZOI-UHFFFAOYSA-N	$>1.1\times10^{1}$		Maniere et al. (2011)	?	242, 166
acrinathrin $C_{26}H_{21}F_6NO_5$ [101007-06-1] YLFSVIMMRPNPFK-WEQBUNFVSA-N	9.3×10^{1}		Maniere et al. (2011)	?	12, 166

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cerivastatin $C_{26}H_{34}FNO_5$ [145599-86-6] SEERZIQQUAZTOL-ANMDKAQQSA-N	1.7×10^{13}		HSDB (2015)	Q	100
flucythrinate, isomer 1 $C_{26}H_{23}F_2NO_4$ [70124-77-5] GBIHOLCMZGAKNG-UHFFFAOYSA-N	1.1×10^{2} 9.3×10^{2}		HSDB (2015) Mackay et al. (2006d)	V V	
PFBHA-methanal $H_2C{=}NOCH_2C_6F_5$ [86356-73-2] SRTQFRQWTUMMTC-UHFFFAOYSA-N	1.6×10^{-2}	7200	Destaillats and Charles (2002)	M	
PFBHA-ethanal $CH_3CH{=}NOCH_2C_6F_5$ [114611-59-5] AKDRYEADQPNLOH-UHFFFAOYSA-N	1.9×10^{-2}	5400	Destaillats and Charles (2002)	M	
PFBHA-propanone $(CH_3)_2C{=}NOCH_2C_6F_5$ [899828-53-6] DLIFNTQMBOCKTL-UHFFFAOYSA-N	1.1×10^{-2}	3800	Destaillats and Charles (2002)	M	
PFBHA-butanone $(C_2H_5)(CH_3)C{=}NOCH_2C_6F_5$ LNDQFOSWZJYEIC-UHFFFAOYSA-N	4.7×10^{-3}	6000	Destaillats and Charles (2002)	M	
PFBHA-2-pentanone $(C_3H_7)(CH_3)C{=}NOCH_2C_6F_5$ YKQOTQPNOJSJFA-UHFFFAOYSA-N	3.7×10^{-3}	2200	Destaillats and Charles (2002)	M	
PFBHA-hexanal $C_5H_{11}CH{=}NOCH_2C_6F_5$ GPAVMFOMYSGJDM-UHFFFAOYSA-N	5.8×10^{-3}		Destaillats and Charles (2002)	M	
PFBHA-octanal $C_7H_{15}CH{=}NOCH_2C_6F_5$ RLSQIXNUITTXKZ-UHFFFAOYSA-N	7.9×10^{-3}		Destaillats and Charles (2002)	M	
PFBHA-decanal $C_9H_{19}CH{=}NOCH_2C_6F_5$ NUGDFCWVLOJWOP-UHFFFAOYSA-N	2.4×10^{-2}		Destaillats and Charles (2002)	M	
PFBHA-propenal $CH_2CHCH{=}NOCH_2C_6F_5$ ICDUEGOPUWNJNF-UHFFFAOYSA-N	9.5×10^{-3}	5400	Destaillats and Charles (2002)	M	

Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(*E*)-PFBHA-propenal $C_{10}H_6F_5NO$ [932710-55-9] ICDUEGOPUWNJNF-HQYXKAPLSA-N	9.5×10^{-3}		Ebert et al. (2023)	?	581
PFBHA-crotonaldehyde $CH_3CHCHCH{=}NOCH_2C_6F_5$ [932710-52-6] QNPFFCQTVXPCLD-UHFFFAOYSA-N	6.8×10^{-3}	3400	Destaillats and Charles (2002)	M	
PFBHA-benzaldehyde $C_6H_5CH{=}NOCH_2C_6F_5$ UKSAZCDAGVHMRF-UHFFFAOYSA-N	5.0×10^{-3}	2000	Destaillats and Charles (2002)	M	
PFBHA-4-methyl-benzaldehyde $C_8H_8{=}NOCH_2C_6F_5$ UCASBURGYXMQLW-UHFFFAOYSA-N	6.6×10^{-3}		Destaillats and Charles (2002)	M	
PFBHA-9-fluorenone $C_{13}H_8{=}NOCH_2C_6F_5$ UABDVZDYKDIZFO-UHFFFAOYSA-N	1.1×10^{-2}		Destaillats and Charles (2002)	M	
PFBHA-ethanedial $(HC{=}NOCH_2C_6F_5)_2$ [618858-54-1] VNVBOBJSRGZDCW-UHFFFAOYSA-N	1.6×10^{-2}		Destaillats and Charles (2002)	M	
PFBHA-1-hydroxypropanone $(CH_2OH)(CH_3)C{=}NOCH_2C_6F_5$ BCTASVPUYLXFBW-UHFFFAOYSA-N	2.7×10^{-2}		Destaillats and Charles (2002)	M	
PFBHA-3-hydroxy-3-methyl-2-butanone $(HOC_3H_6)(CH_3)C{=}NOCH_2C_6F_5$ VNWPJWLGZUDTBZ-UHFFFAOYSA-N	1.2×10^{-2}		Destaillats and Charles (2002)	M	

A6 Organic species with chlorine (Cl)

A6.1 Chlorocarbons (C, H, Cl)

Table A6.1: Chlorocarbons (C, H, Cl)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chloromethane	1.0×10^{-3}	2900	Schwardt et al. (2021)	L	1
CH_3Cl	1.0×10^{-3}	2900	Burkholder et al. (2019)	L	1
(methyl chloride)	8.7×10^{-4}	3400	Burkholder et al. (2019)	L	71
[74-87-3]	1.1×10^{-3}	3300	Burkholder et al. (2015)	L	
NEHMKBQYUWJMIP-UHFFFAOYSA-N	8.7×10^{-4}	3400	Burkholder et al. (2015)	L	71
	1.0×10^{-3}	2800	Brockbank (2013)	L	1
	1.3×10^{-3}	3300	Sander et al. (2011)	L	648
	1.1×10^{-3}	3300	Warneck (2007)	L	
	1.3×10^{-3}	3300	Sander et al. (2006)	L	649
	1.1×10^{-3}	3300	Staudinger and Roberts (2001)	L	
	1.1×10^{-3}		Mackay and Shiu (1981)	L	
	1.0×10^{-3}	2800	Wilhelm et al. (1977)	L	
	7.9×10^{-4}	2400	Hiatt (2013)	M	
	9.1×10^{-4}	2000	Chen et al. (2012)	M	
	8.8×10^{-4}	3200	Moore (2000)	M	71
	9.3×10^{-4}	3300	Moore et al. (1995)	M	71
	8.5×10^{-4}	2800	Reichl (1995)	M	650
	1.1×10^{-3}	3000	Elliott and Rowland (1993)	M	
	1.2×10^{-3}	4200	Gossett (1987)	M	
	1.4×10^{-3}		Pearson and McConnell (1975)	M	651, 12
	1.1×10^{-3}	2600	Swain and Thornton (1962)	M	
	9.9×10^{-4}	2500	Boggs and Buck (1958)	M	
	1.0×10^{-3}	2900	Glew and Moelwyn-Hughes (1953)	M	652
	1.0×10^{-3}		Mackay et al. (2006b)	V	
	4.2×10^{-4}		Lide and Frederikse (1995)	V	
	1.0×10^{-3}		Mackay et al. (1993)	V	
	1.1×10^{-3}		Dilling (1977)	V	653
	1.2×10^{-3}		Dilling (1977)	V	12
	9.9×10^{-4}		Hine and Mookerjee (1975)	V	
	1.2×10^{-3}		Yaws (2003)	X	238
	2.9×10^{-4}	-630	Goldstein (1982)	X	299
	2.5×10^{-5}		Ryan et al. (1988)	C	
	1.1×10^{-3}		Hayer et al. (2022)	Q	20
	2.7×10^{-4}		Wang et al. (2017)	Q	81, 239
	1.4×10^{-3}		Wang et al. (2017)	Q	81, 240
	1.8×10^{-3}		Wang et al. (2017)	Q	81, 241
	9.9×10^{-4}		Li et al. (2014)	Q	242
	6.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	247

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.0×10^{-3}		Hilal et al. (2008)	Q	
	1.9×10^{-3}		Modarresi et al. (2007)	Q	68
		2600	Kühne et al. (2005)	Q	
	1.1×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	8.6×10^{-4}		Yao et al. (2002)	Q	230
	1.0×10^{-3}		English and Carroll (2001)	Q	231, 232
	3.7×10^{-4}		Katritzky et al. (1998)	Q	
	8.6×10^{-4}		Suzuki et al. (1992)	Q	233
	3.9×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	8.6×10^{-4}		Irmann (1965)	Q	
	1.1×10^{-3}		Mackay et al. (2006b)	?	
		2700	Kühne et al. (2005)	?	
	1.2×10^{-3}		Yaws (1999)	?	21
	6.9×10^{-4}		Abraham and Weathersby (1994)	?	21
	1.2×10^{-3}		Yaws and Yang (1992)	?	21
	1.0×10^{-3}		Abraham et al. (1990)	?	
dichloromethane	3.9×10^{-3}	3500	Schwardt et al. (2021)	L	1
CH_2Cl_2	3.9×10^{-3}	3700	Burkholder et al. (2019)	L	
(methylene chloride)	3.5×10^{-3}	3900	Burkholder et al. (2019)	L	71
[75-09-2]	3.9×10^{-3}	3700	Burkholder et al. (2015)	L	
YMWUJEATGCHHMB-UHFFFAOYSA-N	3.5×10^{-3}	3900	Burkholder et al. (2015)	L	71
	3.7×10^{-3}	3300	Brockbank (2013)	L	1
	3.6×10^{-3}	4100	Sander et al. (2011)	L	
	3.9×10^{-3}	3700	Warneck (2007)	L	
	3.6×10^{-3}	4100	Sander et al. (2006)	L	
	3.6×10^{-3}	4100	Staudinger and Roberts (2001)	L	
	3.6×10^{-3}	4100	Staudinger and Roberts (1996)	L	
	3.8×10^{-3}		Mackay and Shiu (1981)	L	
	4.0×10^{-3}	3900	Hiatt (2013)	M	
	3.5×10^{-3}	2300	Chen et al. (2012)	M	
	3.6×10^{-3}	3700	Ooki and Yokouchi (2011)	M	71
	3.2×10^{-3}		Helburn et al. (2008)	M	
	4.3×10^{-3}	3500	Lutsyk et al. (2005)	M	
	3.3×10^{-3}	4200	Moore (2000)	M	71
	3.9×10^{-3}		David et al. (2000)	M	73
	3.4×10^{-3}		McIntosh and Heffron (2000)	M	14
	4.1×10^{-3}		Ryu and Park (1999)	M	
	3.4×10^{-3}		Chiang et al. (1998)	M	654, 12
	3.7		Welke et al. (1998)	M	
	5.1×10^{-3}		Hovorka and Dohnal (1997)	M	12
	3.7×10^{-3}	3200	Kondoh and Nakajima (1997)	M	
	4.3×10^{-3}	3500	Park et al. (1997)	M	
	4.1×10^{-3}		Hoff et al. (1993)	M	
	3.8×10^{-3}		Li et al. (1993)	M	
	3.9×10^{-3}	3400	Wright et al. (1992)	M	655

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.9×10^{-3}	3500	Tse et al. (1992)	M	
	4.4×10^{-3}		Yu (1992)	M	12
	3.4×10^{-3}		Guitart et al. (1989)	M	14
	3.4×10^{-3}	4200	Ashworth et al. (1988)	M	279
	4.6×10^{-3}	3800	Gossett (1987)	M	
	5.7×10^{-3}		Hellmann (1987)	M	88
	5.2×10^{-3}		Yurteri et al. (1987)	M	12
	3.8×10^{-3}	4500	Gossett et al. (1985)	M	
	3.4×10^{-3}	4200	Lincoff and Gossett (1984)	M	
	3.0×10^{-3}	3600	Leighton and Calo (1981)	M	
	3.1×10^{-3}		Warner et al. (1980)	M	
	2.8×10^{-3}		Sato and Nakajima (1979b)	M	14
	3.3×10^{-3}		Pearson and McConnell (1975)	M	651, 12
	4.2×10^{-3}	4400	Hartkopf and Karger (1973)	M	
	4.1×10^{-3}	4000	Rex (1906)	M	
	2.7×10^{-3}		Mackay et al. (2006b)	V	
	3.5×10^{-3}	4100	Fogg and Sangster (2003)	V	
	4.0×10^{-3}		Park et al. (1997)	V	
	5.9×10^{-3}		Mackay et al. (1993)	V	
	2.9×10^{-3}		Hwang et al. (1992)	V	
	3.2×10^{-3}		Warner et al. (1980)	V	
	4.0×10^{-3}		Dilling (1977)	V	653
	1.2×10^{-2}		Dilling (1977)	V	154
	4.3×10^{-3}		Hine and Mookerjee (1975)	V	
	4.0×10^{-3}		Dilling et al. (1975)	V	
	4.0×10^{-3}		Yaws (2003)	X	238
	3.1×10^{-3}	3600	Goldstein (1982)	X	299
	4.2×10^{-3}		Harrison et al. (1993)	C	
	3.4×10^{-3}		Harrison et al. (1993)	C	
	4.7×10^{-3}		Ryan et al. (1988)	C	
	3.1×10^{-3}		Shen (1982)	C	
	3.7×10^{-3}		Dilling (1977)	C	
	3.7×10^{-3}		Dilling et al. (1975)	C	
	5.6×10^{-3}		Hayer et al. (2022)	Q	20
	8.8×10^{-3}		Keshavarz et al. (2022)	Q	
	2.6×10^{-3}		Duchowicz et al. (2020)	Q	
	6.2×10^{-4}		Wang et al. (2017)	Q	81, 239
	1.4×10^{-2}		Wang et al. (2017)	Q	81, 240
	9.3×10^{-3}		Wang et al. (2017)	Q	81, 241
	2.9×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	4.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
	9.0×10^{-3}		Hilal et al. (2008)	Q	
	1.8×10^{-3}		Modarresi et al. (2007)	Q	68

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		3000	Kühne et al. (2005)	Q	
	3.8×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	3.0×10^{-3}		Yao et al. (2002)	Q	230
	1.8×10^{-3}		English and Carroll (2001)	Q	231, 261
	6.4×10^{-4}		Katritzky et al. (1998)	Q	
	2.2×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	3.0×10^{-3}		Duchowicz et al. (2020)	?	186, 21
	3.3×10^{-3}		Mackay et al. (2006b)	?	
		3900	Kühne et al. (2005)	?	
	4.0×10^{-3}		Yaws (1999)	?	21
	2.9×10^{-3}		Abraham and Weathersby (1994)	?	21
	3.3×10^{-3}		Mackay et al. (1993)	?	
	4.0×10^{-3}		Yaws and Yang (1992)	?	21
	3.7×10^{-3}		Abraham et al. (1990)	?	
dichloromethane-d2 CD_2Cl_2 (methylene chloride-d2) [1665-00-5] YMWUJEATGCHHMB-DICFDUPASA-N	3.8×10^{-3}	4600	Hiatt (2013)	M	
trichloromethane $CHCl_3$ (chloroform) [67-66-3] HEDRZPFGACZZDS-UHFFFAOYSA-N	2.7×10^{-3}	4200	Schwardt et al. (2021)	L	1
	2.6×10^{-3}	4300	Burkholder et al. (2019)	L	
	2.0×10^{-3}	4400	Burkholder et al. (2019)	L	71
	2.6×10^{-3}	4300	Burkholder et al. (2015)	L	
	2.0×10^{-3}	4400	Burkholder et al. (2015)	L	71
	2.3×10^{-3}	4200	Brockbank (2013)	L	1, 656
	2.5×10^{-3}	4500	Sander et al. (2011)	L	
	2.6×10^{-3}	4300	Warneck (2007)	L	
	2.5×10^{-3}	4500	Sander et al. (2006)	L	
	2.5×10^{-3}	4500	Staudinger and Roberts (2001)	L	
	2.5×10^{-3}	4500	Staudinger and Roberts (1996)	L	
	2.6×10^{-3}		Mackay and Shiu (1981)	L	
	1.6×10^{-3}		Steward et al. (1973)	L	14
	2.6×10^{-3}	3900	Allott et al. (1973)	L	
	2.8×10^{-3}	4500	Hiatt (2013)	M	
	2.5×10^{-3}	3900	Chen et al. (2012)	M	
	3.1×10^{-3}		Ruiz-Bevia and Fernandez-Torres (2010)	M	
	2.7×10^{-3}	4500	Lutsyk et al. (2005)	M	
	1.4×10^{-3}		Zhang et al. (2002)	M	14
	2.3×10^{-3}	4200	Görgényi et al. (2002)	M	657
	2.0×10^{-3}	4600	Moore (2000)	M	71
	2.4×10^{-3}		David et al. (2000)	M	73
	2.7×10^{-3}		Ryu and Park (1999)	M	
	3.0×10^{-3}		Dohnal and Hovorka (1999)	M	12
	3.0×10^{-3}		Chiang et al. (1998)	M	12

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.4×10^{-3}		Welke et al. (1998)	M	
	3.2×10^{-3}		Hovorka and Dohnal (1997)	M	12
	2.7×10^{-3}	3400	Kondoh and Nakajima (1997)	M	
	2.6×10^{-3}	3400	Park et al. (1997)	M	
	2.2×10^{-3}	4700	Turner et al. (1996)	M	
	2.2×10^{-3}	4200	Moore et al. (1995)	M	658, 71
	2.6×10^{-3}	4400	Dewulf et al. (1995)	M	
	2.5×10^{-3}		Hoff et al. (1993)	M	
	2.4×10^{-3}		Li et al. (1993)	M	
	2.6×10^{-3}	4000	Wright et al. (1992)	M	659
	4.8×10^{-3}	7300	Tancrède and Yanagisawa (1990)	M	
	2.4×10^{-3}	2000	Lamarche and Droste (1989)	M	347
	2.1×10^{-3}		Guitart et al. (1989)	M	14
	2.3×10^{-3}	5000	Ashworth et al. (1988)	M	279
	2.7×10^{-3}	4600	Gossett (1987)	M	
	2.6×10^{-3}	4300	Munz and Roberts (1987)	M	
	2.9×10^{-3}		Hellmann (1987)	M	88
	3.3×10^{-3}		Munz and Roberts (1986)	M	
	2.5×10^{-3}	4300	Gossett et al. (1985)	M	
	2.5×10^{-3}	5200	Nicholson et al. (1984)	M	
	2.3×10^{-3}	4200	Lincoff and Gossett (1984)	M	
	2.0×10^{-3}	3900	Hunter-Smith et al. (1983)	M	71, 660
	2.5×10^{-3}	4000	Leighton and Calo (1981)	M	
	1.5×10^{-3}	5600	Ervin et al. (1980)	M	
	2.9×10^{-3}		Warner et al. (1980)	M	
	2.4×10^{-3}	7200	Balls (1980)	M	
	1.4×10^{-3}		Sato and Nakajima (1979b)	M	14
	3.5×10^{-3}		Pearson and McConnell (1975)	M	651, 12
	2.8×10^{-3}	5100	Hartkopf and Karger (1973)	M	
	1.6×10^{-3}		Bachofen and Farhi (1971)	M	14
	2.6×10^{-3}	4600	Rex (1906)	M	
	2.6×10^{-3}		Mackay et al. (2006b)	V	
	2.6×10^{-3}	4400	Fogg and Sangster (2003)	V	
	2.5×10^{-3}		Park et al. (1997)	V	
	2.6×10^{-3}		Mackay et al. (1993)	V	
	2.6×10^{-3}		Hwang et al. (1992)	V	
	5.5×10^{-3}		McLachlan et al. (1990)	V	375
	3.1×10^{-3}		Warner et al. (1980)	V	
	2.8×10^{-3}		Smith and Bomberger (1980)	V	24
	2.5×10^{-3}		Dilling (1977)	V	653
	9.0×10^{-3}		Dilling (1977)	V	154
	2.3×10^{-3}		Hine and Mookerjee (1975)	V	
	2.5×10^{-3}		Dilling et al. (1975)	V	
	2.2×10^{-3}	4700	Winkler (1906)	V	
	2.5×10^{-3}	4100	Barr and Newsham (1987)	X	299
	3.0×10^{-3}	4400	Goldstein (1982)	X	299

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.4×10^{-3}		Harrison et al. (1993)	C	
	3.4×10^{-3}		Harrison et al. (1993)	C	
	3.4×10^{-3}		Ryan et al. (1988)	C	
	2.7×10^{-3}		Nicholson et al. (1984)	C	
	2.1×10^{-3}		Nicholson et al. (1984)	C	12
	2.9×10^{-3}		Shen (1982)	C	
	3.1×10^{-3}		Dilling (1977)	C	
	3.1×10^{-3}		Dilling et al. (1975)	C	
	2.6×10^{-3}		Hayer et al. (2022)	Q	20
	1.1×10^{-3}		Wang et al. (2017)	Q	81, 239
	4.3×10^{-3}		Wang et al. (2017)	Q	81, 240
	4.5×10^{-3}		Wang et al. (2017)	Q	81, 241
	3.7×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	3.2×10^{-3}		Hilal et al. (2008)	Q	
	1.3×10^{-3}		Modarresi et al. (2007)	Q	68
		3300	Kühne et al. (2005)	Q	
	4.1×10^{-3}		Yao et al. (2002)	Q	230
	1.0×10^{-3}		English and Carroll (2001)	Q	231, 275
	2.6×10^{-4}		Katritzky et al. (1998)	Q	
	3.9×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	2.3×10^{-3}		Arbuckle (1983)	Q	
	2.3×10^{-3}		Mackay et al. (2006b)	?	
		4300	Kühne et al. (2005)	?	
	2.4×10^{-3}		Yaws (1999)	?	21
	1.6×10^{-3}		Abraham and Weathersby (1994)	?	21
	2.3×10^{-3}		Mackay et al. (1993)	?	
	2.4×10^{-3}		Yaws and Yang (1992)	?	21
	2.5×10^{-3}		Abraham et al. (1990)	?	
tetrachloromethane CCl_4 (carbontetrachloride) [56-23-5] VZGDMQKNWNREIO-UHFFFAOYSA-N	3.4×10^{-4}	4200	Schwardt et al. (2021)	L	1
	3.6×10^{-4}	4300	Burkholder et al. (2019)	L	
	2.6×10^{-4}	4200	Burkholder et al. (2019)	L	71
	3.6×10^{-4}	4300	Burkholder et al. (2015)	L	
	2.6×10^{-4}	4200	Burkholder et al. (2015)	L	71
	3.5×10^{-4}	4200	Brockbank (2013)	L	1, 661
	3.4×10^{-4}	4200	Sander et al. (2011)	L	
	3.6×10^{-4}	4300	Warneck (2007)	L	
	3.4×10^{-4}	4200	Sander et al. (2006)	L	
	3.4×10^{-4}	4200	Staudinger and Roberts (2001)	L	
	3.4×10^{-4}	4200	Staudinger and Roberts (1996)	L	
	5.0×10^{-4}		Mackay and Shiu (1981)	L	
	5.0×10^{-4}	4500	Hiatt (2013)	M	
	3.0×10^{-4}	4400	Chen et al. (2012)	M	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.4×10^{-4}	3800	Lutsyk et al. (2005)	M	
	3.8×10^{-4}		Ryu and Park (1999)	M	
	4.0×10^{-4}		Chiang et al. (1998)	M	12
	2.9×10^{-4}	3700	Bullister and Wisegarver (1998)	M	662
	4.4×10^{-4}	1900	Kondoh and Nakajima (1997)	M	
	3.9×10^{-4}	2600	Park et al. (1997)	M	
	3.8×10^{-4}	4400	Dewulf et al. (1995)	M	
	3.6×10^{-4}		Hoff et al. (1993)	M	
	3.3×10^{-4}	3600	Hansen et al. (1993)	M	282
	2.3×10^{-4}		Li and Carr (1993)	M	
	2.9×10^{-4}	4500	Wright et al. (1992)	M	663
	3.8×10^{-4}	3600	Tse et al. (1992)	M	
	3.4×10^{-4}	4100	Tancrède and Yanagisawa (1990)	M	
	2.8×10^{-4}	5600	Bissonette et al. (1990)	M	
	3.3×10^{-4}	4000	Ashworth et al. (1988)	M	279
	3.3×10^{-4}	4400	Gossett (1987)	M	
	3.3×10^{-4}	4300	Munz and Roberts (1987)	M	
	3.3×10^{-4}		Hellmann (1987)	M	88
	4.3×10^{-4}		Yurteri et al. (1987)	M	12
	4.2×10^{-4}		Munz and Roberts (1986)	M	
	4.1×10^{-4}	3200	Hunter-Smith et al. (1983)	M	660
	3.6×10^{-4}	4400	Leighton and Calo (1981)	M	
	3.3×10^{-4}		Warner et al. (1980)	M	
	3.2×10^{-4}	3300	Balls (1980)	M	
	9.7×10^{-5}		Sato and Nakajima (1979b)	M	14
	4.5×10^{-4}		Pearson and McConnell (1975)	M	651, 12
	3.7×10^{-4}	5200	Hartkopf and Karger (1973)	M	
	3.5×10^{-4}	4400	Rex (1906)	M	
	3.4×10^{-4}		Mackay et al. (2006b)	V	
	3.6×10^{-4}	4200	Fogg and Sangster (2003)	V	
	4.3×10^{-4}		Park et al. (1997)	V	
	3.4×10^{-4}		Mackay et al. (1993)	V	
	3.4×10^{-4}		Hwang et al. (1992)	V	
	6.7×10^{-5}		Ballschmiter and Wittlinger (1991)	V	
	3.5×10^{-4}		Warner et al. (1980)	V	
	4.6×10^{-4}		Smith and Bomberger (1980)	V	24
	3.4×10^{-4}		Dilling (1977)	V	
	3.4×10^{-4}		Hine and Mookerjee (1975)	V	
	2.0×10^{-4}		Pierotti (1965)	T	
	3.4×10^{-4}		Yaws (2003)	X	238
	3.3×10^{-4}	1100	Goldstein (1982)	X	299
	3.8×10^{-4}		Harrison et al. (1993)	C	
	2.1×10^{-4}		Harrison et al. (1993)	C	
	4.5×10^{-4}		Ryan et al. (1988)	C	
	3.3×10^{-4}		Shen (1982)	C	
	4.6×10^{-4}		Dilling (1977)	C	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.7×10^{-4}		Liss and Slater (1974)	C	
	4.9×10^{-4}		Hayer et al. (2022)	Q	20
	5.4×10^{-4}		Keshavarz et al. (2022)	Q	
	6.3×10^{-4}		Duchowicz et al. (2020)	Q	
	3.4×10^{-4}		Li et al. (2014)	Q	242
	3.2×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
	5.4×10^{-4}		Hilal et al. (2008)	Q	
	2.3×10^{-4}		Modarresi et al. (2007)	Q	68
		3700	Kühne et al. (2005)	Q	
	3.5×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	2.1×10^{-4}		English and Carroll (2001)	Q	231, 232
	3.4×10^{-5}		Katritzky et al. (1998)	Q	
	3.5×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	4.1×10^{-4}		Arbuckle (1983)	Q	
	3.6×10^{-4}		Duchowicz et al. (2020)	?	186, 21
	1.2×10^{-4}		MacBean (2012a)	?	
	3.3×10^{-4}		Mackay et al. (2006b)	?	
		4300	Kühne et al. (2005)	?	
	3.4×10^{-4}		Yaws (1999)	?	21
	1.0×10^{-4}		Abraham and Weathersby (1994)	?	21
	3.3×10^{-4}		Mackay et al. (1993)	?	
	3.3×10^{-4}		Yaws and Yang (1992)	?	21
	3.5×10^{-4}		Abraham et al. (1990)	?	
	4.3×10^{-4}		Mackay and Yeun (1983)	?	
	1.1×10^{-3}		Chiou et al. (1980)	?	80
chloroethane	8.1×10^{-4}	3000	Schwardt et al. (2021)	L	1
C_2H_5Cl	8.1×10^{-4}	2900	Burkholder et al. (2019)	L	1
[75-00-3]	8.3×10^{-4}	2800	Burkholder et al. (2015)	L	
HRYZWHHZPQKTII-UHFFFAOYSA-N	8.1×10^{-4}	2900	Brockbank (2013)	L	1
	8.3×10^{-4}	2800	Warneck (2007)	L	
	8.4×10^{-4}	2900	Staudinger and Roberts (2001)	L	
	8.3×10^{-4}	2900	Staudinger and Roberts (1996)	L	
	5.0×10^{-3}		Mackay and Shiu (1981)	L	
	4.7×10^{-4}		Steward et al. (1973)	L	14
	7.3×10^{-4}	3500	Allott et al. (1973)	L	
	8.5×10^{-4}	3200	Hiatt (2013)	M	
	7.6×10^{-4}	3100	Chen et al. (2012)	M	
	8.9×10^{-4}	3200	Maaßen (1995)	M	664
	9.3×10^{-4}	3300	Reichl (1995)	M	665
	7.9×10^{-4}	2600	Ashworth et al. (1988)	M	279
	8.8×10^{-4}	3100	Gossett (1987)	M	
	5.5×10^{-3}		Mackay et al. (2006b)	V	
	5.5×10^{-3}		Mackay et al. (1993)	V	
	5.6×10^{-4}		Hwang et al. (1992)	V	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.8×10^{-4}		Dilling (1977)	V	
	1.2×10^{-3}		Hine and Mookerjee (1975)	V	
	1.4×10^{-3}		Yaws (2003)	X	238, 12
	6.8×10^{-4}	750	Goldstein (1982)	X	299
	6.6×10^{-4}		Ryan et al. (1988)	C	
	6.3×10^{-4}		Irmann (1965)	C	
	8.0×10^{-4}		Hayer et al. (2022)	Q	20
	2.2×10^{-4}		Wang et al. (2017)	Q	81, 239
	1.4×10^{-3}		Wang et al. (2017)	Q	81, 240
	1.7×10^{-3}		Wang et al. (2017)	Q	81, 241
	7.9×10^{-4}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	9.3×10^{-4}		Gharagheizi et al. (2010)	Q	247
	1.2×10^{-3}		Hilal et al. (2008)	Q	
	1.0×10^{-3}		Modarresi et al. (2007)	Q	68
		3000	Kühne et al. (2005)	Q	
	1.1×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	4.8×10^{-4}		Yao et al. (2002)	Q	230
	9.7×10^{-4}		English and Carroll (2001)	Q	231, 232
	9.0×10^{-4}		Katritzky et al. (1998)	Q	
	6.1×10^{-4}		Suzuki et al. (1992)	Q	233
	7.9×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	7.6×10^{-4}		Irmann (1965)	Q	
	9.8×10^{-4}		Mackay et al. (2006b)	?	
		2900	Kühne et al. (2005)	?	
	1.4×10^{-3}		Yaws (1999)	?	21, 12
	4.8×10^{-4}		Abraham and Weathersby (1994)	?	21
	9.8×10^{-4}		Mackay et al. (1993)	?	
	1.4×10^{-3}		Yaws and Yang (1992)	?	21, 12
	1.2×10^{-3}		Abraham et al. (1990)	?	
1,1-dichloroethane $CHCl_2CH_3$ [75-34-3] SCYULBFZEHDVBN-UHFFFAOYSA-N	1.7×10^{-3}	3900	Schwardt et al. (2021)	L	1
	1.7×10^{-3}	4000	Burkholder et al. (2019)	L	1
	1.5×10^{-3}	3900	Burkholder et al. (2019)	L	71
	1.7×10^{-3}	4100	Burkholder et al. (2015)	L	
	1.5×10^{-3}	3900	Burkholder et al. (2015)	L	71
	1.7×10^{-3}	4000	Brockbank (2013)	L	1
	1.7×10^{-3}	4100	Warneck (2007)	L	
	1.8×10^{-3}	4100	Fogg and Sangster (2003)	L	
	1.6×10^{-3}	3700	Staudinger and Roberts (2001)	L	
	1.5×10^{-3}	3600	Staudinger and Roberts (1996)	L	
	1.7×10^{-3}		Mackay and Shiu (1981)	L	
	2.0×10^{-3}	3900	Hiatt (2013)	M	
	1.9×10^{-3}	3300	Chen et al. (2012)	M	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.0×10^{-3}		Bobadilla et al. (2003)	M	
	1.6×10^{-3}	3900	Görgényi et al. (2002)	M	666
	2.2×10^{-3}		Hovorka and Dohnal (1997)	M	12
	1.8×10^{-3}	2600	Kondoh and Nakajima (1997)	M	
	2.0×10^{-3}	4300	Dewulf et al. (1995)	M	
	1.5×10^{-3}	4900	Wright et al. (1992)	M	667
	1.7×10^{-3}	3700	Tse et al. (1992)	M	
	1.7×10^{-3}	2100	Lamarche and Droste (1989)	M	347
	1.5×10^{-3}	3100	Ashworth et al. (1988)	M	279
	1.8×10^{-3}	4100	Gossett (1987)	M	
	1.3×10^{-3}	4900	Ervin et al. (1980)	M	
	1.8×10^{-3}		Warner et al. (1980)	M	
	1.0×10^{-3}		Sato and Nakajima (1979b)	M	14
	1.8×10^{-3}	4400	Rex (1906)	M	
	1.7×10^{-3}		Mackay et al. (2006b)	V	
	1.6×10^{-3}		Mackay et al. (1993)	V	
	1.8×10^{-3}		Warner et al. (1980)	V	
	1.7×10^{-3}		Smith and Bomberger (1980)	V	24
	1.7×10^{-3}		Dilling (1977)	V	
	1.7×10^{-3}		Hine and Mookerjee (1975)	V	
	1.7×10^{-3}		Yaws (2003)	X	238
	1.7×10^{-3}	3800	Barr and Newsham (1987)	X	299
	1.8×10^{-3}	1700	Goldstein (1982)	X	299
	2.4×10^{-3}		Ryan et al. (1988)	C	
	1.8×10^{-3}		Shen (1982)	C	
	5.1×10^{-4}		Wang et al. (2017)	Q	81, 239
	4.2×10^{-3}		Wang et al. (2017)	Q	81, 240
	6.5×10^{-3}		Wang et al. (2017)	Q	81, 241
	2.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.6×10^{-3}		Gharagheizi et al. (2010)	Q	247
	3.2×10^{-3}		Hilal et al. (2008)	Q	
	1.4×10^{-3}		Modarresi et al. (2007)	Q	68
		3300	Kühne et al. (2005)	Q	
	1.8×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	5.0×10^{-4}		English and Carroll (2001)	Q	231, 275
	1.1×10^{-3}		Katritzky et al. (1998)	Q	
	1.4×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.8×10^{-3}		Mackay et al. (2006b)	?	
		3900	Kühne et al. (2005)	?	
	1.7×10^{-3}		Yaws (1999)	?	21
	1.1×10^{-3}		Abraham and Weathersby (1994)	?	21
	1.6×10^{-3}		Mackay et al. (1993)	?	
	1.7×10^{-3}		Yaws and Yang (1992)	?	21

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.7×10^{-3}		Abraham et al. (1990)	?	
1,2-dichloroethane	7.5×10^{-3}	4400	Schwardt et al. (2021)	L	1
CH_2ClCH_2Cl	8.9×10^{-3}	4300	Burkholder et al. (2019)	L	
[107-06-2]	7.6×10^{-3}	3700	Burkholder et al. (2019)	L	71
WSLDOOZREJYCGB-UHFFFAOYSA-N	8.9×10^{-3}	4300	Burkholder et al. (2015)	L	
	7.6×10^{-3}	3700	Burkholder et al. (2015)	L	71
	8.4×10^{-3}	4200	Brockbank (2013)	L	1
	8.9×10^{-3}	4300	Warneck (2007)	L	
	9.1×10^{-3}	4300	Fogg and Sangster (2003)	L	
	7.8×10^{-3}	4200	Staudinger and Roberts (2001)	L	
	7.1×10^{-3}	4200	Staudinger and Roberts (1996)	L	
	9.1×10^{-3}		Mackay and Shiu (1981)	L	
	8.2×10^{-3}	4400	Hiatt (2013)	M	
	9.1×10^{-3}	6100	Chen et al. (2012)	M	
	5.4×10^{-3}		Ayuttaya et al. (2001)	M	342
	5.7×10^{-4}		Ayuttaya et al. (2001)	M	343
	4.2×10^{-3}		Ayuttaya et al. (2001)	M	344
	8.1×10^{-3}		Ayuttaya et al. (2001)	M	345
	7.5×10^{-3}		Welke et al. (1998)	M	
	1.1×10^{-2}		Hovorka and Dohnal (1997)	M	12
	6.2×10^{-3}	3700	Kondoh and Nakajima (1997)	M	
	9.3×10^{-3}	4600	Dewulf et al. (1995)	M	
	8.3×10^{-3}		Hoff et al. (1993)	M	
	8.2×10^{-3}		Li et al. (1993)	M	
	8.4×10^{-3}	4300	Wright et al. (1992)	M	668
	8.0×10^{-3}	3600	Tse et al. (1992)	M	
	6.4×10^{-3}	4500	Bissonette et al. (1990)	M	
	5.8×10^{-3}	3000	Lamarche and Droste (1989)	M	347
	7.6×10^{-3}		Guitart et al. (1989)	M	14
	6.4×10^{-3}	1500	Ashworth et al. (1988)	M	33, 279
	8.4×10^{-3}	3500	Leighton and Calo (1981)	M	
	9.0×10^{-3}		Warner et al. (1980)	M	
	4.4×10^{-3}		Sato and Nakajima (1979b)	M	14
	1.1×10^{-2}		Pearson and McConnell (1975)	M	651, 12
	7.9×10^{-3}	4400	Hartkopf and Karger (1973)	M	
	7.2×10^{-3}		Saylor et al. (1938)	M	38
	8.6×10^{-3}	4400	Rex (1906)	M	
	8.2×10^{-3}		Mackay et al. (2006b)	V	
	8.3×10^{-3}		Mackay et al. (1993)	V	
	7.3×10^{-3}		Warner et al. (1980)	V	
	8.1×10^{-3}		Dilling (1977)	V	
	7.5×10^{-3}		Hine and Mookerjee (1975)	V	
	8.3×10^{-3}		Yaws (2003)	X	238
	8.5×10^{-3}	3700	Barr and Newsham (1987)	X	299
	9.0×10^{-3}	2400	Goldstein (1982)	X	299

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.6×10^{-3}		Harrison et al. (1993)	C	
	9.0×10^{-3}		Harrison et al. (1993)	C	
	1.1×10^{-2}		Ryan et al. (1988)	C	
	9.0×10^{-3}		Shen (1982)	C	
	1.0×10^{-2}		Dilling (1977)	C	
	1.1×10^{-2}		Hayer et al. (2022)	Q	20
	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	3.8×10^{-3}		Duchowicz et al. (2020)	Q	185
	1.5×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.2×10^{-2}		Wang et al. (2017)	Q	81, 240
	2.0×10^{-2}		Wang et al. (2017)	Q	81, 241
	7.5×10^{-3}		Li et al. (2014)	Q	242
	6.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.1×10^{-2}		Gharagheizi et al. (2010)	Q	247
	1.0×10^{-2}		Hilal et al. (2008)	Q	
	5.1×10^{-3}		Modarresi et al. (2007)	Q	68
		3300	Kühne et al. (2005)	Q	
	8.2×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	3.4×10^{-3}		English and Carroll (2001)	Q	231, 232
	2.2×10^{-3}		Katritzky et al. (1998)	Q	
	7.7×10^{-3}		Russell et al. (1992)	Q	280
	1.8×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	8.4×10^{-3}		Duchowicz et al. (2020)	?	186, 21
	4.2×10^{-3}		MacBean (2012a)	?	
	7.0×10^{-3}		Mackay et al. (2006b)	?	
		3600	Kühne et al. (2005)	?	
	8.4×10^{-3}		Yaws (1999)	?	21
	4.5×10^{-3}		Abraham and Weathersby (1994)	?	21
	7.0×10^{-3}		Mackay et al. (1993)	?	
	8.3×10^{-3}		Yaws and Yang (1992)	?	21
	8.2×10^{-3}		Abraham et al. (1990)	?	
	1.2×10^{-2}		Chiou et al. (1980)	?	80
1,2-dichloroethane-d4 CD_2ClCD_2Cl [17060-07-0] WSLDOOZREJYCGB-LNLMKGTHSA-N	8.7×10^{-3}	4300	Hiatt (2013)	M	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1,1-trichloroethane	6.0×10^{-4}	3800	Schwardt et al. (2021)	L	1
CH_3CCl_3	6.0×10^{-4}	3700	Burkholder et al. (2019)	L	
(methylchloroform; MCF)	4.2×10^{-4}	4200	Burkholder et al. (2019)	L	71
[71-55-6]	6.0×10^{-4}	3700	Burkholder et al. (2015)	L	
UOCLXMDMGBRAIB-UHFFFAOYSA-N	4.2×10^{-4}	4200	Burkholder et al. (2015)	L	71
	5.8×10^{-4}	4100	Brockbank (2013)	L	1
	6.0×10^{-4}	3700	Warneck (2007)	L	
	6.2×10^{-4}	3900	Fogg and Sangster (2003)	L	
	5.9×10^{-4}	4000	Staudinger and Roberts (2001)	L	
	5.8×10^{-4}	3900	Staudinger and Roberts (1996)	L	
	3.6×10^{-4}		Mackay and Shiu (1981)	L	
	6.9×10^{-4}	4000	Hiatt (2013)	M	
	5.4×10^{-4}	4100	Chen et al. (2012)	M	
	6.2×10^{-4}	3500	Vane and Giroux (2000)	M	
	7.1×10^{-4}		Chiang et al. (1998)	M	12
	7.9×10^{-4}		Hovorka and Dohnal (1997)	M	12
	6.7×10^{-4}	1900	Kondoh and Nakajima (1997)	M	
	4.8×10^{-4}		Turner et al. (1996)	M	
	6.7×10^{-4}	4100	Dewulf et al. (1995)	M	
	5.5×10^{-4}	2500	Robbins et al. (1993)	M	669
	5.3×10^{-4}		Hoff et al. (1993)	M	
	5.9×10^{-4}	3100	Hansen et al. (1993)	M	282
	5.7×10^{-4}		Li et al. (1993)	M	
	6.0×10^{-4}	3300	Wright et al. (1992)	M	670
	6.3×10^{-4}	3700	Tse et al. (1992)	M	
	7.9×10^{-4}	1300	Kolb et al. (1992)	M	278
	5.1×10^{-4}	5200	Bissonette et al. (1990)	M	
	3.2×10^{-4}		Guitart et al. (1989)	M	14
	5.7×10^{-4}	3400	Ashworth et al. (1988)	M	279
	5.9×10^{-4}	4100	Gossett (1987)	M	
	5.8×10^{-4}	4100	Munz and Roberts (1987)	M	
	6.3×10^{-4}		Yurteri et al. (1987)	M	12
	5.7×10^{-4}	4200	Gossett et al. (1985)	M	
	5.9×10^{-4}	4300	Lincoff and Gossett (1984)	M	
	7.6×10^{-4}	3200	Hunter-Smith et al. (1983)	M	660
	4.9×10^{-4}	4400	Leighton and Calo (1981)	M	
	2.7×10^{-4}	7000	Ervin et al. (1980)	M	
	2.0×10^{-3}		Warner et al. (1980)	M	
	3.6×10^{-4}		Sato and Nakajima (1979b)	M	14
	2.9×10^{-4}		Pearson and McConnell (1975)	M	651, 12
	5.9×10^{-4}		Mackay et al. (2006b)	V	
	6.8×10^{-4}		Mackay et al. (1993)	V	
	7.0×10^{-4}	4700	McLinden (1989)	V	
	2.4×10^{-3}		Warner et al. (1980)	V	
	3.4×10^{-4}		Dilling (1977)	V	653
	4.0×10^{-4}		Dilling (1977)	V	12

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^{-3}		Dilling (1977)	V	154
	6.1×10^{-4}		Hine and Mookerjee (1975)	V	
	5.9×10^{-4}		Dilling et al. (1975)	V	
	4.5×10^{-4}		Yaws (2003)	X	238
	5.8×10^{-4}	4000	Barr and Newsham (1987)	X	299
	2.2×10^{-3}	1700	Goldstein (1982)	X	299
	3.1×10^{-4}		Ryan et al. (1988)	C	
	2.0×10^{-3}		Shen (1982)	C	
	2.3×10^{-4}		Wang et al. (2017)	Q	81, 239
	7.6×10^{-4}		Wang et al. (2017)	Q	81, 240
	2.0×10^{-3}		Wang et al. (2017)	Q	81, 241
	2.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	4.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
	9.0×10^{-4}		Hilal et al. (2008)	Q	
	1.3×10^{-3}		Modarresi et al. (2007)	Q	68
		3700	Kühne et al. (2005)	Q	
	6.1×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	7.9×10^{-4}		English and Carroll (2001)	Q	231, 261
	5.4×10^{-4}		Katritzky et al. (1998)	Q	
	2.3×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.6×10^{-3}		Arbuckle (1983)	Q	
	5.7×10^{-4}		Mackay et al. (2006b)	?	
		3700	Kühne et al. (2005)	?	
	4.6×10^{-4}		Yaws (1999)	?	21
	3.8×10^{-4}		Abraham and Weathersby (1994)	?	21
	5.7×10^{-4}		Mackay et al. (1993)	?	
	5.6×10^{-4}		Abraham et al. (1990)	?	
	1.6×10^{-3}		Chiou et al. (1980)	?	80
1,1,2-trichloroethane	1.1×10^{-2}	4400	Schwardt et al. (2021)	L	1
$CHCl_2CH_2Cl$	1.1×10^{-2}	4100	Burkholder et al. (2019)	L	
[79-00-5]	1.1×10^{-2}	4100	Burkholder et al. (2015)	L	
UBOXGVDOUJQMTN-UHFFFAOYSA-N	1.1×10^{-2}	4400	Brockbank (2013)	L	1, 671
	1.1×10^{-2}	4100	Warneck (2007)	L	
	1.2×10^{-2}	4200	Fogg and Sangster (2003)	L	
	1.1×10^{-2}	4900	Staudinger and Roberts (2001)	L	
	1.1×10^{-2}	4900	Staudinger and Roberts (1996)	L	
	8.3×10^{-3}		Mackay and Shiu (1981)	L	
	7.3×10^{-3}	2400	Schwardt et al. (2021)	M	672, 11
	1.4×10^{-2}	5400	Hiatt (2013)	M	
	1.2×10^{-2}		Bobadilla et al. (2003)	M	
	1.1×10^{-2}	4700	Dewulf et al. (1999)	M	
	1.5×10^{-2}		Dohnal and Hovorka (1999)	M	12

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.5×10^{-2}		Hovorka and Dohnal (1997)	M	12
	1.1×10^{-2}	5100	Kondoh and Nakajima (1997)	M	
	1.2×10^{-2}	5900	Hansen et al. (1993)	M	282
	1.1×10^{-2}	4300	Wright et al. (1992)	M	673
	1.1×10^{-2}	4100	Tse et al. (1992)	M	
	1.0×10^{-2}	4800	Ashworth et al. (1988)	M	279
	1.2×10^{-2}	3700	Leighton and Calo (1981)	M	
	6.6×10^{-3}		Sato and Nakajima (1979b)	M	14
	1.1×10^{-2}		Mackay et al. (2006b)	V	
	1.0×10^{-2}		Mackay et al. (1993)	V	
	1.1×10^{-2}		Dilling (1977)	V	
	1.1×10^{-2}		Hine and Mookerjee (1975)	V	
	1.1×10^{-2}		Yaws (2003)	X	238
	1.1×10^{-2}	4300	Barr and Newsham (1987)	X	299
	1.2×10^{-2}	2700	Goldstein (1982)	X	299
	1.3×10^{-3}		Ryan et al. (1988)	C	
	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	7.7×10^{-3}		Duchowicz et al. (2020)	Q	
	4.9×10^{-3}		Wang et al. (2017)	Q	81, 239
	2.1×10^{-2}		Wang et al. (2017)	Q	81, 240
	4.1×10^{-2}		Wang et al. (2017)	Q	81, 241
	1.1×10^{-2}		Li et al. (2014)	Q	242
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
	1.5×10^{-2}		Hilal et al. (2008)	Q	
	6.7×10^{-3}		Modarresi et al. (2007)	Q	68
		3700	Kühne et al. (2005)	Q	
	8.6×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.9×10^{-3}		Katritzky et al. (1998)	Q	
	3.3×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	7.6×10^{-3}		Arbuckle (1983)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	1.1×10^{-2}		Mackay et al. (2006b)	?	
		4200	Kühne et al. (2005)	?	
	1.1×10^{-2}		Yaws (1999)	?	21
	6.9×10^{-3}		Abraham and Weathersby (1994)	?	21
	1.1×10^{-2}		Mackay et al. (1993)	?	
	1.0×10^{-2}		Yaws and Yang (1992)	?	21
	1.2×10^{-2}		Abraham et al. (1990)	?	
1,1,2-trichloroethane-d3 $CDCl_2CD_2Cl$ [171086-93-4] UBOXGVDOUJQMTN-FUDHJZNOSA-N	1.3×10^{-2}	5100	Hiatt (2013)	M	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1,1,2-tetrachloroethane	5.0×10^{-3}	6700	Schwardt et al. (2021)	L	1
CCl_3CH_2Cl	4.2×10^{-3}	4600	Burkholder et al. (2019)	L	
[630-20-6]	4.2×10^{-3}	4600	Burkholder et al. (2015)	L	
QVLAWKAXOMEXPM-UHFFFAOYSA-N	4.2×10^{-3}	4900	Brockbank (2013)	L	
	4.2×10^{-3}	4600	Warneck (2007)	L	
	2.4×10^{-2}	3200	Staudinger and Roberts (2001)	L	
	3.6×10^{-3}		Mackay and Shiu (1981)	L	
	4.5×10^{-3}	11000	Schwardt et al. (2021)	M	674
	4.8×10^{-3}	4800	Hiatt (2013)	M	
	4.3×10^{-3}	4100	Kondoh and Nakajima (1997)	M	
	4.0×10^{-3}	4400	Wright et al. (1992)	M	675
	4.5×10^{-3}	4600	Tse et al. (1992)	M	
	2.1×10^{-3}		Sato and Nakajima (1979b)	M	14
	4.0×10^{-3}		Mackay et al. (2006b)	V	
	4.2×10^{-3}	5000	Fogg and Sangster (2003)	V	
	4.1×10^{-3}		Mackay et al. (1993)	V	
	3.7×10^{-3}		Dilling (1977)	V	
	4.1×10^{-3}		Yaws (2003)	X	238
	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	185
	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	3.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
	3.9×10^{-3}		Hilal et al. (2008)	Q	
	6.0×10^{-3}		Modarresi et al. (2007)	Q	68
		4100	Kühne et al. (2005)	Q	
	3.8×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	4.5×10^{-3}		English and Carroll (2001)	Q	231, 232
	1.2×10^{-3}		Katritzky et al. (1998)	Q	
	5.4×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	3.9×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4600	Kühne et al. (2005)	?	
	4.1×10^{-3}		Yaws (1999)	?	21
	2.2×10^{-3}		Abraham and Weathersby (1994)	?	21
	3.5×10^{-3}		Abraham et al. (1990)	?	
1,1,2,2-tetrachloroethane	2.3×10^{-2}	3700	Schwardt et al. (2021)	L	1
$CHCl_2CHCl_2$	2.3×10^{-2}	4800	Burkholder et al. (2019)	L	
[79-34-5]	2.3×10^{-2}	4800	Burkholder et al. (2015)	L	
QPFMBZIOSGYJDE-UHFFFAOYSA-N	2.4×10^{-2}	5000	Brockbank (2013)	L	
	2.4×10^{-2}	4800	Warneck (2007)	L	
	2.4×10^{-2}	3200	Staudinger and Roberts (1996)	L	
	2.1×10^{-2}		Mackay and Shiu (1981)	L	
	3.3×10^{-2}	7200	Hiatt (2013)	M	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.0×10^{-2}		Hovorka and Dohnal (1997)	M	12
	2.3×10^{-2}	6800	Kondoh and Nakajima (1997)	M	676
	2.9×10^{-2}		Li and Carr (1993)	M	
	2.2×10^{-2}	3100	Wright et al. (1992)	M	677
	2.6×10^{-2}	4800	Tse et al. (1992)	M	
	2.2×10^{-2}	2900	Ashworth et al. (1988)	M	42, 279
	2.7×10^{-2}	3500	Leighton and Calo (1981)	M	
	1.4×10^{-2}		Sato and Nakajima (1979b)	M	14
	2.1×10^{-2}		Mackay et al. (2006b)	V	
	2.2×10^{-2}		Mackay et al. (1993)	V	
	2.1×10^{-2}		Dilling (1977)	V	
	2.2×10^{-2}		Hine and Mookerjee (1975)	V	
	2.8×10^{-2}		Yaws (2003)	X	238
	1.8×10^{-2}	4200	Barr and Newsham (1987)	X	299
	2.3×10^{-2}	3000	Goldstein (1982)	X	299
	2.5×10^{-2}		Ryan et al. (1988)	C	
	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	1.5×10^{-2}		Duchowicz et al. (2020)	Q	300
	1.6×10^{-2}		Wang et al. (2017)	Q	81, 239
	2.7×10^{-2}		Wang et al. (2017)	Q	81, 240
	9.3×10^{-2}		Wang et al. (2017)	Q	81, 241
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	2.8×10^{-2}		Gharagheizi et al. (2010)	Q	247
	1.9×10^{-2}		Hilal et al. (2008)	Q	
	5.5×10^{-3}		Modarresi et al. (2007)	Q	68
		4100	Kühne et al. (2005)	Q	
	2.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.1×10^{-3}		Katritzky et al. (1998)	Q	
	6.1×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	2.7×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	3.9×10^{-2}		Mackay et al. (2006b)	?	
		4500	Kühne et al. (2005)	?	
	2.8×10^{-2}		Yaws (1999)	?	21
	1.4×10^{-2}		Abraham and Weathersby (1994)	?	21
	3.9×10^{-2}		Mackay et al. (1993)	?	
	3.0×10^{-2}		Yaws and Yang (1992)	?	21
	2.6×10^{-2}		Abraham et al. (1990)	?	
	3.0×10^{-2}		Chiou et al. (1980)	?	80

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pentachloroethane	4.1×10^{-3}	7700	Burkholder et al. (2019)	L	678
$CHCl_2CCl_3$	4.2×10^{-3}	7700	Brockbank (2013)	L	
[76-01-7]	4.5×10^{-3}		Mackay and Shiu (1981)	L	
BNIXVQGCZULYKV-UHFFFAOYSA-N	5.9×10^{-3}	5400	Hiatt (2013)	M	
	5.1×10^{-3}		Duchowicz et al. (2020)	V	187
	5.2×10^{-3}		HSDB (2015)	V	
	4.1×10^{-3}		Mackay et al. (2006b)	V	
	4.0×10^{-3}		Mackay et al. (1993)	V	
	5.3×10^{-3}		Meylan and Howard (1991)	V	
	4.0×10^{-3}		Dilling (1977)	V	
	4.0×10^{-3}		Hine and Mookerjee (1975)	V	
	6.2×10^{-3}		Duchowicz et al. (2020)	Q	
	4.0×10^{-3}		Li et al. (2014)	Q	242
	2.0×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	6.1×10^{-3}		Hilal et al. (2008)	Q	
	3.6×10^{-3}		Modarresi et al. (2007)	Q	68
	4.0×10^{-4}		Katritzky et al. (1998)	Q	
	1.9×10^{-2}		Meylan and Howard (1991)	Q	
	1.0×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	5.1×10^{-3}		Yaws (1999)	?	21
	5.4×10^{-3}		Yaws and Yang (1992)	?	21
	4.2×10^{-3}		Abraham et al. (1990)	?	
hexachloroethane	2.7×10^{-3}	5700	Burkholder et al. (2019)	L	
C_2Cl_6	2.6×10^{-3}	5600	Burkholder et al. (2015)	L	
[67-72-1]	2.8×10^{-3}	6100	Brockbank (2013)	L	
VHHHONWQHHHLTI-UHFFFAOYSA-N	2.5×10^{-3}	5600	Staudinger and Roberts (1996)	L	
	1.2×10^{-3}	2600	Ashworth et al. (1988)	M	33, 279
	2.5×10^{-3}	5600	Munz and Roberts (1987)	M	
	3.4×10^{-3}		Munz and Roberts (1986)	M	
	1.0×10^{-3}		Warner et al. (1980)	M	
	4.2×10^{-3}		Mackay et al. (2006b)	V	
	3.6×10^{-3}		Lide and Frederikse (1995)	V	
	1.5×10^{-2}		Hwang et al. (1992)	V	
	2.2×10^{-4}		Ballschmiter and Wittlinger (1991)	V	
	7.7×10^{-4}		Mackay and Shiu (1981)	V	
	8.1×10^{-3}		Dilling (1977)	V	
	4.3×10^{-3}		Hine and Mookerjee (1975)	V	
	3.9×10^{-4}		Yaws (2003)	X	238
	1.0×10^{-3}	2100	Goldstein (1982)	X	299
	9.8×10^{-4}		Ryan et al. (1988)	C	
	1.0×10^{-3}		Shen (1982)	C	
	7.3×10^{-4}		Keshavarz et al. (2022)	Q	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.5×10^{-3}		Duchowicz et al. (2020)	Q	
	2.4×10^{-3}		Zhang et al. (2010)	Q	288, 289
	1.8×10^{-3}		Zhang et al. (2010)	Q	288, 290
	1.9×10^{-3}		Zhang et al. (2010)	Q	288, 291
	3.9×10^{-3}		Zhang et al. (2010)	Q	288, 292
	3.7×10^{-4}		Gharagheizi et al. (2010)	Q	247
	3.9×10^{-3}		Hilal et al. (2008)	Q	
	9.3×10^{-4}		Modarresi et al. (2007)	Q	68
	8.0×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	2.4×10^{-4}		Yao et al. (2002)	Q	230
	1.0×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	2.5×10^{-3}		Duchowicz et al. (2020)	?	186, 21
	1.2×10^{-3}		Mackay et al. (2006b)	?	
	3.9×10^{-4}		Yaws (1999)	?	21
	1.2×10^{-3}		Mackay et al. (1993)	?	
	4.4×10^{-4}		Yaws and Yang (1992)	?	21
1-chloropropane	7.6×10^{-4}	4500	Brockbank (2013)	L	
C_3H_7Cl	6.9×10^{-4}		Li et al. (1993)	M	
[540-54-5]	4.3×10^{-4}		Sato and Nakajima (1979b)	M	14
SNMVRZFUUCLYTO-UHFFFAOYSA-N	7.7×10^{-4}	4400	Rex (1906)	M	
	7.5×10^{-4}		Duchowicz et al. (2020)	V	187
	7.6×10^{-4}		HSDB (2015)	V	
	6.9×10^{-4}		Mackay et al. (2006b)	V	
	7.1×10^{-4}		Mackay et al. (1993)	V	
	7.1×10^{-4}		Abraham (1984)	V	
	7.3×10^{-4}		Hine and Mookerjee (1975)	V	
	9.2×10^{-4}		Yaws (2003)	X	238, 12
	1.3×10^{-3}		Duchowicz et al. (2020)	Q	
	7.3×10^{-4}		Li et al. (2014)	Q	242
	4.3×10^{-4}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	6.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
	1.1×10^{-3}		Hilal et al. (2008)	Q	
	1.0×10^{-3}		Modarresi et al. (2007)	Q	68
		3300	Kühne et al. (2005)	Q	
			Yaffe et al. (2003)	Q	358
	2.8×10^{-4}		Yao et al. (2002)	Q	230
	7.3×10^{-4}		English and Carroll (2001)	Q	231, 232
	1.2×10^{-3}		Katritzky et al. (1998)	Q	
	4.7×10^{-4}		Suzuki et al. (1992)	Q	233
	6.2×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
		3500	Kühne et al. (2005)	?	
	7.5×10^{-4}		Yaws (1999)	?	21, 12

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.4×10^{-4}		Abraham and Weathersby (1994)	?	21
	9.1×10^{-4}		Yaws and Yang (1992)	?	21, 12
	7.0×10^{-4}		Abraham et al. (1990)	?	
2-chloropropane	5.7×10^{-4}	4400	Brockbank (2013)	L	
C_3H_7Cl	5.4×10^{-4}		Li et al. (1993)	M	
[75-29-6]	5.6×10^{-4}	4300	Rex (1906)	M	
ULYZAYCEDJDHCC-UHFFFAOYSA-N	5.6×10^{-4}		Duchowicz et al. (2020)	V	187
	5.5×10^{-4}		HSDB (2015)	V	
	5.6×10^{-4}		Mackay et al. (2006b)	V	
	5.5×10^{-4}		Mackay et al. (1993)	V	
	6.1×10^{-4}		Hine and Mookerjee (1975)	V	
	6.8×10^{-4}		Yaws (2003)	X	238, 12
	5.9×10^{-4}		Duchowicz et al. (2020)	Q	
	9.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	4.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
	6.0×10^{-4}		Hilal et al. (2008)	Q	
	8.1×10^{-4}		Modarresi et al. (2007)	Q	68
	6.1×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	6.2×10^{-4}		English and Carroll (2001)	Q	231, 261
	1.5×10^{-3}		Katritzky et al. (1998)	Q	
	9.5×10^{-4}		Russell et al. (1992)	Q	280
	4.1×10^{-4}		Suzuki et al. (1992)	Q	233
	5.1×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	5.6×10^{-4}		Yaws (1999)	?	21, 12
	6.8×10^{-4}		Yaws and Yang (1992)	?	21, 12
	6.1×10^{-4}		Abraham et al. (1990)	?	
1,1-dichloropropane	2.6×10^{-3}		Duchowicz et al. (2020)	V	187
$C_3H_6Cl_2$	3.3×10^{-3}		Duchowicz et al. (2020)	V	187
[78-99-9]	2.6×10^{-3}		HSDB (2015)	V	
WIHMGGWNMISDNJ-UHFFFAOYSA-N	2.7×10^{-3}		Duchowicz et al. (2020)	Q	
	2.7×10^{-3}		Duchowicz et al. (2020)	Q	
1,2-dichloropropane	3.7×10^{-3}	4100	Schwardt et al. (2021)	L	1
$C_3H_6Cl_2$	3.4×10^{-3}	4300	Burkholder et al. (2019)	L	
[78-87-5]	3.4×10^{-3}	4300	Burkholder et al. (2015)	L	
KNKRKFALVUDBJE-UHFFFAOYSA-N	3.4×10^{-3}	4000	Brockbank (2013)	L	1
	3.4×10^{-3}	4300	Staudinger and Roberts (2001)	L	
	3.4×10^{-3}	4300	Staudinger and Roberts (1996)	L	
	4.3×10^{-3}	4400	Hiatt (2013)	M	
	4.2×10^{-3}		Bobadilla et al. (2003)	M	
	3.5×10^{-3}	4300	Dewulf et al. (1999)	M	
	4.4×10^{-3}		Dohnal and Hovorka (1999)	M	12

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.5×10^{-3}		Welke et al. (1998)	M	
	4.6×10^{-3}		Hovorka and Dohnal (1997)	M	12
	4.3×10^{-3}	3700	Kondoh and Nakajima (1997)	M	
	3.6×10^{-3}	4200	Wright et al. (1992)	M	679
	3.8×10^{-3}	3800	Tse et al. (1992)	M	
	3.0×10^{-3}	3800	Bissonette et al. (1990)	M	
	3.8×10^{-3}	4700	Ashworth et al. (1988)	M	33, 279
	4.9×10^{-3}		Albanese et al. (1987)	M	
	3.4×10^{-3}	4300	Leighton and Calo (1981)	M	
	3.5×10^{-3}		Warner et al. (1980)	M	
	2.1×10^{-3}		Sato and Nakajima (1979b)	M	14
	3.7×10^{-3}		Mackay et al. (2006b)	V	
	3.7×10^{-3}		Mackay et al. (1993)	V	
	3.6×10^{-3}		Warner et al. (1980)	V	
	3.4×10^{-3}		Hine and Mookerjee (1975)	V	
	3.5×10^{-3}		Yaws (2003)	X	238
	3.4×10^{-3}	2100	Goldstein (1982)	X	299
	3.5×10^{-3}		Horvath and Getzen (1999)	C	
	3.4×10^{-3}		Ryan et al. (1988)	C	
	3.5×10^{-3}		Shen (1982)	C	
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	1.8×10^{-3}		Duchowicz et al. (2020)	Q	185
	1.4×10^{-3}		Wang et al. (2017)	Q	81, 239
	6.2×10^{-3}		Wang et al. (2017)	Q	81, 240
	8.9×10^{-3}		Wang et al. (2017)	Q	81, 241
	4.7×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	4.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
	5.4×10^{-3}		Hilal et al. (2008)	Q	
	3.6×10^{-3}		Modarresi et al. (2007)	Q	68
		3700	Kühne et al. (2005)	Q	
	3.8×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	2.1×10^{-3}		English and Carroll (2001)	Q	231, 232
	2.8×10^{-3}		Katritzky et al. (1998)	Q	
	1.2×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	3.5×10^{-3}		Duchowicz et al. (2020)	?	186, 21
	8.5×10^{-4}		MacBean (2012a)	?	
	3.5×10^{-3}		Mackay et al. (2006b)	?	
		4000	Kühne et al. (2005)	?	
	3.5×10^{-3}		Yaws (1999)	?	21
	2.2×10^{-3}		Abraham and Weathersby (1994)	?	21
	3.5×10^{-3}		Mackay et al. (1993)	?	
	3.7×10^{-3}		Yaws and Yang (1992)	?	21
	3.4×10^{-3}		Abraham et al. (1990)	?	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.8×10^{-3}		Mackay and Yeun (1983)	?	
	5.9×10^{-3}		Chiou et al. (1980)	?	80
1,2-dichloropropane-d6 $C_3D_6Cl_2$ [93952-08-0] KNKRKFALVUDBJE-LIDOUZCJSA-N	3.6×10^{-3}	4600	Hiatt (2013)	M	
1,3-dichloropropane	1.0×10^{-2}	3900	Burkholder et al. (2019)	L	
$C_3H_6Cl_2$	1.0×10^{-2}	3900	Burkholder et al. (2015)	L	
[142-28-9]	1.2×10^{-2}	3100	Brockbank (2013)	L	
YHRUOJUYPBUZOS-UHFFFAOYSA-N	1.3×10^{-2}	5300	Hiatt (2013)	M	
	1.1×10^{-2}	5000	Kondoh and Nakajima (1997)	M	
	8.5×10^{-3}		Albanese et al. (1987)	M	
	1.0×10^{-2}	3900	Leighton and Calo (1981)	M	
	9.9×10^{-3}		Hine and Mookerjee (1975)	V	
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	3.6×10^{-3}		Duchowicz et al. (2020)	Q	300
	1.8×10^{-2}		Hilal et al. (2008)	Q	
	5.8×10^{-3}		Modarresi et al. (2007)	Q	68
		3700	Kühne et al. (2005)	Q	
	5.6×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	3.0×10^{-3}		Katritzky et al. (1998)	Q	
	1.4×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.0×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		3900	Kühne et al. (2005)	?	
	1.0×10^{-2}		Yaws (1999)	?	21
	9.9×10^{-3}		Yaws and Yang (1992)	?	21
	9.9×10^{-3}		Abraham et al. (1990)	?	
2,2-dichloropropane	4.4×10^{-4}	7400	Hiatt (2013)	M	
$C_3H_6Cl_2$	8.1×10^{-4}	3900	Bakierowska and Trzeszczyński (2003)	M	
[594-20-7]	7.1×10^{-4}	630	Kondoh and Nakajima (1997)	M	
ZEOVXNVKXIPWMS-UHFFFAOYSA-N		3700	Kühne et al. (2005)	Q	
		3900	Kühne et al. (2005)	?	
1,1,1-trichloropropane	3.1×10^{-3}		Duchowicz et al. (2020)	V	187
$C_3H_5Cl_3$	3.8×10^{-3}		Yaws et al. (2005)	X	448
[7789-89-1]	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
AVGQTJUPLKNPQP-UHFFFAOYSA-N	1.1×10^{-3}		Hilal et al. (2008)	Q	
	3.1×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	6.5×10^{-4}		Katritzky et al. (1998)	Q	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1,2-trichloropropane	3.1×10^{-2}		Duchowicz et al. (2020)	V	187
$C_3H_5Cl_3$	1.4×10^{-2}		Yaws et al. (2005)	X	448
[598-77-6]	4.0×10^{-3}		Duchowicz et al. (2020)	Q	
GRSQYISVQKPZCW-UHFFFAOYSA-N	7.9×10^{-3}		Hilal et al. (2008)	Q	
	3.1×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.4×10^{-3}		Katritzky et al. (1998)	Q	
1,2,3-trichloropropane	3.6×10^{-2}	3700	Burkholder et al. (2019)	L	
$C_3H_5Cl_3$	3.6×10^{-2}	3700	Burkholder et al. (2015)	L	
[96-18-4]	3.3×10^{-2}	1900	Brockbank (2013)	L	
CFXQEHVMCRXUSD-UHFFFAOYSA-N	3.6×10^{-2}	3700	Staudinger and Roberts (2001)	L	
	3.4×10^{-2}	3700	Staudinger and Roberts (1996)	L	
	4.2×10^{-2}	7200	Hiatt (2013)	M	
	2.8×10^{-2}	5300	Kondoh and Nakajima (1997)	M	
	4.4×10^{-2}	4000	Tancrède and Yanagisawa (1990)	M	
	3.3×10^{-2}		Albanese et al. (1987)	M	
	2.9×10^{-2}	3500	Leighton and Calo (1981)	M	
	2.6×10^{-2}		Mackay et al. (2006b)	V	
	2.6×10^{-2}		Mackay et al. (1993)	V	
	3.1×10^{-2}		Dilling (1977)	V	
	2.6×10^{-2}		Yaws (2003)	X	238
	2.2×10^{-2}		Yaws et al. (2005)	X	448
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	5.3×10^{-3}		Duchowicz et al. (2020)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	2.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	1.4×10^{-2}		Modarresi et al. (2007)	Q	68
		4000	Kühne et al. (2005)	Q	
	2.9×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	3.9×10^{-3}		Katritzky et al. (1998)	Q	
	2.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		4100	Kühne et al. (2005)	?	
	2.6×10^{-2}		Yaws (1999)	?	21
	2.9×10^{-2}		Yaws and Yang (1992)	?	21
1,1,2,2,3-pentachloropropane	1.4×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_3H_3Cl_5$	7.3×10^{-2}		Zhang et al. (2010)	Q	288, 290
[16714-68-4]	6.2×10^{-1}		Zhang et al. (2010)	Q	288, 291
IYFMQUDCYNWFTL-UHFFFAOYSA-N	8.6×10^{-3}		Zhang et al. (2010)	Q	288, 292

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloro-2-methylpropane	8.3×10^{-3}		Mackay and Shiu (1981)	L	
C_4H_9Cl	5.0×10^{-4}		Duchowicz et al. (2020)	V	187
[513-36-0]	5.0×10^{-4}		Duchowicz et al. (2020)	Q	
QTBFPMKWQKYFLR-UHFFFAOYSA-N	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	7.3×10^{-4}		Hilal et al. (2008)	Q	
	8.5×10^{-4}		Modarresi et al. (2007)	Q	68
	8.6×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	6.3×10^{-4}		Yaws and Yang (1992)	?	21, 12
2-chloro-2-methylpropane	1.6×10^{-4}	5600	Clarke et al. (1962)	M	
C_4H_9Cl	7.7×10^{-4}		Duchowicz et al. (2020)	V	187
(*tert*-butyl chloride)	1.2×10^{-3}		Yaws (2003)	X	238, 81
[507-20-0]	2.2×10^{-4}		Duchowicz et al. (2020)	Q	
NBRKLOOSMBRFMH-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.2×10^{-4}		Hilal et al. (2008)	Q	
	6.5×10^{-4}		Modarresi et al. (2007)	Q	68
	6.9×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	3.1×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	7.7×10^{-4}		Yaws (1999)	?	21, 81
	6.4×10^{-5}		Abraham et al. (1990)	?	
1-chlorobutane	5.6×10^{-4}	4500	Brockbank (2013)	L	
C_4H_9Cl	6.7×10^{-4}		Dohnal and Hovorka (1999)	M	12
(butyl chloride)	5.3×10^{-4}		Li et al. (1993)	M	
[109-69-3]	5.9×10^{-4}	3500	Leighton and Calo (1981)	M	
VFWCMGCRMGJXDK-UHFFFAOYSA-N	3.3×10^{-4}		Sato and Nakajima (1979b)	M	14
	4.8×10^{-4}		Mackay et al. (2006b)	V	
	4.8×10^{-4}		Mackay et al. (1993)	V	
	5.3×10^{-4}		Abraham (1984)	V	
	5.1×10^{-4}		Hine and Mookerjee (1975)	V	
	5.9×10^{-4}		Yaws (2003)	X	238
	4.4×10^{-4}		Keshavarz et al. (2022)	Q	
	1.3×10^{-3}		Duchowicz et al. (2020)	Q	
	3.1×10^{-4}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	4.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
	9.0×10^{-4}		Hilal et al. (2008)	Q	
	8.7×10^{-4}		Modarresi et al. (2007)	Q	68
		3700	Kühne et al. (2005)	Q	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.1×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	1.9×10^{-4}		Yao et al. (2002)	Q	230
	5.4×10^{-4}		English and Carroll (2001)	Q	231, 232
	1.4×10^{-3}		Katritzky et al. (1998)	Q	
	1.3×10^{-3}		Russell et al. (1992)	Q	280
	3.6×10^{-4}		Suzuki et al. (1992)	Q	233
	5.0×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	5.9×10^{-4}		Duchowicz et al. (2020)	?	186, 21
	6.5×10^{-4}		Mackay et al. (2006b)	?	
		3700	Kühne et al. (2005)	?	
	5.9×10^{-4}		Yaws (1999)	?	21
	3.4×10^{-4}		Abraham and Weathersby (1994)	?	21
	6.5×10^{-4}		Mackay et al. (1993)	?	
	5.6×10^{-4}		Hoff et al. (1993)	?	21
	5.8×10^{-4}		Yaws and Yang (1992)	?	21
	5.3×10^{-4}		Abraham et al. (1990)	?	
2-chlorobutane	4.1×10^{-4}	4500	Brockbank (2013)	L	
C_4H_9Cl	4.1×10^{-4}	4500	Leighton and Calo (1981)	M	
(*sec*-butyl chloride)	5.3×10^{-4}		Mackay et al. (2006b)	V	
[78-86-4]	5.3×10^{-4}		Mackay et al. (1993)	V	
BSPCSKHALVHRSR-UHFFFAOYSA-N	5.1×10^{-4}		Yaws (2003)	X	238
	4.4×10^{-4}		Keshavarz et al. (2022)	Q	
	5.9×10^{-4}		Duchowicz et al. (2020)	Q	300
	5.3×10^{-4}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	3.7×10^{-4}		Gharagheizi et al. (2010)	Q	247
	6.2×10^{-4}		Hilal et al. (2008)	Q	
	8.2×10^{-4}		Modarresi et al. (2007)	Q	68
		3700	Kühne et al. (2005)	Q	
	4.2×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	1.3×10^{-4}		Yao et al. (2002)	Q	230
	4.7×10^{-4}		English and Carroll (2001)	Q	231, 275
	1.9×10^{-3}		Katritzky et al. (1998)	Q	
	4.2×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	4.1×10^{-4}		Duchowicz et al. (2020)	?	186, 21
	4.4×10^{-4}		Mackay et al. (2006b)	?	
		4500	Kühne et al. (2005)	?	
	5.2×10^{-4}		Yaws (1999)	?	21
	4.4×10^{-4}		Mackay et al. (1993)	?	
	5.3×10^{-4}		Yaws and Yang (1992)	?	21
	4.0×10^{-4}		Abraham et al. (1990)	?	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1-dichlorobutane	1.3×10^{-3}		Duchowicz et al. (2020)	V	187
$C_4H_8Cl_2$	1.3×10^{-3}		Hine and Mookerjee (1975)	V	
[541-33-3]	2.7×10^{-3}		Duchowicz et al. (2020)	Q	
SEQRDAAUNCRFIT-UHFFFAOYSA-N	2.5×10^{-3}		Hilal et al. (2008)	Q	
	9.2×10^{-4}		Modarresi et al. (2007)	Q	68
	1.4×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.6×10^{-3}		English and Carroll (2001)	Q	231, 261
	1.3×10^{-3}		Katritzky et al. (1998)	Q	
	9.2×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
1,4-dichlorobutane	2.0×10^{-2}	3600	Brockbank (2013)	L	
$C_4H_8Cl_2$	1.2×10^{-2}		Albanese et al. (1987)	M	
[110-56-5]	2.0×10^{-2}	3100	Leighton and Calo (1981)	M	
KJDRSWPQXHESDQ-UHFFFAOYSA-N	2.2×10^{-2}		Keshavarz et al. (2022)	Q	
	3.6×10^{-3}		Duchowicz et al. (2020)	Q	300
	2.6×10^{-2}		Hilal et al. (2008)	Q	
	4.5×10^{-3}		Modarresi et al. (2007)	Q	68
		4000	Kühne et al. (2005)	Q	
	2.0×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.9×10^{-3}		English and Carroll (2001)	Q	231, 232
	3.9×10^{-3}		Katritzky et al. (1998)	Q	
	1.1×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	2.0×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		3700	Kühne et al. (2005)	?	
	2.0×10^{-2}		Abraham et al. (1990)	?	
2,3-dichlorobutane	1.4×10^{-3}		Duchowicz et al. (2020)	V	187
$C_4H_8Cl_2$	2.5×10^{-3}		Yaws et al. (2005)	X	448
[7581-97-7]	8.4×10^{-4}		Duchowicz et al. (2020)	Q	
RMISVOPUIFJTEO-UHFFFAOYSA-N	2.8×10^{-3}		Hilal et al. (2008)	Q	
	2.5×10^{-3}		Modarresi et al. (2007)	Q	68
	1.4×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	3.1×10^{-3}		Katritzky et al. (1998)	Q	
1-chloropentane	4.1×10^{-4}	4000	Brockbank (2013)	L	1
$C_5H_{11}Cl$	4.2×10^{-4}		Li et al. (1993)	M	
[543-59-9]	4.1×10^{-4}	4700	Leighton and Calo (1981)	M	
SQCZQTSHSZLZIQ-UHFFFAOYSA-N	2.7×10^{-4}		Sato and Nakajima (1979b)	M	14
	4.5×10^{-4}		Mackay et al. (2006b)	V	
	4.5×10^{-4}		Mackay et al. (1993)	V	
	4.5×10^{-4}		Abraham (1984)	V	
	4.3×10^{-4}		Amoore and Buttery (1978)	V	
	4.5×10^{-4}		Hine and Mookerjee (1975)	V	
	1.9×10^{-4}		Yaws (2003)	X	238
	5.9×10^{-4}		Keshavarz et al. (2022)	Q	
	1.3×10^{-3}		Duchowicz et al. (2020)	Q	300
	2.5×10^{-4}		Gharagheizi et al. (2012)	Q	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
	7.3×10^{-4}		Hilal et al. (2008)	Q	
	7.1×10^{-4}		Modarresi et al. (2007)	Q	68
		4000	Kühne et al. (2005)	Q	
	4.2×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	4.1×10^{-4}		English and Carroll (2001)	Q	231, 232
	1.6×10^{-3}		Katritzky et al. (1998)	Q	
	2.8×10^{-4}		Suzuki et al. (1992)	Q	233
	3.9×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	4.1×10^{-4}		Duchowicz et al. (2020)	?	186, 21
	4.2×10^{-4}		Mackay et al. (2006b)	?	
		4400	Kühne et al. (2005)	?	
	1.9×10^{-4}		Yaws (1999)	?	21
	2.8×10^{-4}		Abraham and Weathersby (1994)	?	21
	4.2×10^{-4}		Mackay et al. (1993)	?	
	2.0×10^{-4}		Yaws and Yang (1992)	?	21
	4.5×10^{-4}		Abraham et al. (1990)	?	
2-chloropentane $C_5H_{11}Cl$ [625-29-6] NFRKUDYZEVQXTE-UHFFFAOYSA-N	6.7×10^{-4}		Duchowicz et al. (2020)	V	187
	3.6×10^{-4}		Hine and Mookerjee (1975)	V	
	5.8×10^{-4}		Duchowicz et al. (2020)	Q	
	4.8×10^{-4}		Hilal et al. (2008)	Q	
	6.0×10^{-4}		Modarresi et al. (2007)	Q	68
	6.7×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	3.6×10^{-4}		English and Carroll (2001)	Q	231, 275
	2.2×10^{-3}		Katritzky et al. (1998)	Q	
	2.5×10^{-4}		Suzuki et al. (1992)	Q	233
	3.3×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	3.6×10^{-4}		Abraham et al. (1990)	?	
3-chloropentane $C_5H_{11}Cl$ [616-20-6] CXQSCYIVCSCSES-UHFFFAOYSA-N	3.8×10^{-4}		Duchowicz et al. (2020)	V	187
	3.8×10^{-4}		Meylan and Howard (1991)	V	
	3.8×10^{-4}		Hine and Mookerjee (1975)	V	
	5.8×10^{-4}		Duchowicz et al. (2020)	Q	
	4.7×10^{-4}		Hilal et al. (2008)	Q	
	5.9×10^{-4}		Modarresi et al. (2007)	Q	68
	4.5×10^{-4}		English and Carroll (2001)	Q	231, 261
	2.5×10^{-4}		Suzuki et al. (1992)	Q	233
	3.9×10^{-4}		Meylan and Howard (1991)	Q	
	3.4×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	3.8×10^{-4}		Abraham et al. (1990)	?	
1,2-dichloropentane $C_5H_{10}Cl_2$ [1674-33-5] PPLBPDUKNRCHGG-UHFFFAOYSA-N	4.8×10^{-3}		Yaws et al. (2005)	X	448
	3.1×10^{-3}		Hilal et al. (2008)	Q	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,5-dichloropentane	1.0×10^{-2}	4000	Brockbank (2013)	L	
$C_5H_{10}Cl_2$	1.8×10^{-2}	1600	Leighton and Calo (1981)	M	
[628-76-2]	2.9×10^{-2}		Keshavarz et al. (2022)	Q	
LBKDGROORAKTLC-UHFFFAOYSA-N	3.6×10^{-3}		Duchowicz et al. (2020)	Q	185
	2.0×10^{-2}		Hilal et al. (2008)	Q	
	3.8×10^{-3}		Modarresi et al. (2007)	Q	68
		4400	Kühne et al. (2005)	Q	
	1.8×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	4.2×10^{-3}		Katritzky et al. (1998)	Q	
	1.8×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		4100	Kühne et al. (2005)	?	
2,3-dichloropentane	2.9×10^{-3}		Yaws et al. (2005)	X	448
$C_5H_{10}Cl_2$	2.8×10^{-3}		Hilal et al. (2008)	Q	
[600-11-3]					
HVFJQRZGBBKTPL-UHFFFAOYSA-N					
2-chloro-2-methylbutane	3.1×10^{-3}		Yaws (1999)	?	21
$C_5H_{11}Cl$	3.0×10^{-3}		Yaws and Yang (1992)	?	21
[594-36-5]					
CRNIHJHMEQZAAS-UHFFFAOYSA-N					
1-chlorohexane	3.1×10^{-4}		Li et al. (1993)	M	
$C_6H_{13}Cl$	4.1×10^{-4}	4500	Leighton and Calo (1981)	M	
[544-10-5]	8.0×10^{-4}		Keshavarz et al. (2022)	Q	
MLRVZFYXUZQSRU-UHFFFAOYSA-N	1.3×10^{-3}		Duchowicz et al. (2020)	Q	300
	6.1×10^{-4}		Hilal et al. (2008)	Q	
	6.1×10^{-4}		Modarresi et al. (2007)	Q	68
		4300	Kühne et al. (2005)	Q	
	3.5×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	3.1×10^{-4}		English and Carroll (2001)	Q	231, 232
	1.7×10^{-3}		Katritzky et al. (1998)	Q	
	3.1×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	4.1×10^{-4}		Duchowicz et al. (2020)	?	186, 21
		4400	Kühne et al. (2005)	?	
	4.0×10^{-4}		Abraham et al. (1990)	?	
2-chlorohexane	5.0×10^{-4}		Yaws et al. (2005)	X	448
$C_6H_{13}Cl$	4.2×10^{-4}		Hilal et al. (2008)	Q	
[638-28-8]					
GLCIPJOIEVLTPR-UHFFFAOYSA-N					
3-chlorohexane	5.0×10^{-4}		Yaws et al. (2005)	X	448
$C_6H_{13}Cl$	5.0×10^{-4}		Hilal et al. (2008)	Q	
[2346-81-8]					
BXSMMAVTEURRGG-UHFFFAOYSA-N					

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloroheptane $C_7H_{15}Cl$ [629-06-1] DZMDPHNGKBEVRE-UHFFFAOYSA-N	2.5×10^{-4} 5.1×10^{-4} 5.1×10^{-4} 2.3×10^{-4} 2.4×10^{-4} 2.5×10^{-4}		Abraham (1984) Hilal et al. (2008) Modarresi et al. (2007) English and Carroll (2001) Nirmalakhandan et al. (1997) Abraham et al. (1990)	V Q Q Q Q ?	 68 231, 232
2-chloroheptane $C_7H_{15}Cl$ [1001-89-4] PTSLUOSUHFGQHV-UHFFFAOYSA-N	3.9×10^{-4} 3.4×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	448
3-chloroheptane $C_7H_{15}Cl$ [999-52-0] DMKNOEJJJSHSML-UHFFFAOYSA-N	3.6×10^{-4} 3.4×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	448
4-chloroheptane $C_7H_{15}Cl$ [998-95-8] MGSGWAXIEMEWCQ-UHFFFAOYSA-N	3.6×10^{-4} 3.5×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	448
1-chlorooctane $C_8H_{17}Cl$ [111-85-3] CNDHHGUSRIZDSL-UHFFFAOYSA-N	2.6×10^{-4} 1.9×10^{-4} 2.6×10^{-4} 1.3×10^{-3} 1.6×10^{-4} 4.2×10^{-4} 2.6×10^{-4} 1.8×10^{-3}	 6100 	Duchowicz et al. (2020) Sarraute et al. (2004) Yaws et al. (2005) Duchowicz et al. (2020) HSDB (2015) Hilal et al. (2008) Yaffe et al. (2003) Katritzky et al. (1998)	V V X Q Q Q Q Q	187 448 100 249, 250
2-chlorooctane $C_8H_{17}Cl$ [628-61-5] HKDCIIMOALDWHF-UHFFFAOYSA-N	2.7×10^{-4} 3.1×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	448
3-(chloromethyl)-heptane $C_8H_{17}Cl$ [123-04-6] WLVCBAMXYMWGLJ-UHFFFAOYSA-N	4.5×10^{-4} 4.9×10^{-4}		Hilal et al. (2008) Modarresi et al. (2007)	Q Q	 68
1,8-dichlorooctane $C_8H_{16}Cl_2$ [2162-99-4] WXYMNDFVLNUAIA-UHFFFAOYSA-N	7.1×10^{-3}	7100	Sarraute et al. (2006)	M	680
1-chlorononane $C_9H_{19}Cl$ [2473-01-0] RKAMCQVGHFRILV-UHFFFAOYSA-N	1.6×10^{-4} 3.5×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	448

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-chlorononane $C_9H_{19}Cl$ [2216-36-6] DTWJISBCMBWFNY-UHFFFAOYSA-N	2.7×10^{-4} 3.0×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	448
5-chlorononane $C_9H_{19}Cl$ [28123-70-8] GHLDSOWZIOPMTC-UHFFFAOYSA-N	2.2×10^{-4} 2.6×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	448
1-chlorodecane $C_{10}H_{21}Cl$ [1002-69-3] ZTEHOZMYMCEYRM-UHFFFAOYSA-N	1.6×10^{-4} 2.5×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	448
1,10-dichlorodecane $C_{10}H_{20}Cl_2$ [2162-98-3] RBBNTRDPSVZESY-UHFFFAOYSA-N	2.0×10^{-3} 5.3×10^{-3}		Drouillard et al. (1998) Hilal et al. (2008)	V Q	
1,2,9,10-tetrachlorodecane $C_{10}H_{18}Cl_4$ [205646-11-3] VXBHNYIEBLRXAW-UHFFFAOYSA-N	5.6×10^{-2} 6.2×10^{-2} 3.9×10^{-2} 6.2×10^{-4} 1.4×10^{-2}		Drouillard et al. (1998) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Hilal et al. (2008)	M Q Q Q Q	 243, 244 245 246
pentachlorodecane isomers $C_{10}H_{17}Cl_5$ [175801-37-3] AMKBEJYNNQNKGD-UHFFFAOYSA-N	2.0×10^{-1} 3.8×10^{-1}		Drouillard et al. (1998) Drouillard et al. (1998)	M M	
1-chloroundecane $C_{11}H_{23}Cl$ [2473-03-2] ZHKKNUKCXPWZOP-UHFFFAOYSA-N	1.7×10^{-4} 2.3×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	448
1,2,10,11-tetrachloroundecane $C_{11}H_{20}Cl_4$ [210049-49-3] VVAAXDBMZVCVPA-UHFFFAOYSA-N	1.6×10^{-1} 4.9×10^{-2} 3.1×10^{-2} 4.9×10^{-4} 1.1×10^{-2}		Drouillard et al. (1998) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Hilal et al. (2008)	M Q Q Q Q	 243, 244 245 246
pentachloroundecane isomers $C_{11}H_{19}Cl_5$ [210175-48-7] BBCUCNDIXLWBNQ-UHFFFAOYSA-N	6.8×10^{-1} 1.5		Drouillard et al. (1998) Drouillard et al. (1998)	M M	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chlorododecane $C_{12}H_{25}Cl$ [112-52-7] YAYNEUUHHLGGAH-UHFFFAOYSA-N	2.3×10^{-4} 1.9×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	448
1,12-dichlorododecane $C_{12}H_{24}Cl_2$ [3922-28-9] RNXPZVYZVHJVHM-UHFFFAOYSA-N	1.5×10^{-3} 3.1×10^{-3}		Drouillard et al. (1998) Hilal et al. (2008)	V Q	
1-chlorotridecane $C_{13}H_{27}Cl$ [822-13-9] ASZMYJSJEOGSBR-UHFFFAOYSA-N	2.9×10^{-4} 1.4×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	448
1-chlorotetradecane $C_{14}H_{29}Cl$ [2425-54-9] RNHWYOLIEJIAMV-UHFFFAOYSA-N	3.9×10^{-4} 1.2×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	448
tetrachlorocyclopentane $C_5H_6Cl_4$ [59808-78-5] ZFMWDTNZPKDVBU-UHFFFAOYSA-N	6.4×10^{-3} 4.1×10^{-1} 1.5 2.9×10^{-2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
1,1,2,3,3,4- hexachlorocyclopentane $C_5H_4Cl_6$ [68258-91-3] RPUFWOAXMFQSDJ-UHFFFAOYSA-N	5.1×10^{-2} 1.9×10^{-1} 1.6 2.2×10^{-2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
1,1,2,3,3,4,5- heptachlorocyclopentane $C_5H_3Cl_7$ [68258-90-2] XCEUTYGYMGYCBG-UHFFFAOYSA-N	1.5×10^{-1} 7.9×10^{-1} 1.6 8.6×10^{-2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
1,2,3,3,4,5- hexachlorocyclopentene $C_5H_2Cl_6$ OSRFTCIVMWPVNP-UHFFFAOYSA-N	1.4×10^{-2} 4.4×10^{-2} 4.4×10^{-1} 6.4×10^{-2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
heptachlorocyclopentene C_5HCl_7 [62111-47-1] AJUXFTIOMRYFRL-UHFFFAOYSA-N	3.9×10^{-2} 3.5×10^{-2} 8.4×10^{-2} 5.4×10^{-2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chlorocyclohexane	2.8×10^{-3}	3300	Bakierowska and Trzeszczyński (2003)	M	
$C_6H_{11}Cl$	3.2×10^{-3}		Hilal et al. (2008)	Q	
[542-18-7]		4200	Kühne et al. (2005)	Q	
UNFUYWDGSFDHCW-UHFFFAOYSA-N		3200	Kühne et al. (2005)	?	
α-1,2,3,4,5,6-hexachlorocyclohexane	1.5		Xiao et al. (2004)	L	368
$C_6H_6Cl_6$	1.4		Xiao et al. (2004)	L	369
(α-lindane; α-HCH)	3.0	5500	Cetin et al. (2006)	M	
[319-84-6]	1.7	7500	Sahsuvar et al. (2003)	M	
JLYXXMFPNIAWKQ-SHFUYGGZSA-N	8.1×10^{-1}		Altschuh et al. (1999)	M	
	1.3	6500	Kucklick et al. (1991)	M	
	4.2×10^{-1}		Atlas et al. (1982)	M	681
	1.1		Mackay et al. (2006d)	V	
	9.1×10^{-1}		Ballschmiter and Wittlinger (1991)	V	
	2.3		Calamari et al. (1991)	V	12
	1.1		Suntio et al. (1988)	V	12
	5.9×10^{-3}	3900	Paasivirta et al. (1999)	T	
	1.8		Suntio et al. (1988)	C	682
	3.9×10^{-2}		Zhang et al. (2010)	Q	288, 289
	7.7		Zhang et al. (2010)	Q	288, 290
	4.0×10^{1}		Zhang et al. (2010)	Q	288, 291
	3.8×10^{-1}		Zhang et al. (2010)	Q	288, 292
	1.1		Modarresi et al. (2007)	Q	68
		7100	Kühne et al. (2005)	Q	
		7100	Kühne et al. (2005)	?	
β-1,2,3,4,5,6-hexachlorocyclohexane	2.7×10^{1}		Xiao et al. (2004)	L	368
$C_6H_6Cl_6$	2.7×10^{1}		Xiao et al. (2004)	L	369
(β-lindane; β-HCH)	2.8×10^{1}	7800	Sahsuvar et al. (2003)	M	
[319-85-7]	2.2×10^{1}		Altschuh et al. (1999)	M	
JLYXXMFPNIAWKQ-CDRYSYESSA-N	8.6		Mackay et al. (2006d)	V	
	1.4×10^{1}		Ballschmiter and Wittlinger (1991)	V	
	8.3		Suntio et al. (1988)	V	12
	5.6×10^{1}		Suntio et al. (1988)	C	683
	6.7×10^{-1}		Ryan et al. (1988)	C	
	5.8		Keshavarz et al. (2022)	Q	
	3.0×10^{-2}		Duchowicz et al. (2020)	Q	185
	1.1		Modarresi et al. (2007)	Q	68
		7100	Kühne et al. (2005)	Q	
	2.2×10^{1}		Duchowicz et al. (2020)	?	186, 21
		7800	Kühne et al. (2005)	?	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
γ-1,2,3,4,5,6- hexachlorocyclohexane	3.7		Xiao et al. (2004)	L	368
$C_6H_6Cl_6$	3.3		Xiao et al. (2004)	L	369
(γ-lindane; lindane; γ-HCH)	3.1		Mackay and Shiu (1981)	L	
[58-89-9]	3.1		Chao et al. (2017)	M	
JLYXXMFPNIAWKQ-GNIYUCBRSA-N	3.9	3300	Cetin et al. (2006)	M	
	6.0	6200	Xie et al. (2004)	M	
	4.3	7500	Sahsuvar et al. (2003)	M	
	1.9		Altschuh et al. (1999)	M	
	2.8	5500	Kucklick et al. (1991)	M	
	4.9		Fendinger et al. (1989)	M	73
	5.0		Fendinger and Glotfelty (1988)	M	73
	6.7		Mackay et al. (2006d)	V	
	3.3		Siebers et al. (1994)	V	
	1.0×10^{1}		Ballschmiter and Wittlinger (1991)	V	
	5.9		Calamari et al. (1991)	V	12
	3.7		McLachlan et al. (1990)	V	375
	7.7		Suntio et al. (1988)	V	12
	6.7×10^{-1}		Caron et al. (1985)	V	
	7.9		Burkhard and Guth (1981)	V	
	3.1		Chiou et al. (1980)	V	
	2.0×10^{1}		Mackay and Leinonen (1975)	V	
	6.2×10^{-2}	7100	Paasivirta et al. (1999)	T	
	3.1×10^{1}		McCarty (1980)	X	370
	2.0×10^{1}		Suntio et al. (1988)	C	12
	5.0		Suntio et al. (1988)	C	683
	1.4		Suntio et al. (1988)	C	
	5.8		Keshavarz et al. (2022)	Q	
	3.0×10^{-2}		Duchowicz et al. (2020)	Q	
	3.9×10^{-2}		Zhang et al. (2010)	Q	288, 289
	7.7		Zhang et al. (2010)	Q	288, 290
	4.7×10^{1}		Zhang et al. (2010)	Q	288, 291
	3.8×10^{-1}		Zhang et al. (2010)	Q	288, 292
	5.3		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	68
		7100	Kühne et al. (2005)	Q	
	1.9		Duchowicz et al. (2020)	?	186, 21
		6200	Kühne et al. (2005)	?	
	2.2×10^{1}		Brimblecombe (1986)	?	81

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
δ-1,2,3,4,5,6- hexachlorocyclohexane	2.3×10^{1}		Duchowicz et al. (2020)	V	187
$C_6H_6Cl_6$	2.3×10^{1}		HSDB (2015)	V	
(δ-lindane; δ-HCH)	1.4×10^{1}		Mackay et al. (2006d)	V	
[319-86-8]	1.4×10^{1}		Suntio et al. (1988)	V	12
JLYXXMFPNIAWKQ-GPIVLXJGSA-N	5.6×10^{1}		Suntio et al. (1988)	C	683
	3.0×10^{-2}		Duchowicz et al. (2020)	Q	
	1.1		Modarresi et al. (2007)	Q	68
4,5,6,7,8,8-hexachloro-3a,4,7,7a- tetrahydro-4,7-methano-1H-indene	2.0×10^{-2}		HSDB (2015)	Q	100
$C_{10}H_6Cl_6$	2.0×10^{-2}		Zhang et al. (2010)	Q	288, 289
[3734-48-3]	6.2×10^{-3}		Zhang et al. (2010)	Q	288, 290
XCJXQCUJXDUNDN-UHFFFAOYSA-N	2.2		Zhang et al. (2010)	Q	288, 291
	4.2×10^{-1}		Zhang et al. (2010)	Q	288, 292
dienochlor	1.8×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{10}Cl_{10}$	1.2×10^{-2}		Duchowicz et al. (2020)	Q	
[2227-17-0]					
LWLJUMBEZJHXHV-UHFFFAOYSA-N					
mirex	1.2×10^{-2}	11000	Yin and Hassett (1986)	M	
$C_{10}Cl_{12}$	1.2×10^{-3}		Mackay et al. (2006d)	V	
(dodecachloropentacyclodecane)	5.8×10^{-2}		McLachlan et al. (1990)	V	375
[2385-85-5]	1.2×10^{-3}		Suntio et al. (1988)	V	12
GVYLCNUFSHDAAW-UHFFFAOYSA-N	5.2×10^{-2}		Smith and Bomberger (1980)	V	24
	9.9×10^{-4}		Suntio et al. (1988)	C	12
	1.3×10^{-1}		Keshavarz et al. (2022)	Q	
	4.3		Duchowicz et al. (2020)	Q	
	3.9×10^{-3}		Hilal et al. (2008)	Q	
		10000	Kühne et al. (2005)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		11000	Kühne et al. (2005)	?	
dechlorane plus	1.3		HSDB (2015)	Q	100
$C_{18}H_{12}Cl_{12}$	1.3		Zhang et al. (2010)	Q	288, 289
[13560-89-9]	7.0×10^{-2}		Zhang et al. (2010)	Q	288, 290
UGQQAJOWXNCOPY-UHFFFAOYSA-N	2.1×10^{3}		Zhang et al. (2010)	Q	288, 291
	4.6×10^{1}		Zhang et al. (2010)	Q	288, 292
chloroethene	4.1×10^{-4}	2500	Schwardt et al. (2021)	L	1
CH_2CHCl	3.8×10^{-4}	3100	Burkholder et al. (2019)	L	
(vinyl chloride)	3.8×10^{-4}	3100	Burkholder et al. (2015)	L	
[75-01-4]	4.3×10^{-4}	3000	Brockbank (2013)	L	1
BZHJMEDXRYGGRV-UHFFFAOYSA-N	3.8×10^{-4}	3100	Warneck (2007)	L	
	3.9×10^{-4}	3100	Staudinger and Roberts (2001)	L	
	3.9×10^{-4}	3100	Staudinger and Roberts (1996)	L	
	4.5×10^{-4}	3000	Wilhelm et al. (1977)	L	
	3.9×10^{-4}	2400	Schwardt et al. (2021)	M	684, 11

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.9×10^{-4}	3200	Hiatt (2013)	M	
	4.1×10^{-4}	2300	Chen et al. (2012)	M	
			Chiang et al. (1998)	M	654
	4.0×10^{-4}	2900	Ashworth et al. (1988)	M	279
	3.7×10^{-4}	3300	Gossett (1987)	M	
	8.5×10^{-6}		Pearson and McConnell (1975)	M	651, 375
			Mackay et al. (2006b)	V	685
	9.1×10^{-4}		Lide and Frederikse (1995)	V	
	1.2×10^{-4}		Mackay et al. (1993)	V	
	1.1×10^{-4}		Hwang et al. (1992)	V	
	5.4×10^{-4}		Smith and Bomberger (1980)	V	24
	9.4×10^{-6}		Dilling (1977)	V	
	4.2×10^{-4}		Dilling (1977)	V	
	1.8×10^{-4}		Hine and Mookerjee (1975)	V	
	4.4×10^{-4}		Yaws (2003)	X	238
	6.5×10^{-4}		Ryan et al. (1988)	C	
	6.0×10^{-4}		Wang et al. (2017)	Q	81, 239
	2.4×10^{-4}		Wang et al. (2017)	Q	81, 240
	6.3×10^{-4}		Wang et al. (2017)	Q	81, 241
	3.4×10^{-3}		Li et al. (2014)	Q	242
	4.9×10^{-4}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	2.6×10^{-4}		Gharagheizi et al. (2010)	Q	247
	2.1×10^{-4}		Hilal et al. (2008)	Q	
	1.2×10^{-3}		Modarresi et al. (2007)	Q	68
	4.2×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	1.4×10^{-3}		Yao et al. (2002)	Q	230
	2.4×10^{-3}		Suzuki et al. (1992)	Q	233
	2.0×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	8.1×10^{-4}		Irmann (1965)	Q	
	3.7×10^{-4}		Mackay et al. (2006b)	?	
	4.4×10^{-4}		Yaws (1999)	?	21
	3.9×10^{-4}	2700	Yaws et al. (1999)	?	21
	3.7×10^{-4}		Mackay et al. (1993)	?	
	4.4×10^{-4}		Yaws and Yang (1992)	?	21
	4.5×10^{-4}		Abraham et al. (1990)	?	
chloroethene-d3 CD_2CDCl (vinyl chloride-d3) [6745-35-3] BZHJMEDXRYGGRV-FUDHJZNOSA-N	3.8×10^{-4}	3100	Hiatt (2013)	M	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1-dichloroethene	3.7×10^{-4}	3500	Schwardt et al. (2021)	L	1
CH_2CCl_2	3.7×10^{-4}	3400	Burkholder et al. (2019)	L	
[75-35-4]	3.7×10^{-4}	3400	Burkholder et al. (2015)	L	
LGXVIGDEPROXKC-UHFFFAOYSA-N	3.1×10^{-4}	3900	Brockbank (2013)	L	1, 686
	3.7×10^{-4}	3400	Warneck (2007)	L	
	4.0×10^{-4}	3800	Fogg and Sangster (2003)	L	
	3.4×10^{-4}	4000	Staudinger and Roberts (2001)	L	
	3.4×10^{-4}	3900	Staudinger and Roberts (1996)	L	
	4.0×10^{-4}	3400	Schwardt et al. (2021)	M	687
	4.1×10^{-4}	4600	Hiatt (2013)	M	
	3.7×10^{-4}	4200	Dewulf et al. (1999)	M	
	4.4×10^{-4}		Chiang et al. (1998)	M	12
	4.6×10^{-4}	1600	Kondoh and Nakajima (1997)	M	
	3.5×10^{-4}	3300	Tse et al. (1992)	M	
	3.4×10^{-4}	4500	Bissonette et al. (1990)	M	
	3.7×10^{-4}	2900	Ashworth et al. (1988)	M	279, 688
	3.8×10^{-4}	3700	Gossett (1987)	M	
	1.3×10^{-4}		Yurteri et al. (1987)	M	12
	2.6×10^{-4}	4600	Leighton and Calo (1981)	M	
	1.4×10^{-4}	6600	Ervin et al. (1980)	M	
	6.6×10^{-4}		Warner et al. (1980)	M	
	6.6×10^{-5}		Pearson and McConnell (1975)	M	651, 12
	4.3×10^{-4}		Mackay et al. (2006b)	V	
	3.3×10^{-4}		Lide and Frederikse (1995)	V	
	4.3×10^{-4}		Mackay et al. (1993)	V	
	7.5×10^{-5}		Mackay and Shiu (1981)	V	
	6.5×10^{-4}		Warner et al. (1980)	V	
	5.2×10^{-5}		Dilling (1977)	V	653
	6.1×10^{-5}		Dilling (1977)	V	12
	4.3×10^{-4}		Yaws (2003)	X	238
	6.4×10^{-4}	1200	Goldstein (1982)	X	299
	2.2×10^{-3}		Ryan et al. (1988)	C	
	6.6×10^{-4}		Shen (1982)	C	
	1.0×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.3×10^{-4}		Wang et al. (2017)	Q	81, 240
	4.5×10^{-4}		Wang et al. (2017)	Q	81, 241
	1.3×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
	1.3×10^{-4}		Hilal et al. (2008)	Q	
	8.9×10^{-4}		Modarresi et al. (2007)	Q	68
		3300	Kühne et al. (2005)	Q	
	3.8×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	2.6×10^{-3}		Yao et al. (2002)	Q	230, 268

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.7×10^{-4}		Katritzky et al. (1998)	Q	
	3.8×10^{-4}		Mackay et al. (2006b)	?	
		3700	Kühne et al. (2005)	?	
	4.3×10^{-4}		Yaws (1999)	?	21
	3.8×10^{-4}		Mackay et al. (1993)	?	
	4.3×10^{-4}		Yaws and Yang (1992)	?	21
	2.7×10^{-4}		Abraham et al. (1990)	?	
1,2-dichloroethene	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
$C_2H_2Cl_2$	5.1×10^{-3}		Duchowicz et al. (2020)	Q	300
[540-59-0]	3.7×10^{-4}		Hilal et al. (2008)	Q	
KFUSEUYYWQURPO-UHFFFAOYSA-N	2.3×10^{-3}		Modarresi et al. (2007)	Q	68
	1.4×10^{-3}		Yaffe et al. (2003)	Q	249, 273
	6.2×10^{-4}		Katritzky et al. (1998)	Q	
	4.5×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	2.4×10^{-3}		Duchowicz et al. (2020)	?	186, 21
(*Z*)-1,2-dichloroethene	2.3×10^{-3}	3400	Schwardt et al. (2021)	L	1
CHClCHCl	2.6×10^{-3}	3700	Burkholder et al. (2019)	L	
(*cis*-1,2-dichloroethene)	2.6×10^{-3}	3700	Burkholder et al. (2015)	L	
[156-59-2]	2.4×10^{-3}	4000	Brockbank (2013)	L	1
KFUSEUYYWQURPO-UPHRSURJSA-N	2.6×10^{-3}	3700	Warneck (2007)	L	
	2.5×10^{-3}	4000	Fogg and Sangster (2003)	L	
	2.3×10^{-3}	3900	Staudinger and Roberts (2001)	L	
	2.3×10^{-3}	3900	Staudinger and Roberts (1996)	L	
	2.7×10^{-3}	3800	Hiatt (2013)	M	
	2.5×10^{-3}	3900	Chen et al. (2012)	M	
	2.2×10^{-3}	3100	Shimotori and Arnold (2003)	M	
	1.5×10^{-3}		Ryu and Park (1999)	M	
	3.2×10^{-3}		Hovorka and Dohnal (1997)	M	12
	2.5×10^{-3}	3000	Kondoh and Nakajima (1997)	M	
	1.3×10^{-3}	3100	Park et al. (1997)	M	
	2.4×10^{-3}	4000	Wright et al. (1992)	M	689
	2.5×10^{-3}	3800	Tse et al. (1992)	M	
	2.5×10^{-3}	4200	Bissonette et al. (1990)	M	
	2.1×10^{-3}	3200	Ashworth et al. (1988)	M	279
	2.6×10^{-3}	4200	Gossett (1987)	M	
	2.2×10^{-3}		Yurteri et al. (1987)	M	12
	2.2×10^{-3}	4100	Ervin et al. (1980)	M	
	1.1×10^{-3}		Sato and Nakajima (1979b)	M	14
	1.3×10^{-3}		Mackay et al. (2006b)	V	
	1.3×10^{-3}		Park et al. (1997)	V	
	1.3×10^{-3}		Mackay et al. (1993)	V	
	1.3×10^{-3}		Mackay and Shiu (1981)	V	
	1.3×10^{-3}		Dilling (1977)	V	
	2.9×10^{-3}		Hine and Mookerjee (1975)	V	
	1.3×10^{-3}		Yaws (2003)	X	238

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.8×10^{-3}		Wang et al. (2017)	Q	315, 81, 239
	4.9×10^{-4}		Wang et al. (2017)	Q	315, 81, 240
	1.1×10^{-3}		Wang et al. (2017)	Q	315, 81, 241
	3.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.3×10^{-3}		Modarresi et al. (2007)	Q	68
		3300	Kühne et al. (2005)	Q	
	1.4×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	5.2×10^{-3}		Yao et al. (2002)	Q	230
	2.7×10^{-3}		English and Carroll (2001)	Q	231, 232
	2.2×10^{-3}		Mackay et al. (2006b)	?	
		4200	Kühne et al. (2005)	?	
	1.3×10^{-3}		Yaws (1999)	?	21
	1.2×10^{-3}		Abraham and Weathersby (1994)	?	21
	2.2×10^{-3}		Mackay et al. (1993)	?	
	1.3×10^{-3}		Yaws and Yang (1992)	?	21
	1.3×10^{-3}		Abraham et al. (1990)	?	
(*E*)-1,2-dichloroethene	9.9×10^{-4}	3600	Schwardt et al. (2021)	L	1
CHClCHCl	1.0×10^{-3}	3600	Burkholder et al. (2019)	L	
(*trans*-1,2-dichloroethene)	1.0×10^{-3}	3600	Burkholder et al. (2015)	L	
[156-60-5]	1.0×10^{-3}	3900	Brockbank (2013)	L	
KFUSEUYYWQURPO-OWOJBTEDSA-N	1.0×10^{-3}	3500	Warneck (2007)	L	
	1.1×10^{-3}	4200	Fogg and Sangster (2003)	L	
	9.0×10^{-4}	4100	Staudinger and Roberts (2001)	L	
	9.0×10^{-4}	4100	Staudinger and Roberts (1996)	L	
	9.2×10^{-4}	2600	Schwardt et al. (2021)	M	690, 11
	1.0×10^{-3}	4000	Hiatt (2013)	M	
	1.0×10^{-3}	3500	Shimotori and Arnold (2003)	M	
	1.6×10^{-3}		Ryu and Park (1999)	M	
	1.3×10^{-3}		Hovorka and Dohnal (1997)	M	12
	1.1×10^{-3}	2200	Kondoh and Nakajima (1997)	M	
	1.8×10^{-3}	6200	Park et al. (1997)	M	
	9.3×10^{-4}	4900	Khalfaoui and Newsham (1994b)	M	691
	9.8×10^{-4}	3400	Hansen et al. (1993)	M	282
	1.0×10^{-3}	4200	Wright et al. (1992)	M	692
	1.0×10^{-3}	3700	Tse et al. (1992)	M	
	9.7×10^{-4}	5000	Cooling et al. (1992)	M	693
	8.4×10^{-4}	4800	Bissonette et al. (1990)	M	
	9.9×10^{-4}	3000	Ashworth et al. (1988)	M	279, 688
	1.1×10^{-3}	4200	Gossett (1987)	M	
	1.1×10^{-3}		Yurteri et al. (1987)	M	12
	7.0×10^{-4}	5400	Ervin et al. (1980)	M	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.9×10^{-3}		Warner et al. (1980)	M	
	8.1×10^{-4}		Sato and Nakajima (1979b)	M	14
	1.5×10^{-3}		Mackay et al. (2006b)	V	
	1.5×10^{-3}		Park et al. (1997)	V	
	1.5×10^{-3}		Mackay et al. (1993)	V	
	1.5×10^{-3}		Hwang et al. (1992)	V	
	1.5×10^{-3}		Mackay and Shiu (1981)	V	
	2.4×10^{-3}		Warner et al. (1980)	V	
	1.5×10^{-3}		Dilling (1977)	V	
	1.5×10^{-3}		Hine and Mookerjee (1975)	V	
	1.5×10^{-3}		Yaws (2003)	X	238
	1.9×10^{-3}	1700	Goldstein (1982)	X	299
	1.5×10^{-3}		Ryan et al. (1988)	C	
	1.9×10^{-3}		Shen (1982)	C	
	1.8×10^{-3}		Wang et al. (2017)	Q	315, 81, 239
	4.9×10^{-4}		Wang et al. (2017)	Q	315, 81, 240
	1.1×10^{-3}		Wang et al. (2017)	Q	315, 81, 241
	2.1×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.3×10^{-3}		Modarresi et al. (2007)	Q	68
		3300	Kühne et al. (2005)	Q	
	2.2×10^{-3}		Yao et al. (2002)	Q	230
	2.3×10^{-3}		English and Carroll (2001)	Q	231, 232
	1.0×10^{-3}		Mackay et al. (2006b)	?	
		4300	Kühne et al. (2005)	?	
	1.5×10^{-3}		Yaws (1999)	?	21
	8.4×10^{-4}		Abraham and Weathersby (1994)	?	21
	1.0×10^{-3}		Mackay et al. (1993)	?	
	1.5×10^{-3}		Yaws and Yang (1992)	?	21
	1.5×10^{-3}		Abraham et al. (1990)	?	
trichloroethene	1.1×10^{-3}	4100	Schwardt et al. (2021)	L	1
C_2HCl_3	1.1×10^{-3}	4300	Burkholder et al. (2019)	L	
(trichloroethylene)	8.6×10^{-4}	4200	Burkholder et al. (2019)	L	71
[79-01-6]	1.1×10^{-3}	4300	Burkholder et al. (2015)	L	
XSTXAVWGXDQKEL-UHFFFAOYSA-N	8.6×10^{-4}	4200	Burkholder et al. (2015)	L	71
	1.0×10^{-3}	4200	Brockbank (2013)	L	1
	1.1×10^{-3}	4300	Warneck (2007)	L	
	1.0×10^{-3}	4300	Fogg and Sangster (2003)	L	
	1.0×10^{-3}	4600	Staudinger and Roberts (2001)	L	
	9.9×10^{-4}	4600	Staudinger and Roberts (1996)	L	
	6.6×10^{-4}		Steward et al. (1973)	L	14
	1.1×10^{-3}	4100	Allott et al. (1973)	L	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.0×10^{-3}	4200	Schwardt et al. (2021)	M	694
	1.2×10^{-3}	4700	Hiatt (2013)	M	
	1.6×10^{-3}	2800	Zhang et al. (2013)	M	326
	1.3×10^{-3}		Zhang et al. (2013)	M	327
	1.0×10^{-3}	3900	Chen et al. (2012)	M	
	9.4×10^{-4}		Helburn et al. (2008)	M	
	1.0×10^{-3}	3900	Shimotori and Arnold (2003)	M	
	9.5×10^{-4}	4300	Görgényi et al. (2002)	M	695
	1.2×10^{-3}	3600	Bierwagen and Keller (2001)	M	
	7.6×10^{-4}	4900	Moore (2000)	M	71
	1.0×10^{-3}		David et al. (2000)	M	73
	1.1×10^{-3}	3900	Vane and Giroux (2000)	M	
	1.1×10^{-3}	4800	Knauss et al. (2000)	M	696
	9.5×10^{-4}	4900	Dewulf et al. (1999)	M	
	9.5×10^{-4}		Ryu and Park (1999)	M	
	9.3×10^{-4}	3700	Heron et al. (1998)	M	
	1.1×10^{-3}		Chiang et al. (1998)	M	12
	1.4×10^{-3}		Peng and Wan (1998)	M	
	8.7×10^{-4}	4000	Peng and Wan (1998)	M	71
	1.1×10^{-3}	3800	Peng and Wan (1997)	M	
	1.3×10^{-3}		Hovorka and Dohnal (1997)	M	12
	1.1×10^{-3}	2200	Kondoh and Nakajima (1997)	M	
	8.8×10^{-4}	3600	Park et al. (1997)	M	
	8.5×10^{-4}		Turner et al. (1996)	M	
	8.3×10^{-4}		Ramachandran et al. (1996)	M	
	1.2×10^{-3}	3900	Dewulf et al. (1995)	M	
	1.3×10^{-3}		Nielsen et al. (1994)	M	
	9.5×10^{-4}	5000	Khalfaoui and Newsham (1994b)	M	697
	9.4×10^{-4}	3100	Robbins et al. (1993)	M	698
	1.1×10^{-3}		Hoff et al. (1993)	M	
	1.0×10^{-3}		Li et al. (1993)	M	
	1.1×10^{-3}	3700	Wright et al. (1992)	M	699
	1.1×10^{-3}	4200	Tse et al. (1992)	M	
	9.7×10^{-4}	4900	Cooling et al. (1992)	M	700
	1.3×10^{-3}	5200	Tancrède and Yanagisawa (1990)	M	
	1.0×10^{-3}	5200	Bissonette et al. (1990)	M	
	9.7×10^{-4}	2000	Lamarche and Droste (1989)	M	347
	5.5×10^{-4}		Guitart et al. (1989)	M	14
	9.5×10^{-4}	3700	Ashworth et al. (1988)	M	279
	1.0×10^{-3}	4800	Gossett (1987)	M	
	9.6×10^{-4}	4700	Munz and Roberts (1987)	M	
	9.8×10^{-4}		Hellmann (1987)	M	88
	9.4×10^{-4}		Yurteri et al. (1987)	M	12
	9.0×10^{-4}	5400	Schoene and Steinhanses (1985)	M	
	1.1×10^{-3}	4300	Gossett et al. (1985)	M	
	1.0×10^{-3}		Garbarini and Lion (1985)	M	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.7×10^{-4}	4900	Lincoff and Gossett (1984)	M	
	1.0×10^{-3}	4600	Leighton and Calo (1981)	M	
	7.4×10^{-4}	4800	Ervin et al. (1980)	M	
	8.4×10^{-4}		Warner et al. (1980)	M	
	5.0×10^{-4}		Sato and Nakajima (1979b)	M	14
	1.1×10^{-3}		Pearson and McConnell (1975)	M	651, 12
	8.5×10^{-4}		Mackay et al. (2006b)	V	
	9.9×10^{-4}		Park et al. (1997)	V	
	8.4×10^{-4}		Mackay et al. (1993)	V	
	1.1×10^{-3}		Hwang et al. (1992)	V	
	8.1×10^{-4}		Mackay and Shiu (1981)	V	
	8.4×10^{-4}		Warner et al. (1980)	V	
	8.2×10^{-4}		Dilling (1977)	V	653
	1.0×10^{-3}		Dilling (1977)	V	12
	2.4×10^{-3}		Dilling (1977)	V	154
	8.4×10^{-4}		Hine and Mookerjee (1975)	V	
	8.4×10^{-4}		Dilling et al. (1975)	V	
	8.6×10^{-4}		Yaws (2003)	X	259
	8.5×10^{-4}		Yaws (2003)	X	238
	8.8×10^{-4}	1600	Goldstein (1982)	X	299
	1.1×10^{-3}		Ryan et al. (1988)	C	
	8.4×10^{-4}		Shen (1982)	C	
	6.2×10^{-4}		Dupeux et al. (2022)	Q	260
	2.2×10^{-3}		Keshavarz et al. (2022)	Q	
	2.9×10^{-3}		Duchowicz et al. (2020)	Q	185
	2.9×10^{-3}		Wang et al. (2017)	Q	81, 239
	2.2×10^{-4}		Wang et al. (2017)	Q	81, 240
	6.9×10^{-4}		Wang et al. (2017)	Q	81, 241
	8.4×10^{-4}		Li et al. (2014)	Q	242
	5.5×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	8.7×10^{-4}		Gharagheizi et al. (2010)	Q	247
	3.0×10^{-4}		Hilal et al. (2008)	Q	
	1.8×10^{-3}		Modarresi et al. (2007)	Q	68
		3600	Kühne et al. (2005)	Q	
	1.1×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.1×10^{-3}		English and Carroll (2001)	Q	231, 275
	4.0×10^{-4}		Katritzky et al. (1998)	Q	
	8.4×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.0×10^{-3}		Duchowicz et al. (2020)	?	186, 21
	9.7×10^{-4}		Mackay et al. (2006b)	?	
		4200	Kühne et al. (2005)	?	
	8.5×10^{-4}		Yaws (1999)	?	21
	5.2×10^{-4}		Abraham and Weathersby (1994)	?	21

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.7×10^{-4}		Mackay et al. (1993)	?	
	8.4×10^{-4}		Yaws and Yang (1992)	?	21
	8.4×10^{-4}		Abraham et al. (1990)	?	
tetrachloroethene	5.7×10^{-4}	4700	Schwardt et al. (2021)	L	1
C_2Cl_4	5.5×10^{-4}	4500	Burkholder et al. (2019)	L	
(tetrachloroethylene)	4.6×10^{-4}	4400	Burkholder et al. (2019)	L	71
[127-18-4]	5.5×10^{-4}	4500	Burkholder et al. (2015)	L	
CYTYCFOTNPOANT-UHFFFAOYSA-N	4.6×10^{-4}	4400	Burkholder et al. (2015)	L	71
	5.6×10^{-4}	4700	Brockbank (2013)	L	1
	6.2×10^{-4}	4500	Warneck (2007)	L	
	6.0×10^{-4}	4200	Fogg and Sangster (2003)	L	
	5.9×10^{-4}	4800	Staudinger and Roberts (2001)	L	
	5.8×10^{-4}	4800	Staudinger and Roberts (1996)	L	
	4.3×10^{-4}		Mackay and Shiu (1981)	L	
	5.8×10^{-4}	4500	Schwardt et al. (2021)	M	701
	9.9×10^{-4}	4600	Hiatt (2013)	M	
	6.2×10^{-4}	4200	Chen et al. (2012)	M	
	5.8×10^{-4}	4200	Shimotori and Arnold (2003)	M	
	4.1×10^{-4}	5300	Moore (2000)	M	71
	6.0×10^{-4}	4100	Vane and Giroux (2000)	M	
	4.8×10^{-4}	4400	Knauss et al. (2000)	M	702
	5.3×10^{-4}		Ryu and Park (1999)	M	
	8.6×10^{-4}		Dohnal and Hovorka (1999)	M	12
	6.2×10^{-4}		Chiang et al. (1998)	M	12
	7.8×10^{-4}		Peng and Wan (1998)	M	
	4.7×10^{-4}	4100	Peng and Wan (1998)	M	71
	6.1×10^{-4}	4200	Peng and Wan (1997)	M	
	8.4×10^{-4}		Hovorka and Dohnal (1997)	M	12
	6.9×10^{-4}	2200	Kondoh and Nakajima (1997)	M	
	5.5×10^{-4}	4200	Park et al. (1997)	M	
	6.9×10^{-4}	4800	Dewulf et al. (1995)	M	
	5.8×10^{-4}	5200	Robbins et al. (1993)	M	703
	6.3×10^{-4}		Hoff et al. (1993)	M	
	6.3×10^{-4}		Li et al. (1993)	M	
	8.1×10^{-4}	2100	Kolb et al. (1992)	M	33, 278
	5.9×10^{-4}	5500	Tancrède and Yanagisawa (1990)	M	
	6.2×10^{-4}	5300	Bissonette et al. (1990)	M	
	5.4×10^{-4}	4400	Ashworth et al. (1988)	M	279
	5.6×10^{-4}	4900	Gossett (1987)	M	
	5.4×10^{-4}	4400	Munz and Roberts (1987)	M	
	7.7×10^{-4}		Hellmann (1987)	M	88
	7.5×10^{-4}		Yurteri et al. (1987)	M	12
	6.5×10^{-4}	4600	Gossett et al. (1985)	M	
	5.7×10^{-4}	5100	Lincoff and Gossett (1984)	M	
	6.1×10^{-4}	4700	Leighton and Calo (1981)	M	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.7×10^{-4}	5200	Ervin et al. (1980)	M	
	3.4×10^{-4}		Warner et al. (1980)	M	
	1.1×10^{-3}	4300	Gossett (1980)	M	
	1.7×10^{-4}		Sato and Nakajima (1979b)	M	14
	5.0×10^{-4}		Pearson and McConnell (1975)	M	651, 12
	3.7×10^{-4}		Mackay et al. (2006b)	V	
	3.4×10^{-4}		Park et al. (1997)	V	
	3.7×10^{-4}		Mackay et al. (1993)	V	
	3.6×10^{-4}		Hwang et al. (1992)	V	
	9.1×10^{-4}		Addison et al. (1983)	V	
	3.5×10^{-4}		Warner et al. (1980)	V	
	3.4×10^{-4}		Dilling (1977)	V	653
	4.0×10^{-4}		Dilling (1977)	V	12
	1.2×10^{-3}		Dilling (1977)	V	154
	3.7×10^{-4}		Hine and Mookerjee (1975)	V	
	9.8×10^{-4}		Dilling et al. (1975)	V	
	3.6×10^{-4}		Yaws (2003)	X	238
	3.6×10^{-4}	1500	Goldstein (1982)	X	299
	6.3×10^{-4}		Ryan et al. (1988)	C	
	3.4×10^{-4}		Shen (1982)	C	
	8.1×10^{-4}		Dilling (1977)	C	
	8.1×10^{-4}		Dilling et al. (1975)	C	
	4.4×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.2×10^{-4}		Wang et al. (2017)	Q	81, 240
	2.5×10^{-4}		Wang et al. (2017)	Q	81, 241
	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-4}		Gharagheizi et al. (2010)	Q	247
	1.7×10^{-4}		Hilal et al. (2008)	Q	
	1.2×10^{-3}		Modarresi et al. (2007)	Q	68
		3900	Kühne et al. (2005)	Q	
	5.6×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	3.1×10^{-4}		English and Carroll (2001)	Q	231, 232
	9.9×10^{-5}		Katritzky et al. (1998)	Q	
	8.8×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	5.8×10^{-4}		Mackay et al. (2006b)	?	
		5100	Kühne et al. (2005)	?	
	3.7×10^{-4}		Yaws (1999)	?	21
	1.7×10^{-4}		Abraham and Weathersby (1994)	?	21
	5.8×10^{-4}		Mackay et al. (1993)	?	
	3.7×10^{-4}		Yaws and Yang (1992)	?	21
	3.4×10^{-4}		Abraham et al. (1990)	?	
	2.9×10^{-3}		Chiou et al. (1980)	?	80

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dichloroethyne C_2Cl_2 [7572-29-4] ZMJOVJSTYLQINE-UHFFFAOYSA-N	4.9×10^{-4}		HSDB (2015)	Q	100
1-chloro-1-propene C_3H_5Cl [590-21-6] OWXJKYNZGFSVRC-UHFFFAOYSA-N	1.8×10^{-4}		HSDB (2015)	Q	100
2-chloro-1-propene C_3H_5Cl [557-98-2] PNLQPWWBHXMFCA-UHFFFAOYSA-N	1.4×10^{-4}		HSDB (2015)	Q	100
3-chloro-1-propene	9.1×10^{-4}		Mackay and Shiu (1981)	L	
C_3H_5Cl	1.3×10^{-3}	4500	Hiatt (2013)	M	
(allyl chloride)	3.7×10^{-3}		Welke et al. (1998)	M	
[107-05-1]	9.0×10^{-4}		Duchowicz et al. (2020)	V	187
OSDWBNJEKMUWAV-UHFFFAOYSA-N	9.0×10^{-4}		HSDB (2015)	V	
	4.6×10^{-4}		Mackay et al. (1993)	V	
	9.2×10^{-4}		Dilling (1977)	V	
	1.1×10^{-3}		Hine and Mookerjee (1975)	V	
	1.1×10^{-3}		Yaws (2003)	X	238
	4.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.1×10^{-3}		Li et al. (2014)	Q	242
	1.4×10^{-3}		Gharagheizi et al. (2012)	Q	
	8.4×10^{-4}		Gharagheizi et al. (2010)	Q	247
	4.0×10^{-3}		Hilal et al. (2008)	Q	
	2.8×10^{-3}		Modarresi et al. (2007)	Q	68
	5.9×10^{-4}		Yao et al. (2002)	Q	230
	1.1×10^{-3}		English and Carroll (2001)	Q	231, 232
	1.8×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	1.9×10^{-3}		Suzuki et al. (1992)	Q	233
	1.7×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.1×10^{-3}		Yaws (1999)	?	21
	1.1×10^{-3}		Yaws and Yang (1992)	?	21
	1.1×10^{-3}		Abraham et al. (1990)	?	
1,1-dichloropropene	6.1×10^{-4}	4200	Hiatt (2013)	M	
$C_3H_4Cl_2$	5.4×10^{-4}	1900	Kondoh and Nakajima (1997)	M	
[563-58-6]					
ZAIDIVBQUMFXEC-UHFFFAOYSA-N					
1,2-dichloropropene	2.0×10^{-3}		HSDB (2015)	V	
$C_3H_4Cl_2$	3.1×10^{-4}		Hilal et al. (2008)	Q	
[563-54-2]	1.8×10^{-3}		Modarresi et al. (2007)	Q	68
PPKPKFIWDXDAGC-UHFFFAOYSA-N					

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3-dichloropropene	6.4×10^{-3}	4300	Wright et al. (1992)	M	704
$C_3H_4Cl_2$	2.8×10^{-3}		Warner et al. (1980)	M	
[542-75-6]	7.3×10^{-3}		Warner et al. (1980)	V	
UOORRWUZONOOLO-UHFFFAOYSA-N	2.4×10^{-5}		Barcelo and Hennion (1997)	X	569
	2.8×10^{-3}	1500	Goldstein (1982)	X	299
	5.8×10^{-3}		Hilal et al. (2008)	C	
	2.8×10^{-3}		Horvath and Getzen (1999)	C	
	8.1×10^{-3}		Ryan et al. (1988)	C	
	2.8×10^{-3}		Shen (1982)	C	
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	5.1×10^{-5}		Goodarzi et al. (2010)	Q	570
	5.7×10^{-3}		Hilal et al. (2008)	Q	
	5.1×10^{-3}		Modarresi et al. (2007)	Q	68
cis-1,3-dichloropropene	4.2×10^{-3}		Mackay and Shiu (1981)	L	
$C_3H_4Cl_2$	9.5×10^{-3}	5500	Hiatt (2013)	M	
[10061-01-5]	1.0×10^{-2}		Thomas et al. (2006)	M	155, 705
UOORRWUZONOOLO-UPHRSURJSA-N	6.3×10^{-3}	4300	Kondoh and Nakajima (1997)	M	
	4.2×10^{-3}		Albanese et al. (1987)	M	
	5.0×10^{-3}	5800	Leistra (1970)	M	
	4.2×10^{-3}		Dilling (1977)	V	
	8.7×10^{-3}		Thomas et al. (2006)	?	155, 706
	5.5×10^{-3}		Yates and Gan (1998)	?	
trans-1,3-dichloropropene	5.6×10^{-3}		Mackay and Shiu (1981)	L	
$C_3H_4Cl_2$	5.8×10^{-3}	4800	Hiatt (2013)	M	
[10061-02-6]	1.5×10^{-2}		Thomas et al. (2006)	M	155, 705
UOORRWUZONOOLO-OWOJBTEDSA-N	1.0×10^{-2}	5000	Kondoh and Nakajima (1997)	M	
	5.6×10^{-3}		Albanese et al. (1987)	M	
	8.1×10^{-3}	5700	Leistra (1970)	M	
	5.6×10^{-3}		Dilling (1977)	V	
	1.5×10^{-2}		Thomas et al. (2006)	?	155, 706
	9.4×10^{-3}		Yates and Gan (1998)	?	
2,3-dichloropropene	2.8×10^{-3}		Mackay and Shiu (1981)	L	
$C_3H_4Cl_2$	3.5×10^{-3}		Albanese et al. (1987)	M	
[78-88-6]	2.4×10^{-3}		Duchowicz et al. (2020)	V	187
FALCMQXTWHPRIH-UHFFFAOYSA-N	2.7×10^{-3}		Dilling (1977)	V	
	2.4×10^{-3}		Yaws (2003)	X	238
	4.0×10^{-3}		Duchowicz et al. (2020)	Q	
	4.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	2.4×10^{-3}		Gharagheizi et al. (2010)	Q	247

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.8×10^{-3}		Hilal et al. (2008)	Q	
	3.8×10^{-3}		Modarresi et al. (2007)	Q	68
	2.9×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.8×10^{-3}		Yao et al. (2002)	Q	230, 268
	2.0×10^{-3}		Katritzky et al. (1998)	Q	
	2.4×10^{-3}		Yaws (1999)	?	21
1,2,3-trichloro-1-propene $C_3H_3Cl_3$ [96-19-5] HIILBTHBHCLUER-UHFFFAOYSA-N	5.5×10^{-4}		HSDB (2015)	Q	100
1,1,2,3,3,3-hexachloro-1-propene C_3Cl_6 [1888-71-7] VFDYKPARTDCDCU-UHFFFAOYSA-N	2.1×10^{-3}		Duchowicz et al. (2020)	V	187
	1.3×10^{-3}		Duchowicz et al. (2020)	Q	
	6.2×10^{-3}		HSDB (2015)	Q	100
	9.9×10^{-4}		Hilal et al. (2008)	Q	
	3.8×10^{-3}		Modarresi et al. (2007)	Q	68
	2.1×10^{-3}		Yaffe et al. (2003)	Q	249, 250
3-chloro-1-butene C_4H_7Cl [563-52-0] VZGLVCFVUREVDP-UHFFFAOYSA-N	5.6×10^{-4}		Ebert et al. (2023)	?	317
3-chloro-2-methyl-1-propene C_4H_7Cl [563-47-3] OHXAOPZTJOUYKM-UHFFFAOYSA-N	1.1×10^{-3}		Duchowicz et al. (2020)	V	187
	1.1×10^{-3}		HSDB (2015)	V	
	1.5×10^{-3}		Duchowicz et al. (2020)	Q	
1-chloro-2-butene C_4H_7Cl (crotyl chloride) [591-97-9] YTKRILODNOEEPX-UHFFFAOYSA-N	9.5×10^{-4}		Ebert et al. (2023)	?	319
(*Z*)-1-chloro-2-butene	1.2×10^{-3}	2800	Bakierowska and Trzeszczyński (2003)	M	
C_4H_7Cl		3800	Kühne et al. (2005)	Q	
(*cis*-1-chloro-2-butene) [4628-21-1] YTKRILODNOEEPX-IHWYPQMZSA-N		2800	Kühne et al. (2005)	?	
(*E*)-1-chloro-2-butene	3.1×10^{-3}	3000	Bakierowska and Trzeszczyński (2003)	M	
C_4H_7Cl		3800	Kühne et al. (2005)	Q	
(*trans*-1-chloro-2-butene) [4894-61-5] YTKRILODNOEEPX-NSCUHMNNSA-N		3000	Kühne et al. (2005)	?	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3-dichloro-2-butene $C_4H_6Cl_2$ [926-57-8] WLIADPFXSACYLS-UHFFFAOYSA-N	2.6×10^{-4}		HSDB (2015)	Q	100
1,4-dichloro-2-butene $C_4H_6Cl_2$ [764-41-0] FQDIANVAWVHZIR-UHFFFAOYSA-N	1.2×10^{-3} 1.7×10^{-2} 4.2×10^{-3} 8.9×10^{-3}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Modarresi et al. (2007)	V V Q Q	187 68
(*Z*)-1,4-dichloro-2-butene $C_4H_6Cl_2$ [1476-11-5] FQDIANVAWVHZIR-UPHRSURJSA-N	3.0×10^{-2} 1.0×10^{-2} 8.5×10^{-3} 8.2×10^{-3} 4.2×10^{-3}	9400	Hiatt (2013) Albanese et al. (1987) Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	M M V V Q	 187
(*E*)-1,4-dichloro-2-butene $C_4H_6Cl_2$ [110-57-6] FQDIANVAWVHZIR-OWOJBTEDSA-N	3.5×10^{-2} 1.7×10^{-2} 1.5×10^{-2} 1.5×10^{-2} 4.2×10^{-3} 7.2×10^{-2} 8.9×10^{-3}	6600	Hiatt (2013) Albanese et al. (1987) Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007)	M M V V Q Q Q	 187 68
3,4-dichloro-1-butene $C_4H_6Cl_2$ [760-23-6] XVEASTGLHPVZNA-UHFFFAOYSA-N	1.2×10^{-3} 1.1×10^{-3} 6.4×10^{-3}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
1-chloro-2-methylpropene C_4H_7Cl (dimethylvinyl chloride) [513-37-1] KWISWUFGPUHDRY-UHFFFAOYSA-N	5.2×10^{-4}		HSDB (2015) Haynes (2014)	V W	 707
2-chloro-1,3-butadiene C_4H_5Cl [126-99-8] YACLQRRMGMJLJV-UHFFFAOYSA-N	4.7×10^{-2} 1.8×10^{-4}		Mackay et al. (1993) HSDB (2015)	V Q	 100
hexachlorobutadiene $CCl_2CClCClCCl_2$ [87-68-3] RWNKSTSCBHKHTB-UHFFFAOYSA-N	5.6×10^{-4} 8.3×10^{-4} 2.3×10^{-3} 6.2×10^{-4} 7.0×10^{-4} 2.3×10^{-3} 9.6×10^{-4} 4.0×10^{-4} 6.1×10^{-4} 6.5×10^{-4}	5500 3100 6200 4900 2500	Brockbank (2013) Fogg and Sangster (2003) Hiatt (2013) Dewulf et al. (1999) Kondoh and Nakajima (1997) Oliver (1985) Warner et al. (1980) Pearson and McConnell (1975) Mackay et al. (2006b) Mackay et al. (1993)	L L M M M M M M V V	 651, 12

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.1×10^{-4}		Ballschmiter and Wittlinger (1991)	V	
	3.8×10^{-4}		Warner et al. (1980)	V	
	4.2×10^{-4}		Yaws (2003)	X	238
	9.8×10^{-4}	4600	Goldstein (1982)	X	299
	9.7×10^{-4}		Hilal et al. (2008)	C	
	9.6×10^{-4}		Horvath and Getzen (1999)	C	
	9.4×10^{-4}		Ryan et al. (1988)	C	
	9.6×10^{-4}		Shen (1982)	C	
	9.0×10^{-4}		Zhang et al. (2010)	Q	288, 289
	5.0×10^{-4}		Zhang et al. (2010)	Q	288, 290
	2.3×10^{-3}		Zhang et al. (2010)	Q	288, 291
	1.7×10^{-2}		Zhang et al. (2010)	Q	288, 292
	4.3×10^{-4}		Gharagheizi et al. (2010)	Q	247
	6.2×10^{-4}		Hilal et al. (2008)	Q	
	7.6×10^{-3}		Modarresi et al. (2007)	Q	68
		5300	Kühne et al. (2005)	Q	
	2.7×10^{-4}		Yao et al. (2002)	Q	230
		3500	Kühne et al. (2005)	?	
	4.2×10^{-4}		Yaws (1999)	?	21
hexachlorocyclopentadiene	3.7×10^{-4}		Wolfe et al. (1982)	M	
C_5Cl_6	6.0×10^{-4}		Warner et al. (1980)	M	
[77-47-4]	6.1×10^{-4}		Mackay et al. (2006b)	V	
VUNCWTMEJYMOOR-UHFFFAOYSA-N	6.0×10^{-4}		Mackay et al. (1993)	V	
	6.2×10^{-4}		Wolfe et al. (1982)	V	
	2.7×10^{-4}		Warner et al. (1980)	V	
	6.0×10^{-4}	1500	Goldstein (1982)	X	299
	2.7×10^{-4}		Ryan et al. (1988)	C	
	6.0×10^{-4}		Shen (1982)	C	
	4.6×10^{-3}		Zhang et al. (2010)	Q	288, 289
	5.3×10^{-3}		Zhang et al. (2010)	Q	288, 290
	1.4×10^{-2}		Zhang et al. (2010)	Q	288, 291
	1.6×10^{-2}		Zhang et al. (2010)	Q	288, 292
	2.3×10^{-3}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	68
	3.7×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	2.4×10^{-3}		Katritzky et al. (1998)	Q	
chlordane	1.8×10^{-1}		Fendinger et al. (1989)	M	73
$C_{10}H_6Cl_8$	1.2×10^{-1}		Fendinger et al. (1989)	M	647
[57-74-9]	2.1×10^{-1}		Warner et al. (1980)	M	
BIWJNBZANLAXMG-UHFFFAOYSA-N	1.1×10^{-1}		Suntio et al. (1988)	V	12
	1.1×10^{-3}		Barcelo and Hennion (1997)	X	569
	2.0×10^{-1}		Suntio et al. (1988)	C	
	1.1×10^{-1}		Suntio et al. (1988)	C	
	1.0×10^{-1}		Ryan et al. (1988)	C	
	2.1×10^{-1}		Shen (1982)	C	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.3×10^{-1}		Keshavarz et al. (2022)	Q	
	3.6×10^{-2}		Duchowicz et al. (2020)	Q	185
	1.4×10^{-1}		Zhang et al. (2010)	Q	288, 289
	4.8×10^{-2}		Zhang et al. (2010)	Q	288, 290
	2.4×10^{1}		Zhang et al. (2010)	Q	288, 291
	1.5		Zhang et al. (2010)	Q	288, 292
	2.1×10^{-4}		Goodarzi et al. (2010)	Q	570, 571
	5.3×10^{-2}		Hilal et al. (2008)	Q	
	2.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
cis-chlordane	1.7×10^{-1}		Shen and Wania (2005)	L	368
$C_{10}H_6Cl_8$	1.8×10^{-1}		Shen and Wania (2005)	L	369
(α-chlordane)	3.7×10^{-2}	4100	Jantunen and Bidleman (2006)	M	
[5103-71-9]	1.5×10^{-1}	6100	Cetin et al. (2006)	M	
BIWJNBZANLAXMG-KMMBHOGFSA-N	1.1×10^{-2}		Atlas et al. (1982)	M	681
	2.8×10^{-2}		Duchowicz et al. (2020)	V	187
			Mackay et al. (2006d)	V	560
	4.8×10^{-3}	7300	Paasivirta et al. (1999)	T	
	3.6×10^{-2}		Duchowicz et al. (2020)	Q	
trans-chlordane	1.7×10^{-1}		Shen and Wania (2005)	L	368
$C_{10}H_6Cl_8$	1.5×10^{-1}		Shen and Wania (2005)	L	369
(β-chlordane)	3.4×10^{-2}	3500	Jantunen and Bidleman (2006)	M	
[5103-74-2]	6.3×10^{-2}	7600	Cetin et al. (2006)	M	
BIWJNBZANLAXMG-OESJLNMISA-N	7.4×10^{-3}		Atlas et al. (1982)	M	681
	2.0×10^{-2}		Duchowicz et al. (2020)	V	187
			Mackay et al. (2006d)	V	560
	3.6×10^{-3}	7100	Paasivirta et al. (1999)	T	
	3.6×10^{-2}		Duchowicz et al. (2020)	Q	
	1.0		Modarresi et al. (2007)	Q	68
γ-chlordane $C_{10}H_6Cl_8$ [5566-34-7] JBZJEPYXXVKOKF-UHFFFAOYSA-N	6.3×10^{-2}		Ebert et al. (2023)	?	581
cis-nonachlor $C_{10}H_5Cl_9$ [5103-73-1] OCHOKXCPKDPNQU-BBXWSCHTSA-N	1.4	5100	Cetin et al. (2006)	M	
trans-nonachlor	3.1×10^{-2}	4800	Jantunen and Bidleman (2006)	M	
$C_{10}H_5Cl_9$	8.8×10^{-2}	8000	Cetin et al. (2006)	M	
[39765-80-5]	7.9×10^{-4}	7600	Paasivirta et al. (1999)	T	
OCHOKXCPKDPNQU-FLVMBEMLSA-N					

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chlorobenzene	2.4×10^{-3}	3700	Schwardt et al. (2021)	L	1, 708
C_6H_5Cl	2.6×10^{-3}	3600	Brockbank (2013)	L	1
[108-90-7]	2.7×10^{-3}	3800	Staudinger and Roberts (2001)	L	
MVPPADPHJFYWMZ-UHFFFAOYSA-N	2.7×10^{-3}	3800	Staudinger and Roberts (1996)	L	
	2.9×10^{-3}		Mackay and Shiu (1981)	L	
	2.0×10^{-3}	3800	Schwardt et al. (2021)	M	709
	3.7×10^{-3}	4400	Hiatt (2013)	M	
	1.7×10^{-3}	1300	Lau et al. (2010)	M	33, 11
	2.4×10^{-3}		Li et al. (2008)	M	
	1.5×10^{-3}	2300	Lei et al. (2004)	M	329
	2.5×10^{-3}	4300	Dewulf et al. (1999)	M	
	1.9×10^{-3}		Ryu and Park (1999)	M	
	3.6×10^{-3}		Dohnal and Hovorka (1999)	M	12
	3.4×10^{-3}		de Wolf and Lieder (1998)	M	88
	2.7×10^{-3}		Welke et al. (1998)	M	
	3.2×10^{-3}		Shiu and Mackay (1997)	M	
	3.5×10^{-3}		Hovorka and Dohnal (1997)	M	12
	3.0×10^{-3}	3600	Kondoh and Nakajima (1997)	M	
	1.9×10^{-3}	1700	Park et al. (1997)	M	
	2.9×10^{-3}		Ramachandran et al. (1996)	M	
	3.0×10^{-3}	2900	Khalfaoui and Newsham (1994b)	M	710
	2.6×10^{-3}		Hoff et al. (1993)	M	
	3.1×10^{-3}	2900	Ettre et al. (1993)	M	11
	2.5×10^{-3}		Li and Carr (1993)	M	
	3.0×10^{-3}	3100	Cooling et al. (1992)	M	711
	2.4×10^{-3}	4700	Bissonette et al. (1990)	M	
	2.5×10^{-3}	2700	Ashworth et al. (1988)	M	279
	2.9×10^{-3}		Hellmann (1987)	M	88
	3.1×10^{-3}		Yurteri et al. (1987)	M	12
	3.2×10^{-3}		Mackay and Shiu (1981)	M	
	3.0×10^{-3}	3500	Leighton and Calo (1981)	M	
	2.9×10^{-3}	4200	Ervin et al. (1980)	M	
	2.5×10^{-3}		Warner et al. (1980)	M	
	2.6×10^{-3}		Mackay et al. (1979)	M	
	1.6×10^{-3}		Sato and Nakajima (1979b)	M	14
	2.8×10^{-3}	4900	Hartkopf and Karger (1973)	M	
	2.7×10^{-3}		Mackay et al. (2006b)	V	
	2.9×10^{-3}	2400	Fogg and Sangster (2003)	V	
	2.7×10^{-3}		Shiu and Mackay (1997)	V	
	2.8×10^{-3}		Park et al. (1997)	V	
	2.9×10^{-3}		Lide and Frederikse (1995)	V	
	2.7×10^{-3}		Mackay et al. (1993)	V	
	2.7×10^{-3}		Mackay et al. (1992a)	V	
	2.5×10^{-3}		Hwang et al. (1992)	V	
	2.7×10^{-3}		Bobra et al. (1985)	V	
	2.7×10^{-3}		Yoshida et al. (1983)	V	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.7×10^{-3}		Cabani et al. (1981)	V	
	2.7×10^{-3}		Warner et al. (1980)	V	
	2.2×10^{-3}		Hine and Mookerjee (1975)	V	
	2.7×10^{-3}		Mackay et al. (1979)	T	
	2.2×10^{-3}		Yaws (2003)	X	238
	2.5×10^{-3}	2100	Goldstein (1982)	X	299
	2.7×10^{-3}		Schüürmann (2000)	C	21
	2.7×10^{-3}		Ryan et al. (1988)	C	
	2.5×10^{-3}		Shen (1982)	C	
	2.4×10^{-2}		Hayer et al. (2022)	Q	20
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	8.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.5×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
	4.0×10^{-3}		Hilal et al. (2008)	Q	
	8.6×10^{-3}		Modarresi et al. (2007)	Q	68
		4000	Kühne et al. (2005)	Q	
	2.9×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	2.8×10^{-3}		Delgado and Alderete (2002)	Q	
	3.6×10^{-3}		Yao et al. (2002)	Q	230
	4.0×10^{-3}		English and Carroll (2001)	Q	231, 232
	1.7×10^{-3}		Katritzky et al. (1998)	Q	
	1.5×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	2.2×10^{-3}		Suzuki et al. (1992)	Q	233
	4.2×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.8×10^{-3}		Arbuckle (1983)	Q	
	3.2×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4000	Kühne et al. (2005)	?	
	2.2×10^{-3}		Yaws (1999)	?	21
	1.6×10^{-3}		Abraham and Weathersby (1994)	?	21
	2.6×10^{-3}		Mackay et al. (1993)	?	
	2.2×10^{-3}		Yaws and Yang (1992)	?	21
	2.8×10^{-3}		Abraham et al. (1990)	?	
	3.8×10^{-3}		Mackay and Yeun (1983)	?	
chlorobenzene-d5 C_6D_5Cl [3114-55-4] MVPPADPHJFYWMZ-RALIUCGRSA-N	3.6×10^{-3}	4500	Hiatt (2013)	M	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-dichlorobenzene	5.6×10^{-3}	3700	Schwardt et al. (2021)	L	1
$C_6H_4Cl_2$	5.9×10^{-3}	5200	Brockbank (2013)	L	1, 712
(*o*-dichlorobenzene)	6.8×10^{-3}	5300	Fogg and Sangster (2003)	L	713
[95-50-1]	5.4×10^{-3}	5900	Staudinger and Roberts (2001)	L	
RFFLAFLAYFXFSW-UHFFFAOYSA-N	5.4×10^{-3}	5900	Staudinger and Roberts (1996)	L	
	5.3×10^{-3}		Mackay and Shiu (1981)	L	
	8.0×10^{-3}	4200	Hiatt (2013)	M	
	6.3×10^{-3}		Li et al. (2008)	M	
	4.7×10^{-3}		Ryu and Park (1999)	M	
	5.1×10^{-3}		Shiu and Mackay (1997)	M	
	7.2×10^{-3}		Hovorka and Dohnal (1997)	M	12
	6.2×10^{-3}	5000	Kondoh and Nakajima (1997)	M	
	4.9×10^{-3}	4400	Park et al. (1997)	M	
	4.8×10^{-3}		Li and Carr (1993)	M	
	3.5×10^{-3}		Yu (1992)	M	12
	4.9×10^{-3}	5100	Bissonette et al. (1990)	M	
	5.3×10^{-3}	1400	Ashworth et al. (1988)	M	42, 279
	8.2×10^{-3}		Oliver (1985)	M	
	5.9×10^{-3}	6700	Gossett et al. (1985)	M	
	5.2×10^{-3}		Mackay and Shiu (1981)	M	
	5.1×10^{-3}		Warner et al. (1980)	M	
	3.5×10^{-3}		Sato and Nakajima (1979b)	M	14
	5.6×10^{-3}		Mackay et al. (2006b)	V	
	4.1×10^{-3}		Shiu and Mackay (1997)	V	
	8.6×10^{-3}		Park et al. (1997)	V	
	8.3×10^{-3}		Lide and Frederikse (1995)	V	
	4.1×10^{-3}		Mackay et al. (1992a)	V	
	6.0×10^{-3}		Hwang et al. (1992)	V	
	4.1×10^{-3}		Bobra et al. (1985)	V	
	4.9×10^{-3}		Warner et al. (1980)	V	
	4.0×10^{-3}		Hine and Mookerjee (1975)	V	
	3.5×10^{-3}		Yaws (2003)	X	238
	5.2×10^{-3}	2800	Goldstein (1982)	X	299
	5.2×10^{-3}		Schüürmann (2000)	C	21
	2.7×10^{-3}		Ryan et al. (1988)	C	
	5.1×10^{-3}		Shen (1982)	C	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	1.5×10^{-2}		Duchowicz et al. (2020)	Q	185
	4.0×10^{-3}		Li et al. (2014)	Q	242
	4.7×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	3.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
	8.2×10^{-3}		Hilal et al. (2008)	Q	
	4.5×10^{-3}		Modarresi et al. (2007)	Q	68

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		4400	Kühne et al. (2005)	Q	
	5.6×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	7.1×10^{-3}		Delgado and Alderete (2002)	Q	
	8.0×10^{-3}		Yao et al. (2002)	Q	230
	4.7×10^{-3}		English and Carroll (2001)	Q	231, 232
	3.3×10^{-3}		Katritzky et al. (1998)	Q	
	2.3×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	8.4×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	5.1×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4800	Kühne et al. (2005)	?	
	3.5×10^{-3}		Yaws (1999)	?	21
	3.6×10^{-3}		Abraham and Weathersby (1994)	?	21
	3.3×10^{-3}		Yaws and Yang (1992)	?	21
	5.1×10^{-3}		Abraham et al. (1990)	?	
	6.2×10^{-3}		Chiou et al. (1980)	?	80
1,2-dichlorobenzene-d4 $C_6D_4Cl_2$ (*o*-dichlorobenzene-d4) [2199-69-1] RFFLAFLAYFXFSW-RHQRLBAQSA-N	8.2×10^{-3}	4200	Hiatt (2013)	M	
1,3-dichlorobenzene $C_6H_4Cl_2$ (*m*-dichlorobenzene) [541-73-1] ZPQOPVIELGIULI-UHFFFAOYSA-N	3.1×10^{-3}	3700	Schwardt et al. (2021)	L	1
	3.1×10^{-3}	4400	Brockbank (2013)	L	
	3.4×10^{-3}	4300	Fogg and Sangster (2003)	L	
	2.8×10^{-3}		Mackay and Shiu (1981)	L	
	5.2×10^{-3}	4800	Hiatt (2013)	M	
	2.9×10^{-3}		Li et al. (2008)	M	
	3.7×10^{-3}		de Wolf and Lieder (1998)	M	88
	4.7×10^{-3}		Hovorka and Dohnal (1997)	M	12
	3.8×10^{-3}	4400	Kondoh and Nakajima (1997)	M	
	3.4×10^{-3}		Hoff et al. (1993)	M	
	3.0×10^{-3}	2600	Ashworth et al. (1988)	M	33, 279
	5.5×10^{-3}		Oliver (1985)	M	
	3.8×10^{-3}		Warner et al. (1980)	M	
	2.1×10^{-3}		Sato and Nakajima (1979b)	M	14
	3.1×10^{-3}		Mackay et al. (2006b)	V	
	2.7×10^{-3}		Shiu and Mackay (1997)	V	
	5.6×10^{-3}		Lide and Frederikse (1995)	V	
	2.7×10^{-3}		Mackay et al. (1992a)	V	
	2.7×10^{-3}		Bobra et al. (1985)	V	
	3.3×10^{-3}		Warner et al. (1980)	V	
	2.1×10^{-3}		Hine and Mookerjee (1975)	V	
	2.9×10^{-3}		Yaws (2003)	X	238
	3.9×10^{-3}	2400	Goldstein (1982)	X	299
	3.7×10^{-3}		Ryan et al. (1988)	C	
	3.8×10^{-3}		Shen (1982)	C	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	9.2×10^{-3}		Duchowicz et al. (2020)	Q	300
	3.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	3.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
	4.7×10^{-3}		Hilal et al. (2008)	Q	
	3.2×10^{-3}		Modarresi et al. (2007)	Q	68
		4100	Kühne et al. (2005)	Q	
	3.8×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	4.5×10^{-3}		Delgado and Alderete (2002)	Q	
	5.0×10^{-3}		Yao et al. (2002)	Q	230, 268
	3.7×10^{-3}		English and Carroll (2001)	Q	231, 275
	4.2×10^{-3}		Katritzky et al. (1998)	Q	
	2.3×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	8.4×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	3.8×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4500	Kühne et al. (2005)	?	
	2.9×10^{-3}		Yaws (1999)	?	21
	2.2×10^{-3}		Abraham and Weathersby (1994)	?	21
	3.0×10^{-3}		Yaws and Yang (1992)	?	21
	2.7×10^{-3}		Abraham et al. (1990)	?	
1,4-dichlorobenzene	3.2×10^{-3}	3800	Schwardt et al. (2021)	L	1
$C_6H_4Cl_2$	3.8×10^{-3}	6000	Brockbank (2013)	L	1
(p-dichlorobenzene)	4.5×10^{-3}	4400	Fogg and Sangster (2003)	L	
[106-46-7]	6.3×10^{-3}		Mackay and Shiu (1981)	L	
OCJBOOLMMGQPQU-UHFFFAOYSA-N	5.8×10^{-3}	4600	Hiatt (2013)	M	
	3.3×10^{-3}		Li et al. (2008)	M	
	2.5×10^{-3}		Chiang et al. (1998)	M	12
	4.1×10^{-3}		Shiu and Mackay (1997)	M	
	5.4×10^{-3}		Hovorka and Dohnal (1997)	M	12
	4.7×10^{-3}	4800	Kondoh and Nakajima (1997)	M	
	3.1×10^{-3}	2700	Ashworth et al. (1988)	M	279
	5.2×10^{-3}		Yurteri et al. (1987)	M	12
	6.6×10^{-3}		Oliver (1985)	M	
	4.2×10^{-3}		Mackay and Shiu (1981)	M	
	3.6×10^{-3}		Warner et al. (1980)	M	
	4.1×10^{-3}		Mackay et al. (2006b)	V	
	6.3×10^{-3}		Shiu and Mackay (1997)	V	
	6.7×10^{-3}		Lide and Frederikse (1995)	V	
	6.3×10^{-3}		Mackay et al. (1992a)	V	
	3.8×10^{-3}		Suntio et al. (1988)	V	12
	5.8×10^{-3}		Bobra et al. (1985)	V	
	2.2×10^{-3}		Hine and Mookerjee (1975)	V	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.3×10^{-3}		Yaws (2003)	X	238
	3.7×10^{-3}	2700	Goldstein (1982)	X	299
	4.1×10^{-3}		Schüürmann (2000)	C	21
	4.1×10^{-3}		Ryan et al. (1988)	C	
	3.6×10^{-3}		Shen (1982)	C	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	8.4×10^{-3}		Duchowicz et al. (2020)	Q	185
	3.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	3.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
	6.5×10^{-3}		Hilal et al. (2008)	Q	
	3.0×10^{-3}		Modarresi et al. (2007)	Q	68
		4100	Kühne et al. (2005)	Q	
	4.1×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	4.1×10^{-3}		Delgado and Alderete (2002)	Q	
	4.3×10^{-3}		Katritzky et al. (1998)	Q	
	2.3×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	8.4×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	2.1×10^{-3}		Arbuckle (1983)	Q	
	4.1×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		3700	Kühne et al. (2005)	?	
	2.3×10^{-3}		Yaws and Yang (1992)	?	21
	3.8×10^{-3}		Abraham et al. (1990)	?	
1,2,3-trichlorobenzene	6.2×10^{-3}	4600	Brockbank (2013)	L	
$C_6H_3Cl_3$	1.5×10^{-2}	4800	Hiatt (2013)	M	
[87-61-6]	6.3×10^{-3}	4600	Brockbank et al. (2013)	M	
RELMFMZEBKVZJC-UHFFFAOYSA-N	8.0×10^{-3}		Lee et al. (2012)	M	
	3.6×10^{-3}	4200	Dewulf et al. (1999)	M	
	7.9×10^{-3}		Shiu and Mackay (1997)	M	
	1.5×10^{-2}	7300	Kondoh and Nakajima (1997)	M	
	1.4×10^{-2}		ten Hulscher et al. (1992)	M	12
	1.1×10^{-2}		Oliver (1985)	M	
	7.9×10^{-3}		Mackay and Shiu (1981)	M	
	4.1×10^{-3}		Mackay et al. (2006b)	V	
	5.8×10^{-3}		Fogg and Sangster (2003)	V	
	2.1×10^{-3}		Fogg and Sangster (2003)	V	
	4.1×10^{-3}		Shiu and Mackay (1997)	V	
	3.3×10^{-3}		Abraham et al. (1994a)	V	
	4.1×10^{-3}		Mackay et al. (1992a)	V	
	4.2×10^{-3}		Bobra et al. (1985)	V	
	4.3×10^{-3}		Mackay and Shiu (1981)	V	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	2.1×10^{-2}		Duchowicz et al. (2020)	Q	300

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.0×10^{-3}		Abraham et al. (2019)	Q	
	8.0×10^{-3}		Li et al. (2014)	Q	242
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	4.5×10^{-3}		Zhang et al. (2010)	Q	288, 289
	6.9×10^{-3}		Zhang et al. (2010)	Q	288, 290
	1.6×10^{-2}		Zhang et al. (2010)	Q	288, 291
	5.2×10^{-3}		Zhang et al. (2010)	Q	288, 292
	8.0×10^{-3}		Hilal et al. (2008)	Q	
	4.6×10^{-3}		Modarresi et al. (2007)	Q	68
		4800	Kühne et al. (2005)	Q	
	1.1×10^{-2}		Delgado and Alderete (2002)	Q	
	3.4×10^{-3}		English and Carroll (2001)	Q	231, 232
	4.4×10^{-3}		Katritzky et al. (1998)	Q	
	3.5×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	1.8×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	7.9×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4200	Kühne et al. (2005)	?	
1,2,3-trichlorobenzene-d3 $C_6D_3Cl_3$ [3907-98-0] SMNOERSLNYGGOU-UHFFFAOYSA-N	1.5×10^{-2}	4600	Hiatt (2013)	M	
1,2,4-trichlorobenzene $C_6H_3Cl_3$ [120-82-1] PBKONEOXTCPAFI-UHFFFAOYSA-N	3.9×10^{-3}	3100	Schwardt et al. (2021)	L	1
	4.2×10^{-3}	6400	Brockbank (2013)	L	
	1.1×10^{-2}	5100	Hiatt (2013)	M	
	5.8×10^{-3}		Lee et al. (2012)	M	
	2.4×10^{-3}	3500	Dewulf et al. (1999)	M	714
	2.7×10^{-3}		Ryu and Park (1999)	M	
	6.5×10^{-3}	5500	Kondoh and Nakajima (1997)	M	
	9.9×10^{-3}		ten Hulscher et al. (1992)	M	12
	4.6×10^{-3}	3900	Ashworth et al. (1988)	M	33, 279
	8.2×10^{-3}		Oliver (1985)	M	
	7.0×10^{-3}		Warner et al. (1980)	M	
			Mackay et al. (2006b)	V	685
	7.1×10^{-3}		Fogg and Sangster (2003)	V	
	8.6×10^{-3}		Fogg and Sangster (2003)	V	
	3.6×10^{-3}		Shiu and Mackay (1997)	V	
	7.1×10^{-3}		Lide and Frederikse (1995)	V	
	3.6×10^{-3}		Mackay et al. (1992a)	V	
	4.8×10^{-3}		McLachlan et al. (1990)	V	375
	3.6×10^{-3}		Bobra et al. (1985)	V	
	2.5×10^{-3}		Yoshida et al. (1983)	V	
	2.6×10^{-3}		Mackay and Shiu (1981)	V	
	4.3×10^{-3}		Warner et al. (1980)	V	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.3×10^{-3}		Yaws (2003)	X	238
	7.0×10^{-3}		Goldstein (1982)	X	448
	7.0×10^{-3}	2500	Goldstein (1982)	X	299
	6.9×10^{-3}		Meylan and Howard (1991)	C	
	4.2×10^{-4}		Ryan et al. (1988)	C	
	7.0×10^{-3}		Shen (1982)	C	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	Q	
	2.5×10^{-3}		Abraham et al. (2019)	Q	
	4.5×10^{-3}		Zhang et al. (2010)	Q	288, 289
	7.7×10^{-3}		Zhang et al. (2010)	Q	288, 290
	1.5×10^{-2}		Zhang et al. (2010)	Q	288, 291
	4.6×10^{-3}		Zhang et al. (2010)	Q	288, 292
	2.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
	9.9×10^{-3}		Hilal et al. (2008)	Q	
	4.2×10^{-3}		Modarresi et al. (2007)	Q	68
		4500	Kühne et al. (2005)	Q	
	2.4×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	6.7×10^{-3}		Delgado and Alderete (2002)	Q	
	7.4×10^{-3}		Yao et al. (2002)	Q	230
	3.4×10^{-3}		English and Carroll (2001)	Q	231, 261
	6.4×10^{-3}		Katritzky et al. (1998)	Q	
	1.6×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	3.5×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	4.5×10^{-3}		Meylan and Howard (1991)	Q	
	6.9×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		3200	Kühne et al. (2005)	?	
	3.3×10^{-3}		Yaws (1999)	?	21
1,2,4-trichlorobenzene-d3 $C_6D_3Cl_3$ [2199-72-6] PBKONEOXTCPAFI-CBYSEHNBSA-N	9.8×10^{-3}	4600	Hiatt (2013)	M	
1,3,5-trichlorobenzene $C_6H_3Cl_3$ [108-70-3] XKEFYDZQGKAQCN-UHFFFAOYSA-N	1.8×10^{-3}	4100	Dewulf et al. (1999)	M	715
	5.2×10^{-3}		ten Hulscher et al. (1992)	M	12
	3.5×10^{-2}		Hellmann (1987)	M	88
	5.2×10^{-3}		Oliver (1985)	M	
			Mackay et al. (2006b)	V	685
	1.4×10^{-3}		Fogg and Sangster (2003)	V	
	8.5×10^{-4}		Fogg and Sangster (2003)	V	
	9.1×10^{-4}		Shiu and Mackay (1997)	V	
	1.0×10^{-2}		Lide and Frederikse (1995)	V	
	1.5×10^{-3}		Abraham et al. (1994a)	V	
	9.1×10^{-4}		Mackay et al. (1992a)	V	
	9.1×10^{-4}		Bobra et al. (1985)	V	
	6.2×10^{-3}		Mackay and Shiu (1981)	V	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	7.5×10^{-3}		Duchowicz et al. (2020)	Q	185
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	4.6×10^{-3}		Hilal et al. (2008)	Q	
	4.2×10^{-3}		Modarresi et al. (2007)	Q	68
		4200	Kühne et al. (2005)	Q	
	4.5×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	4.6×10^{-3}		Delgado and Alderete (2002)	Q	
	1.6×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	3.5×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	4.5×10^{-3}		Meylan and Howard (1991)	Q	
	1.8×10^{-3}		Rumble (2021)	?	716
	5.2×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4400	Kühne et al. (2005)	?	
1,2,3,4-tetrachlorobenzene	3.5×10^{-3}		Ryu and Park (1999)	M	
$C_6H_2Cl_4$	1.3×10^{-2}	4800	ten Hulscher et al. (1992)	M	
[634-66-2]	5.7×10^{-2}		Hellmann (1987)	M	88
GBDZXPJXOMHESU-UHFFFAOYSA-N	1.4×10^{-2}		Oliver (1985)	M	
	9.0×10^{-3}		Mackay et al. (2006b)	V	
	6.9×10^{-3}		Shiu and Mackay (1997)	V	
	6.9×10^{-3}		Mackay et al. (1992a)	V	
	5.8×10^{-3}		McLachlan et al. (1990)	V	375
	6.9×10^{-3}		Bobra et al. (1985)	V	
	3.8×10^{-3}		Mackay and Shiu (1981)	V	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	2.0×10^{-2}		Duchowicz et al. (2020)	Q	300
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	6.1×10^{-3}		Zhang et al. (2010)	Q	288, 289
	7.7×10^{-3}		Zhang et al. (2010)	Q	288, 290
	2.1×10^{-2}		Zhang et al. (2010)	Q	288, 291
	4.6×10^{-3}		Zhang et al. (2010)	Q	288, 292
	8.6×10^{-3}		Hilal et al. (2008)	Q	
	5.7×10^{-3}		Modarresi et al. (2007)	Q	68
		5200	Kühne et al. (2005)	Q	
	1.1×10^{-2}		Delgado and Alderete (2002)	Q	
	4.2×10^{-3}		English and Carroll (2001)	Q	231, 232
	5.7×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	6.1×10^{-3}		Meylan and Howard (1991)	Q	
	1.3×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		4500	Kühne et al. (2005)	?	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,5-tetrachlorobenzene	6.3×10^{-3}		Shiu and Mackay (1997)	M	
$C_6H_2Cl_4$	1.0×10^{-2}		ten Hulscher et al. (1992)	M	12
[634-90-2]	6.3×10^{-3}		Mackay and Shiu (1981)	M	
QZYNWJQFTJXIRN-UHFFFAOYSA-N	1.7×10^{-3}		Mackay et al. (2006b)	V	
	2.1×10^{-3}		Fogg and Sangster (2003)	V	
	1.8×10^{-3}		Fogg and Sangster (2003)	V	
	1.7×10^{-3}		Shiu and Mackay (1997)	V	
	1.7×10^{-3}		Mackay et al. (1992a)	V	
	1.7×10^{-3}		Bobra et al. (1985)	V	
	1.7×10^{-3}		Mackay and Shiu (1981)	V	
	6.3×10^{-3}		Meylan and Howard (1991)	C	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	Q	
	1.7×10^{-3}		Li et al. (2014)	Q	242
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	7.7×10^{-3}		Hilal et al. (2008)	Q	
	5.4×10^{-3}		Modarresi et al. (2007)	Q	68
	7.1×10^{-3}		Delgado and Alderete (2002)	Q	
	4.2×10^{-3}		English and Carroll (2001)	Q	231, 275
	3.2×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	5.7×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	6.1×10^{-3}		Meylan and Howard (1991)	Q	
	2.4×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	6.2×10^{-3}		Duchowicz et al. (2020)	?	186, 21
1,2,4,5-tetrachlorobenzene	1.8×10^{-2}		McPhedran et al. (2013)	M	
$C_6H_2Cl_4$	6.6×10^{-3}		Lee et al. (2012)	M	
[95-94-3]	9.9×10^{-3}		Oliver (1985)	M	
JHBKHLUZVFWLAG-UHFFFAOYSA-N	8.2×10^{-3}		Mackay et al. (2006b)	V	
	2.8×10^{-4}		Fogg and Sangster (2003)	V	
	1.1×10^{-3}		Fogg and Sangster (2003)	V	
	8.2×10^{-3}		Shiu and Mackay (1997)	V	
	8.2×10^{-3}		Mackay et al. (1992a)	V	
	8.2×10^{-3}		Bobra et al. (1985)	V	
	3.8×10^{-3}		Mackay and Shiu (1981)	V	
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	6.1×10^{-3}		Zhang et al. (2010)	Q	288, 289
	8.4×10^{-3}		Zhang et al. (2010)	Q	288, 290
	1.8×10^{-2}		Zhang et al. (2010)	Q	288, 291
	4.8×10^{-3}		Zhang et al. (2010)	Q	288, 292
	9.2×10^{-3}		Hilal et al. (2008)	Q	
	6.1×10^{-3}		Modarresi et al. (2007)	Q	68

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.8×10^{-3}		Delgado and Alderete (2002)	Q	
	4.2×10^{-3}		English and Carroll (2001)	Q	231, 232
	3.2×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	5.7×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	6.1×10^{-3}		Meylan and Howard (1991)	Q	
pentachlorobenzene	1.4×10^{-2}	5400	Schwardt et al. (2021)	L	1
C_6HCl_5	1.4×10^{-2}	5200	Shen and Wania (2005)	L	368
[608-93-5]	1.4×10^{-2}	5600	Shen and Wania (2005)	L	369
CEOCDNVZRAIOQZ-UHFFFAOYSA-N	3.0×10^{-2}		McPhedran et al. (2013)	M	
	5.6×10^{-3}		Lee et al. (2012)	M	
	1.4×10^{-2}	5200	ten Hulscher et al. (1992)	M	
	2.0×10^{-1}		Hellmann (1987)	M	88
	1.4×10^{-2}		Oliver (1985)	M	
	1.2×10^{-2}		Mackay et al. (2006b)	V	
	3.5×10^{-2}		Fogg and Sangster (2003)	V	
	2.4×10^{-2}		Fogg and Sangster (2003)	V	
	1.2×10^{-2}		Shiu and Mackay (1997)	V	
	1.2×10^{-2}		Mackay et al. (1992a)	V	
	1.2×10^{-2}		Bobra et al. (1985)	V	
	1.0×10^{-3}		Mackay and Shiu (1981)	V	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	1.5×10^{-2}		Duchowicz et al. (2020)	Q	300
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	8.2×10^{-3}		Zhang et al. (2010)	Q	288, 289
	6.9×10^{-3}		Zhang et al. (2010)	Q	288, 290
	1.8×10^{-2}		Zhang et al. (2010)	Q	288, 291
	7.0×10^{-3}		Zhang et al. (2010)	Q	288, 292
	7.2×10^{-3}		Hilal et al. (2008)	Q	
	1.1×10^{-2}		Modarresi et al. (2007)	Q	68
		5700	Kühne et al. (2005)	Q	
	1.0×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	7.9×10^{-3}		Delgado and Alderete (2002)	Q	
	9.4×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	1.4×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		5100	Kühne et al. (2005)	?	
hexachlorobenzene	6.5×10^{-3}	6600	Brockbank (2013)	L	
C_6Cl_6	1.9×10^{-2}	6000	Shen and Wania (2005)	L	368
[118-74-1]	1.5×10^{-2}	6400	Shen and Wania (2005)	L	369
CKAPSXZOOQJIBF-UHFFFAOYSA-N	3.3×10^{-2}		McPhedran et al. (2013)	M	
	7.6×10^{-3}		Lee et al. (2012)	M	
	3.0×10^{-2}	6900	Jantunen and Bidleman (2006)	M	
	4.2×10^{-2}		Altschuh et al. (1999)	M	
	3.8×10^{-5}	570	Hansen et al. (1993)	M	282

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.0×10^{-2}	5700	ten Hulscher et al. (1992)	M	
	2.6		Hellmann (1987)	M	88
	2.1×10^{-2}		Oliver (1985)	M	
	1.4×10^{-2}		Atlas et al. (1983)	M	73
	7.5×10^{-3}		Atlas et al. (1982)	M	681
	5.8×10^{-3}		Warner et al. (1980)	M	
	7.6×10^{-3}		Mackay et al. (2006b)	V	
	7.6×10^{-3}		Shiu and Mackay (1997)	V	
	7.7×10^{-3}		Lide and Frederikse (1995)	V	
	7.6×10^{-3}		Mackay et al. (1992a)	V	
	7.1×10^{-3}		Ballschmiter and Wittlinger (1991)	V	
	1.1×10^{-2}		Calamari et al. (1991)	V	12
	1.4×10^{-1}		Riederer (1990)	V	
	2.5×10^{-2}		McLachlan et al. (1990)	V	375
	1.4×10^{-1}		Suntio et al. (1988)	V	12
	7.2×10^{-3}		Bobra et al. (1985)	V	
	1.6×10^{-2}		Yoshida et al. (1983)	V	
	2.0×10^{-1}		Mackay and Shiu (1981)	V	
	3.0×10^{-3}	3700	Paasivirta et al. (1999)	T	
	2.6×10^{-3}		Yaws (2003)	X	238
	5.8×10^{-3}	1600	Goldstein (1982)	X	299
	1.0×10^{-2}		Hilal et al. (2008)	C	
	1.5×10^{-2}		Suntio et al. (1988)	C	12
	5.8×10^{-3}		Ryan et al. (1988)	C	
	5.8×10^{-3}		Shen (1982)	C	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	1.4×10^{-2}		Duchowicz et al. (2020)	Q	185
	1.1×10^{-2}		Zhang et al. (2010)	Q	288, 289
	6.1×10^{-3}		Zhang et al. (2010)	Q	288, 290
	1.6×10^{-2}		Zhang et al. (2010)	Q	288, 291
	1.0×10^{-2}		Zhang et al. (2010)	Q	288, 292
	2.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.0×10^{-2}		Hilal et al. (2008)	Q	
	1.4×10^{-2}		Modarresi et al. (2007)	Q	68
		6400	Kühne et al. (2005)	Q	
	2.1×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	6.5×10^{-3}		Delgado and Alderete (2002)	Q	
	1.6×10^{-2}		Myrdal and Yalkowsky (1994)	Q	
	8.6×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	5.8×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		7200	Kühne et al. (2005)	?	
	2.4×10^{-5}		Yaws and Yang (1992)	?	21

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(chloromethyl)-benzene	2.2×10^{-2}	4400	Brockbank (2013)	L	
$C_6H_5CH_2Cl$	2.0×10^{-2}	7200	Hiatt (2013)	M	
(benzylchloride)	2.8×10^{-2}		Hovorka and Dohnal (1997)	M	12
[100-44-7]	1.2×10^{-2}		Li and Carr (1993)	M	
KCXMKQUNVWSEMD-UHFFFAOYSA-N	2.4×10^{-2}		Duchowicz et al. (2020)	V	187
	2.4×10^{-2}		HSDB (2015)	V	
	2.9×10^{-2}		Lide and Frederikse (1995)	V	
	1.6×10^{-2}		Mackay and Shiu (1981)	V	
	8.6×10^{-3}		Duchowicz et al. (2020)	Q	
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	272, 244
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	3.0×10^{-2}		Hilal et al. (2008)	Q	
	1.9×10^{-2}		Modarresi et al. (2007)	Q	68
	1.6×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.3×10^{-2}		Katritzky et al. (1998)	Q	
	1.0×10^{-2}		Abraham et al. (1990)	?	
1-chloro-2-methylbenzene	2.2×10^{-3}	4500	Brockbank (2013)	L	
C_7H_7Cl	3.2×10^{-3}	4100	Hiatt (2013)	M	
(*o*-chlorotoluene)	2.4×10^{-3}	3400	Kondoh and Nakajima (1997)	M	
[95-49-8]	2.8×10^{-3}	3500	Leighton and Calo (1981)	M	
IBSQPLPBRSHTTG-UHFFFAOYSA-N	1.9×10^{-2}	3000	Goldstein (1982)	X	299
	2.8×10^{-3}		Schüürmann (2000)	C	21
	5.3×10^{-2}		Keshavarz et al. (2022)	Q	
	4.3×10^{-3}		Duchowicz et al. (2020)	Q	300
	4.3×10^{-3}		Hilal et al. (2008)	Q	
	5.4×10^{-3}		Modarresi et al. (2007)	Q	68
		4400	Kühne et al. (2005)	Q	
	5.7×10^{-3}		Katritzky et al. (1998)	Q	
	3.1×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	2.8×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4900	Kühne et al. (2005)	?	
	2.8×10^{-3}		Abraham et al. (1990)	?	
1-chloro-3-methylbenzene	6.1×10^{-4}		Duchowicz et al. (2020)	V	187
C_7H_7Cl	6.2×10^{-4}		Schüürmann (2000)	V	
(*m*-chlorotoluene)	4.3×10^{-3}		Duchowicz et al. (2020)	Q	
[108-41-8]	3.8×10^{-3}		Hilal et al. (2008)	Q	
OSOUNOBYRMOXQQ-UHFFFAOYSA-N	6.4×10^{-3}		Modarresi et al. (2007)	Q	68
		4400	Kühne et al. (2005)	Q	
	6.1×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	4.8×10^{-3}		Katritzky et al. (1998)	Q	
		4800	Kühne et al. (2005)	?	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloro-4-methylbenzene	2.7×10^{-3}	4900	Brockbank (2013)	L	
C_7H_7Cl	4.1×10^{-3}	4200	Hiatt (2013)	M	
(*p*-chlorotoluene)	2.9×10^{-3}	3900	Kondoh and Nakajima (1997)	M	
[106-43-4]	2.3×10^{-3}		Duchowicz et al. (2020)	V	187
NPDACUSDTOMAMK-UHFFFAOYSA-N	2.2×10^{-3}		HSDB (2015)	V	
	3.1×10^{-3}		Yaws (2003)	X	238, 12
	4.3×10^{-3}		Duchowicz et al. (2020)	Q	
	8.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
	4.0×10^{-3}		Hilal et al. (2008)	Q	
	6.8×10^{-3}		Modarresi et al. (2007)	Q	68
		4400	Kühne et al. (2005)	Q	
	5.1×10^{-3}		Yao et al. (2002)	Q	230
	4.8×10^{-3}		Katritzky et al. (1998)	Q	
		4300	Kühne et al. (2005)	?	
	2.3×10^{-3}		Yaws (1999)	?	21, 12
(dichloromethyl)-benzene	2.5×10^{-2}		Duchowicz et al. (2020)	V	187
$C_7H_6Cl_2$	1.8×10^{-2}		Duchowicz et al. (2020)	Q	
[98-87-3]	1.3×10^{-2}		Zhang et al. (2010)	Q	288, 289
CAHQGWAXKLQREW-UHFFFAOYSA-N	3.4×10^{-2}		Zhang et al. (2010)	Q	288, 290
	1.1×10^{-1}		Zhang et al. (2010)	Q	288, 291
	1.0×10^{-2}		Zhang et al. (2010)	Q	288, 292
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	2.0×10^{-2}		Modarresi et al. (2007)	Q	68
1,2-dichloro-4-methylbenzene	3.8×10^{-3}		Duchowicz et al. (2020)	V	187
$C_7H_6Cl_2$	7.9×10^{-3}		Duchowicz et al. (2020)	Q	
(3,4-dichlorotoluene)	7.9×10^{-3}		Hilal et al. (2008)	Q	
[95-75-0]	4.1×10^{-3}		Modarresi et al. (2007)	Q	68
WYUIWKFIFOJVKW-UHFFFAOYSA-N	4.1×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	9.0×10^{-3}		Katritzky et al. (1998)	Q	
1,3-dichloro-2-methylbenzene	2.3×10^{-3}		HSDB (2015)	Q	100
$C_7H_6Cl_2$	3.1×10^{-3}		Zhang et al. (2010)	Q	288, 289
(2,6-dichlorotoluene)	8.6×10^{-3}		Zhang et al. (2010)	Q	288, 290
[118-69-4]	4.2×10^{-3}		Zhang et al. (2010)	Q	288, 291
DMEDNTFWIHCBRK-UHFFFAOYSA-N	1.8×10^{-3}		Zhang et al. (2010)	Q	288, 292
2,4-dichloro-1-methylbenzene	2.7×10^{-3}	5000	Schwardt et al. (2021)	L	1
$C_7H_6Cl_2$	2.7×10^{-3}	5000	Brockbank (2013)	L	
(2,4-dichlorotoluene)	2.7×10^{-3}	4900	Brockbank et al. (2013)	M	
[95-73-8]	2.3×10^{-3}		HSDB (2015)	Q	100
FUNUTBJJKQIVSY-UHFFFAOYSA-N	3.1×10^{-3}		Zhang et al. (2010)	Q	288, 289
	5.4×10^{-3}		Zhang et al. (2010)	Q	288, 290
	6.7×10^{-3}		Zhang et al. (2010)	Q	288, 291
	1.8×10^{-3}		Zhang et al. (2010)	Q	288, 292
		4400	Kühne et al. (2005)	Q	

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		5500	Kühne et al. (2005)	?	
2,3,6-trichloromethylbenzene	6.6×10^{-3}		Oliver (1985)	M	
$C_7H_5Cl_3$	1.4×10^{-2}		Hilal et al. (2008)	Q	
(2,3,6-trichlorotoluene)	6.0×10^{-3}		Modarresi et al. (2007)	Q	68
[2077-46-5]	4.1×10^{-3}		Meylan and Howard (1991)	Q	
UZYYBZNZSSNYSA-UHFFFAOYSA-N					
2,4,5-trichloromethylbenzene	6.6×10^{-3}		Oliver (1985)	M	
$C_7H_5Cl_3$	1.2×10^{-2}		Hilal et al. (2008)	Q	
(2,4,5-trichlorotoluene)	6.2×10^{-3}		Modarresi et al. (2007)	Q	68
[6639-30-1]	4.1×10^{-3}		Meylan and Howard (1991)	Q	
ZCXHZKNWIYVQNC-UHFFFAOYSA-N					
2,4,6-trichloromethylbenzene	6.5×10^{-3}		Ebert et al. (2023)	?	367
$C_7H_5Cl_3$					
(2,4,6-trichlorotoluene)					
[23749-65-7]					
RCTKUIOMKBEGTG-UHFFFAOYSA-N					
pentachloromethylbenzene	1.3×10^{-2}		Oliver (1985)	M	
$C_7H_3Cl_5$	1.6×10^{-2}		Hilal et al. (2008)	Q	
(2,3,4,5,6-pentachlorotoluene)	1.7×10^{-2}		Modarresi et al. (2007)	Q	68
[877-11-2]	7.4×10^{-3}		Meylan and Howard (1991)	Q	
AVSIMRGRHWKCAY-UHFFFAOYSA-N					
1-chloro-2-(chloromethyl)benzene	6.4×10^{-3}		Zhang et al. (2010)	Q	288, 289
$C_7H_6Cl_2$	7.2×10^{-2}		Zhang et al. (2010)	Q	288, 290
[611-19-8]	2.1×10^{-1}		Zhang et al. (2010)	Q	288, 291
BASMANVIUSSIIM-UHFFFAOYSA-N	6.1×10^{-3}		Zhang et al. (2010)	Q	288, 292
1-chloro-4-(chloromethyl)benzene	2.9×10^{-2}		HSDB (2015)	Q	100
$C_7H_6Cl_2$	6.4×10^{-3}		Zhang et al. (2010)	Q	288, 289
[104-83-6]	7.5×10^{-2}		Zhang et al. (2010)	Q	288, 290
JQZAEUFPPSRDOP-UHFFFAOYSA-N	8.2×10^{-2}		Zhang et al. (2010)	Q	288, 291
	6.1×10^{-3}		Zhang et al. (2010)	Q	288, 292
chloro(dichloromethyl)benzene	1.8×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_7H_5Cl_3$	7.3×10^{-2}		Zhang et al. (2010)	Q	288, 290
[88-66-4]	5.4×10^{-2}		Zhang et al. (2010)	Q	288, 291
BXSVYGKOUULJCL-UHFFFAOYSA-N	1.3×10^{-2}		Zhang et al. (2010)	Q	288, 292
(trichloromethyl)-benzene	3.8×10^{-2}		HSDB (2015)	Q	100
$C_7H_5Cl_3$	3.8×10^{-2}		Zhang et al. (2010)	Q	288, 289
[98-07-7]	7.2×10^{-3}		Zhang et al. (2010)	Q	288, 290
XEMRAKSQROQPBR-UHFFFAOYSA-N	2.0×10^{-2}		Zhang et al. (2010)	Q	288, 291
	4.7×10^{-3}		Zhang et al. (2010)	Q	288, 292

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloro-4-(trichloromethyl)benzene	5.1×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_7H_4Cl_4$	1.8×10^{-2}		Zhang et al. (2010)	Q	288, 290
[5216-25-1]	3.4×10^{-2}		Zhang et al. (2010)	Q	288, 291
LVZPKYYPPLUECL-UHFFFAOYSA-N	6.9×10^{-3}		Zhang et al. (2010)	Q	288, 292
1-chloro-3-ethenylbenzene	4.7×10^{-3}		HSDB (2015)	Q	100
C_8H_7Cl					
[2039-85-2]					
BOVQCIDBZXNFEJ-UHFFFAOYSA-N					
1-chloro-4-ethenylbenzene	4.7×10^{-3}		HSDB (2015)	Q	100
C_8H_7Cl					
[1073-67-2]					
KTZVZZJJVJQZHV-UHFFFAOYSA-N					
1,4-dichloro-2,5-dimethylbenzene	2.7×10^{-3}		Zhang et al. (2010)	Q	288, 289
$C_8H_8Cl_2$	1.2×10^{-2}		Zhang et al. (2010)	Q	288, 290
[1124-05-6]	4.6×10^{-3}		Zhang et al. (2010)	Q	288, 291
UTGSRNVBAFCOEU-UHFFFAOYSA-N	2.3×10^{-3}		Zhang et al. (2010)	Q	288, 292
1,4-bis(trichloromethyl)benzene	7.9×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_8H_4Cl_6$	3.7×10^{-2}		Zhang et al. (2010)	Q	288, 290
[68-36-0]	1.1×10^{-1}		Zhang et al. (2010)	Q	288, 291
OTEKOJQFKOIXMU-UHFFFAOYSA-N	5.8×10^{-3}		Zhang et al. (2010)	Q	288, 292
α,α-dichloro-*o*-xylene	1.0×10^{-1}	11000	Hiatt (2013)	M	
$C_8H_8Cl_2$					
[612-12-4]					
FMGGHNGKHRCJLL-UHFFFAOYSA-N					
2-chlorostyrene	4.7×10^{-3}		HSDB (2015)	Q	100
C_8H_7Cl	6.2×10^{-3}		Hilal et al. (2008)	Q	
[2039-87-4]					
ISRGONDNXBCDBM-UHFFFAOYSA-N					
octachlorostyrene	7.6×10^{-2}		Oliver (1985)	M	
C_8Cl_8	4.3×10^{-2}		HSDB (2015)	Q	100
[29082-74-4]	1.6×10^{-2}		Hilal et al. (2008)	Q	
RUYUCCQRWINUHE-UHFFFAOYSA-N	4.3×10^{-2}		Meylan and Howard (1991)	Q	
heptachlor	3.3×10^{-2}		Shen and Wania (2005)	L	368
$C_{10}H_5Cl_7$	2.6×10^{-2}		Shen and Wania (2005)	L	369
[76-44-8]	1.9×10^{-2}	4300	Cetin et al. (2006)	M	
FRCCEHPWNOQAEU-UHFFFAOYSA-N	3.4×10^{-2}		Altschuh et al. (1999)	M	
	6.7×10^{-3}		Warner et al. (1980)	M	
	2.8×10^{-3}		Mackay et al. (2006d)	V	
	8.9×10^{-3}		Suntio et al. (1988)	V	12
	8.8×10^{-5}		Barcelo and Hennion (1997)	X	569
	4.3×10^{-3}		McCarty (1980)	X	370

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.7×10^{-3}		Meylan and Howard (1991)	C	
	6.5×10^{-3}		Ryan et al. (1988)	C	
	6.7×10^{-3}		Shen (1982)	C	
	1.3×10^{-1}		Keshavarz et al. (2022)	Q	
	2.9×10^{-2}		Duchowicz et al. (2020)	Q	
	2.0×10^{-4}		Goodarzi et al. (2010)	Q	570
	2.4×10^{-2}		Hilal et al. (2008)	Q	
	5.8×10^{-1}		Modarresi et al. (2007)	Q	68
	5.6×10^{-2}		Meylan and Howard (1991)	Q	
	3.4×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	2.8×10^{-3}		MacBean (2012a)	?	
1-chloro-2-methyl-2-phenylpropane	2.0×10^{-3}		Zhang et al. (2010)	Q	288, 289
$C_{10}H_{13}Cl$	9.5×10^{-3}		Zhang et al. (2010)	Q	288, 290
[515-40-2]	1.6×10^{-2}		Zhang et al. (2010)	Q	288, 291
DNXXUUPUQXSUFH-UHFFFAOYSA-N	1.6×10^{-3}		Zhang et al. (2010)	Q	288, 292
1,3-dichloro-5-[(2*S*)-2,4,4,4-tetrachlorobutan-2-yl]benzene	8.4×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{10}H_8Cl_6$	6.1×10^{-2}		Zhang et al. (2010)	Q	288, 290
[73588-42-8]	1.5		Zhang et al. (2010)	Q	288, 291
DELZPCKTBPIBEE-VIFPVBQESA-N	2.9×10^{-3}		Zhang et al. (2010)	Q	288, 292
1,2,3,4,5,6,7,8,8-nonachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H-indene	3.9×10^{-1}		HSDB (2015)	Q	100
$C_{10}H_5Cl_9$					
(nonachlor)					
[3734-49-4]					
OCHOKXCPKDPNQU-UHFFFAOYSA-N					
1,1-dichloro-2,2-bis-(4-chlorophenyl)-ethane	1.5		Shen and Wania (2005)	L	368
$C_{14}H_{10}Cl_4$	2.0		Shen and Wania (2005)	L	369
(p,p'-DDD)	7.6×10^{-1}		Chao et al. (2017)	M	
[72-54-8]	9.1×10^{-1}	5100	Cetin et al. (2006)	M	
AHJKRLASYNVKDZ-UHFFFAOYSA-N	1.5		Altschuh et al. (1999)	M	
			Mackay et al. (2006d)	V	560
	1.1×10^{-1}		Ballschmiter and Wittlinger (1991)	V	
	1.6		Suntio et al. (1988)	V	12
	4.6×10^{-1}		Yoshida et al. (1983)	V	
	2.9×10^{-2}	7300	Paasivirta et al. (1999)	T	
	8.1×10^{-4}		Ryan et al. (1988)	C	
	4.3×10^{-1}		Keshavarz et al. (2022)	Q	
	9.5×10^{-2}		Duchowicz et al. (2020)	Q	185
	2.1		Hilal et al. (2008)	Q	
	3.1×10^{-1}		Modarresi et al. (2007)	Q	68

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.5		Duchowicz et al. (2020)	?	186, 21
mitotane	1.2		Duchowicz et al. (2020)	V	187
$C_{14}H_{10}Cl_4$	1.2		HSDB (2015)	V	
(o,p'-DDD)	1.6		Suntio et al. (1988)	V	12
[53-19-0]	5.6×10^{2}		Suntio et al. (1988)	C	717
JWBOIMRXGHLCPP-UHFFFAOYSA-N	9.5×10^{-2}		Duchowicz et al. (2020)	Q	
	2.3×10^{-1}		Zhang et al. (2010)	Q	288, 289
	1.6		Zhang et al. (2010)	Q	288, 290
	1.1×10^{1}		Zhang et al. (2010)	Q	288, 291
	3.9×10^{-1}		Zhang et al. (2010)	Q	288, 292
1,1-dichloro-2,2-bis-(4-chlorophenyl)-ethene	2.4×10^{-1}		Shen and Wania (2005)	L	368
$C_{14}H_8Cl_4$	2.4×10^{-1}		Shen and Wania (2005)	L	369
(p,p'-DDE)	2.9×10^{-2}	4700	Jantunen and Bidleman (2006)	M	
[72-55-9]	1.6×10^{-1}	7700	Cetin et al. (2006)	M	
UCNVFOCBFJOQAL-UHFFFAOYSA-N	2.4×10^{-1}		Altschuh et al. (1999)	M	
	8.1×10^{-3}		Atlas et al. (1982)	M	681
			Mackay et al. (2006d)	V	560
	2.9×10^{-2}		Ballschmiter and Wittlinger (1991)	V	
	1.6×10^{-1}		Calamari et al. (1991)	V	12
	7.6×10^{-1}		McLachlan et al. (1990)	V	375
	1.3×10^{-1}		Suntio et al. (1988)	V	12
	5.1×10^{-2}		Yoshida et al. (1983)	V	
	1.2×10^{-1}		Addison et al. (1983)	V	
	2.6×10^{-2}	7600	Paasivirta et al. (1999)	T	
	4.5×10^{-1}		Suntio et al. (1988)	C	683
	4.5×10^{-1}		Ryan et al. (1988)	C	
	8.1×10^{-2}		Keshavarz et al. (2022)	Q	
	4.2×10^{-2}		Duchowicz et al. (2020)	Q	
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	68
	2.4×10^{-1}		Duchowicz et al. (2020)	?	186, 21
o,p'-DDE	5.3×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{14}H_8Cl_4$	3.9×10^{-1}		Mackay et al. (2006d)	V	
[3424-82-6]	3.9×10^{-1}		Suntio et al. (1988)	V	12
ZDYJWDIWLRZXDB-UHFFFAOYSA-N	1.4×10^{-1}		Suntio et al. (1988)	C	12
	4.2×10^{-2}		Duchowicz et al. (2020)	Q	
1,1,1-trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	1.3		Duchowicz et al. (2020)	V	187
$C_{14}H_9Cl_5$	2.9		Mackay et al. (2006d)	V	
(o,p'-DDT)	1.9×10^{-2}		Calamari et al. (1991)	V	12
[789-02-6]	4.4×10^{-2}		Duchowicz et al. (2020)	Q	
CVUGPAFCQJIYDT-UHFFFAOYSA-N					

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1,1-trichloro-2,2-bis-(4-chlorophenyl)-ethane	9.1×10^{-1}		Shen and Wania (2005)	L	368
$C_{14}H_9Cl_5$	9.1×10^{-1}		Shen and Wania (2005)	L	369
(DDT; p,p'-DDT)	1.9×10^{-1}		Mackay and Shiu (1981)	L	
[50-29-3]	9.0×10^{-1}	7500	Cetin et al. (2006)	M	
YVGGHNCTFXOJCH-UHFFFAOYSA-N	1.2		Altschuh et al. (1999)	M	
	7.7×10^{-1}		Fendinger et al. (1989)	M	73
	1.2		Fendinger et al. (1989)	M	647
			Mackay et al. (2006d)	V	560
	1.7×10^{-1}		Ballschmiter and Wittlinger (1991)	V	
	3.4×10^{-1}		Calamari et al. (1991)	V	12
	4.2×10^{-1}		Suntio et al. (1988)	V	12
	6.1×10^{-1}		Caron et al. (1985)	V	
	3.7×10^{-1}		Yoshida et al. (1983)	V	
	1.3×10^{-1}		Burkhard and Guth (1981)	V	
	2.5×10^{-1}		Mackay and Leinonen (1975)	V	
	1.9×10^{-2}	7800	Paasivirta et al. (1999)	T	
	4.2×10^{-3}		Barcelo and Hennion (1997)	X	569
	1.7×10^{-1}		Suntio et al. (1988)	C	683
	2.0×10^{-1}		Ryan et al. (1988)	C	
	4.3×10^{-1}		Keshavarz et al. (2022)	Q	
	4.4×10^{-2}		Duchowicz et al. (2020)	Q	300
	6.4×10^{-1}		Zhang et al. (2010)	Q	288, 289
	6.2×10^{-1}		Zhang et al. (2010)	Q	288, 290
	1.6×10^{1}		Zhang et al. (2010)	Q	288, 291
	2.0×10^{-1}		Zhang et al. (2010)	Q	288, 292
	7.7×10^{-3}		Goodarzi et al. (2010)	Q	570
	6.7×10^{-1}		Hilal et al. (2008)	Q	
	3.5×10^{-1}		Modarresi et al. (2007)	Q	68
	1.2		Duchowicz et al. (2020)	?	186, 21
	2.8×10^{-1}		Brimblecombe (1986)	?	81
aldrin	6.7×10^{-2}		Shen and Wania (2005)	L	368
$C_{12}H_8Cl_6$	4.3×10^{-2}		Shen and Wania (2005)	L	369
[309-00-2]	3.6×10^{-1}		Mackay and Shiu (1981)	L	
QBYJBZPUGVGKQQ-SJJAEHHWSA-N	2.6×10^{-1}		Chao et al. (2017)	M	
	2.2×10^{-2}	3900	Cetin et al. (2006)	M	
	2.2×10^{-1}		Altschuh et al. (1999)	M	
	2.0×10^{-2}		Warner et al. (1980)	M	
	1.1×10^{-2}		Mackay et al. (2006d)	V	
	1.1×10^{-2}		Suntio et al. (1988)	V	12
	6.9×10^{-1}		Mackay and Leinonen (1975)	V	
	1.1×10^{-4}		Barcelo and Hennion (1997)	X	569
	2.0×10^{-2}		Hilal et al. (2008)	C	
	2.0×10^{-2}		Meylan and Howard (1991)	C	
	7.0×10^{-1}		Suntio et al. (1988)	C	12

Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.1×10^{-1}		Suntio et al. (1988)	C	
	2.6×10^{-2}		Suntio et al. (1988)	C	683
	2.0×10^{-2}		Suntio et al. (1988)	C	12
	8.2×10^{-1}		Ryan et al. (1988)	C	
	2.0×10^{-2}		Shen (1982)	C	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	2.3×10^{-2}		Duchowicz et al. (2020)	Q	185
	6.4×10^{-4}		Goodarzi et al. (2010)	Q	570, 571
	8.6×10^{-3}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Modarresi et al. (2007)	Q	68
	2.6×10^{-2}		Meylan and Howard (1991)	Q	
	2.2×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	8.4×10^{-1}		Brimblecombe (1986)	?	81
isodrin $C_{12}H_8Cl_6$ [465-73-6] QBYJBZPUGVGKQQ-DIFDVCDBSA-N	2.5×10^{-2}		HSDB (2015)	Q	100
1,1'-(2,2-dichloroethylidene)bis[4-ethylbenzene $C_{18}H_{20}Cl_2$ (perthane) [72-56-0] QFMDFTQOJHFVNR-UHFFFAOYSA-N	5.8×10^{-2}		HSDB (2015)	Q	100

A6.2 Polychlorinated naphthalenes (PCNs)

Table A6.2: Polychlorinated naphthalenes (PCNs)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloronaphthalene	2.8×10^{-2}		Shiu and Mackay (1997)	M	
$C_{10}H_7Cl$	2.8×10^{-3}		Mackay and Shiu (1981)	M	
(PCN-1)	5.0×10^{-2}		Yaws (2003)	X	238
[90-13-1]	4.7×10^{-2}		Yaws et al. (2005)	X	448
JTPNRXUCIXHOKM-UHFFFAOYSA-N	2.4×10^{-2}		Keshavarz et al. (2022)	Q	
	3.3×10^{-2}		Duchowicz et al. (2020)	Q	
	1.1×10^{-2}		Li et al. (2014)	Q	242
	3.1×10^{-1}		Gharagheizi et al. (2012)	Q	
	5.3×10^{-2}		Gharagheizi et al. (2010)	Q	247
	5.7×10^{-2}		Hilal et al. (2008)	Q	
	7.3×10^{-2}		Modarresi et al. (2007)	Q	68
	3.1×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	1.1×10^{-2}		Katritzky et al. (1998)	Q	
	6.5×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.8×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	5.1×10^{-2}		Yaws (1999)	?	21
2-chloronaphthalene	3.0×10^{-2}		Shiu and Mackay (1997)	M	
$C_{10}H_7Cl$	3.1×10^{-2}		Mackay and Shiu (1981)	M	
(PCN-2)	1.5×10^{-2}		Hwang et al. (1992)	V	
[91-58-7]	1.6×10^{-2}	3800	Goldstein (1982)	X	299
CGYGETOMCSJHJU-UHFFFAOYSA-N	3.1×10^{-2}		Ryan et al. (1988)	C	
	2.4×10^{-2}		Keshavarz et al. (2022)	Q	
	3.3×10^{-2}		Duchowicz et al. (2020)	Q	185
	6.0×10^{-2}		Hilal et al. (2008)	Q	
	1.0×10^{-1}		Modarresi et al. (2007)	Q	68
	3.1×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	6.5×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	3.1×10^{-2}		Duchowicz et al. (2020)	?	186, 21
1,2-dichloronaphthalene $C_{10}H_6Cl_2$ (PCN-3) [2050-69-3] MOXLHAPKZWTHEX-UHFFFAOYSA-N	1.2×10^{-1}		Ebert et al. (2023)	?	718
1,3-dichloronaphthalene	3.4×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{10}H_6Cl_2$	7.0×10^{-2}		Zhang et al. (2010)	Q	288, 290
(PCN-4)	4.2×10^{-2}		Zhang et al. (2010)	Q	288, 291
[2198-75-6]	4.7×10^{-2}		Zhang et al. (2010)	Q	288, 292
AMCBMCWLCDERHY-UHFFFAOYSA-N					

Table A6.2: Polychlorinated naphthalenes (PCNs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,4-dichloronaphthalene $C_{10}H_6Cl_2$ (PCN-5) [1825-31-6] JDPKCYMVSKDOGS-UHFFFAOYSA-N	2.4×10^{-2} 3.2×10^{-2}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
1,5-dichloronaphthalene $C_{10}H_6Cl_2$ (PCN-6) [1825-30-5] ZBQZXTBAGBTUAD-UHFFFAOYSA-N	4.0×10^{-2}		Ebert et al. (2023)	?	718
2,7-dichloronaphthalene $C_{10}H_6Cl_2$ (PCN-12) [2198-77-8] DWBQZSYTSNYEEJ-UHFFFAOYSA-N	3.1×10^{-2}		Ebert et al. (2023)	?	719
1,2,4-trichloronaphthalene $C_{10}H_5Cl_3$ (PCN-14) [50402-51-2] MRJBOPVWPORBKZ-UHFFFAOYSA-N	8.3×10^{-2}		Ebert et al. (2023)	?	367
1,2,5-trichloronaphthalene $C_{10}H_5Cl_3$ (PCN-15) [55720-33-7] MMHZKSMAFILONG-UHFFFAOYSA-N	1.1×10^{-1}	5300	Odabasi and Adali (2016)	M	720
1,2,6-trichloronaphthalene $C_{10}H_5Cl_3$ (PCN-16) [51570-44-6] AAUJSCRITBXDJH-UHFFFAOYSA-N	1.7×10^{-1}	6500	Odabasi and Adali (2016)	M	720
1,2,7-trichloronaphthalene $C_{10}H_5Cl_3$ (PCN-17) [55720-34-8] QYYUVUXSJZJCLQ-UHFFFAOYSA-N	1.5×10^{-1}		Ebert et al. (2023)	?	367
1,3,5-trichloronaphthalene $C_{10}H_5Cl_3$ (PCN-19) [51570-43-5] DZHZYPCCEISGSQ-UHFFFAOYSA-N	7.1×10^{-2}	5500	Odabasi and Adali (2016)	M	720

Table A6.2: Polychlorinated naphthalenes (PCNs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,4,5-trichloronaphthalene $C_{10}H_5Cl_3$ (PCN-23) [2437-55-0] VQSNXLCFFHGXTI-UHFFFAOYSA-N	2.2×10^{-1}	5400	Odabasi and Adali (2016)	M	720
1,4,6-trichloronaphthalene $C_{10}H_5Cl_3$ (PCN-24) [2437-54-9] RLTTZFDRZKJVKJ-UHFFFAOYSA-N	8.3×10^{-2}		Ebert et al. (2023)	?	367
1,6,7-trichloronaphthalene $C_{10}H_5Cl_3$ (PCN-25) [55720-39-3] FUEZTEBYLIMNHN-UHFFFAOYSA-N	1.5×10^{-1}		Ebert et al. (2023)	?	367
1,2,3,4-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-27) [20020-02-4] NAQWICRLNQSPPW-UHFFFAOYSA-N	4.1×10^{-2} 4.1×10^{-2} 8.3×10^{-2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
1,2,3,5-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-28) [53555-63-8] HJJKSUVYCQAMBG-UHFFFAOYSA-N	1.3×10^{-1}		Ebert et al. (2023)	?	718
1,2,4,5-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-32) [6733-54-6] BIVDISPRSYAHQQ-UHFFFAOYSA-N	1.5×10^{-1}	5900	Odabasi and Adali (2016)	M	720
1,2,4,6-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-33) [51570-45-7] GLVVZPZGCNEVEM-UHFFFAOYSA-N	7.8×10^{-2}		Ebert et al. (2023)	?	367
1,2,4,7-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-34) [67922-21-8] PWXOBMRJWBBEED-UHFFFAOYSA-N	7.8×10^{-2}		Ebert et al. (2023)	?	367

Table A6.2: Polychlorinated naphthalenes (PCNs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,4,8-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-35) [6529-87-9] WCMSFBRREKZZFL-UHFFFAOYSA-N	1.8×10^{-1}	6000	Odabasi and Adali (2016)	M	720
1,2,5,6-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-36) [67922-22-9] ZPUUGNBIWHBXBM-UHFFFAOYSA-N	1.0×10^{-1}		Ebert et al. (2023)	?	367
1,2,5,7-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-37) [67922-23-0] KQZUIOXHRIVQGR-UHFFFAOYSA-N	7.8×10^{-2}		Ebert et al. (2023)	?	367
1,2,5,8-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-38) [149864-80-2] DLTBLLHAQLBHDR-UHFFFAOYSA-N	2.2×10^{-1}		Ebert et al. (2023)	?	367
1,2,6,8-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-40) [67922-24-1] OVAYDYKVLHHIDQ-UHFFFAOYSA-N	2.2×10^{-1}		Ebert et al. (2023)	?	367
1,3,5,7-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-42) [53555-64-9] OTTCXKPQKOLSJN-UHFFFAOYSA-N	5.6×10^{-2}	5600	Odabasi and Adali (2016)	M	720
1,3,5,8-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-43) [31604-28-1] VFTLNRFRXWCJJK-UHFFFAOYSA-N	1.3×10^{-1}		Ebert et al. (2023)	?	719
1,3,6,8-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-45) [150224-15-0] XXWQPOHDPJIYIN-UHFFFAOYSA-N	1.0×10^{-1}		Ebert et al. (2023)	?	367

Table A6.2: Polychlorinated naphthalenes (PCNs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,4,5,8-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-46) [3432-57-3] LITCKAVLJAKHOE-UHFFFAOYSA-N	3.5×10^{-1}	5700	Odabasi and Adali (2016)	M	720
1,4,6,7-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-47) [55720-43-9] VJZRCIYSYVGDMU-UHFFFAOYSA-N	9.2×10^{-2}	5800	Odabasi and Adali (2016)	M	720
1,2,3,4,6-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-50) [67922-26-3] BAOLNVSMVTYGDA-UHFFFAOYSA-N	7.8×10^{-2}	9000	Odabasi and Adali (2016)	M	720
1,2,3,5,7-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-52) [53555-65-0] OVSKLQPHXHPXDR-UHFFFAOYSA-N	6.9×10^{-2}		Ebert et al. (2023)	?	367
1,2,3,5,8-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-53) [150224-24-1] HVYRFNJXZVEGFK-UHFFFAOYSA-N	1.7×10^{-1}	9700	Odabasi and Adali (2016)	M	720
1,2,4,5,6-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-57) [150224-20-7] KPOZENRUJCHWOA-UHFFFAOYSA-N	1.4×10^{-1}	9500	Odabasi and Adali (2016)	M	720
1,2,4,5,7-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-58) [150224-19-4] WYLDWCYZCFRVRH-UHFFFAOYSA-N	8.9×10^{-2}	8700	Odabasi and Adali (2016)	M	720
1,2,4,5,8-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-59) [150224-25-2] FEIKEVSWLMYFFF-UHFFFAOYSA-N	2.6×10^{-1}	9100	Odabasi and Adali (2016)	M	720

Table A6.2: Polychlorinated naphthalenes (PCNs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,4,6,7-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-60) [150224-17-2] GXQUDLBNLKOIQB-UHFFFAOYSA-N	6.9×10^{-2}		Ebert et al. (2023)	?	367
1,2,4,6,8-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-61) [150224-22-9] HGSDQSUMXKHGTH-UHFFFAOYSA-N	1.0×10^{-1}	8800	Odabasi and Adali (2016)	M	720
1,2,4,7,8-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-62) [150224-21-8] LBCOXKFWBDTJTF-UHFFFAOYSA-N	1.7×10^{-1}	9200	Odabasi and Adali (2016)	M	720
1,2,3,4,5,6-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-63) [58877-88-6] CTLMCQOGOWNFHA-UHFFFAOYSA-N	7.8×10^{-1}	12000	Odabasi and Adali (2016)	M	720
1,2,3,4,5,7-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-64) [67922-27-4] SWRNUKWDDYPZGV-UHFFFAOYSA-N	3.7×10^{-1}		Ebert et al. (2023)	?	367
1,2,3,4,5,8-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-65) [103426-93-3] PGCDNPCENWGYMA-UHFFFAOYSA-N	9.3×10^{-1}	10000	Odabasi and Adali (2016)	M	720
1,2,3,4,6,7-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-66) [103426-96-6] ZRNSVEOEIWQEMU-UHFFFAOYSA-N	4.3×10^{-1}		Ebert et al. (2023)	?	718
1,2,3,5,6,7-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-67) [103426-97-7] XZLJCGGEQLNWDT-UHFFFAOYSA-N	2.5×10^{-1}		Ebert et al. (2023)	?	367

Table A6.2: Polychlorinated naphthalenes (PCNs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,5,6,8-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-68) [103426-95-5] FQELOCOACCYGLL-UHFFFAOYSA-N	3.7×10^{-1}		Ebert et al. (2023)	?	367
1,2,3,5,7,8-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-69) [103426-94-4] JPQLLIUTUFJWMH-UHFFFAOYSA-N	4.3×10^{-1}	12000	Odabasi and Adali (2016)	M	720
1,2,4,5,6,8-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-71) [90948-28-0] JHKLUUFTHIWTKX-UHFFFAOYSA-N	4.5×10^{-1}		Ebert et al. (2023)	?	367
1,2,4,5,7,8-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-72) [103426-92-2] SFZREMCYQNYZMZ-UHFFFAOYSA-N	4.5×10^{-1}		Ebert et al. (2023)	?	367
1,2,3,4,5,6,7-heptachloronaphthalene $C_{10}HCl_7$ (PCN-73) [58863-14-2] NDZIBNJHNBUHKW-UHFFFAOYSA-N	3.6	10000	Odabasi and Adali (2016)	M	720
1,2,3,4,5,6,8-heptachloronaphthalene $C_{10}HCl_7$ (PCN-74) [58863-15-3] QYEGXUUXWMKHHS-UHFFFAOYSA-N	2.4	10000	Odabasi and Adali (2016)	M	720
octachloronaphthalene $C_{10}Cl_8$ (PCN-75) [2234-13-1] RTNLUFLDZOAXIC-UHFFFAOYSA-N	1.2 1.4×10^{-2} 1.4×10^{-2} 7.8×10^{-2}	7800	Odabasi and Adali (2016) Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	M V V Q	720 187

A6.3 Polychlorinated biphenyls (PCBs)

Table A6.3: Polychlorinated biphenyls (PCBs)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-chlorobiphenyl	3.0×10^{-2}		Lau et al. (2006)	M	721
$C_{12}H_9Cl$	2.3×10^{-2}		Lau et al. (2006)	M	722
(PCB-1)	3.0×10^{-2}	5300	Charles and Destaillats (2005)	M	
[2051-60-7]	4.9×10^{-2}	5100	Bamford et al. (2000)	M	
LAXBNTIAOJWAOP-UHFFFAOYSA-N	1.7×10^{-2}	5300	Paasivirta and Sinkkonen (2009)	V	
	1.4×10^{-2}		Mackay et al. (2006b)	V	
	1.4×10^{-2}		Mackay et al. (1992a)	V	
	2.7×10^{-3}		Hwang et al. (1992)	V	
	1.4×10^{-2}		Shiu and Mackay (1986)	V	
	3.5×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	3.9×10^{-2}		Duchowicz et al. (2020)	Q	185
	2.3×10^{-2}		Hilal et al. (2008)	Q	
	7.0×10^{-2}		Modarresi et al. (2007)	Q	68
	1.7×10^{-2}		Lee (2007)	Q	723
	2.2×10^{-2}		Lee (2007)	Q	724
		4600	Kühne et al. (2005)	Q	
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	1.3×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		5400	Kühne et al. (2005)	?	
3-chlorobiphenyl	3.2×10^{-2}	5400	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_9Cl$	1.3×10^{-2}		Mackay et al. (2006b)	V	
(PCB-2)	1.3×10^{-2}		Mackay et al. (1992a)	V	
[2051-61-8]	1.3×10^{-2}		Shiu and Mackay (1986)	V	
NMWSKOLWZZWHPL-UHFFFAOYSA-N	6.9×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	3.9×10^{-2}		Duchowicz et al. (2020)	Q	300
	3.7×10^{-2}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	68
	3.7×10^{-2}		Lee (2007)	Q	723
	3.1×10^{-2}		Lee (2007)	Q	724
	3.5×10^{-2}		Dunnivant et al. (1992)	Q	
	1.6×10^{-2}		Duchowicz et al. (2020)	?	186, 21
4-chlorobiphenyl	2.8×10^{-2}	5700	Li et al. (2003)	L	368
$C_{12}H_9Cl$	4.2×10^{-2}	6100	Li et al. (2003)	L	369
(PCB-3)	3.6×10^{-2}		Lau et al. (2006)	M	721
[2051-62-9]	2.9×10^{-2}		Lau et al. (2006)	M	722
FPWNLURCHDRMHC-UHFFFAOYSA-N	3.5×10^{-2}	6700	Charles and Destaillats (2005)	M	
	5.6×10^{-2}	6700	Bamford et al. (2002)	M	
	1.4×10^{-2}	5100	Paasivirta and Sinkkonen (2009)	V	
	2.3×10^{-2}		Mackay et al. (2006b)	V	
	2.3×10^{-2}		Mackay et al. (1992a)	V	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.3×10^{-2}		Shiu and Mackay (1986)	V	
	7.7×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	3.9×10^{-2}		Duchowicz et al. (2020)	Q	300
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Modarresi et al. (2007)	Q	68
	2.1×10^{-2}		Lee (2007)	Q	723
	3.4×10^{-2}		Lee (2007)	Q	724
	3.6×10^{-2}		Dunnivant et al. (1992)	Q	
	1.7×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,2'-dichlorobiphenyl	4.6×10^{-2}	6000	Bamford et al. (2002)	M	
$C_{12}H_8Cl_2$	4.0×10^{-2}		Fendinger and Glotfelty (1990)	M	
(PCB-4)	2.9×10^{-2}		Dunnivant et al. (1988)	M	
[13029-08-8]	2.9×10^{-2}		Dunnivant and Elzerman (1988)	M	725
JAYCNKDKIKZTAF-UHFFFAOYSA-N	3.3×10^{-2}		Murphy et al. (1987)	M	12
	4.5×10^{-2}		Murphy et al. (1983a)	M	24
	7.1×10^{-3}	5500	Paasivirta and Sinkkonen (2009)	V	
	1.7×10^{-2}		Mackay et al. (2006b)	V	
	1.7×10^{-2}		Mackay et al. (1992a)	V	
	1.7×10^{-2}		Shiu and Mackay (1986)	V	
	1.8×10^{-2}		Burkhard et al. (1985)	V	
	2.6×10^{-2}		Chiou et al. (1980)	V	
	4.5×10^{-2}		Murphy et al. (1983b)	X	726, 24
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.5×10^{-2}		Duchowicz et al. (2020)	Q	300
	2.5×10^{-2}		Hilal et al. (2008)	Q	
	6.9×10^{-2}		Modarresi et al. (2007)	Q	68
	2.7×10^{-2}		Lee (2007)	Q	723
	2.1×10^{-2}		Lee (2007)	Q	724
	4.8×10^{-2}		English and Carroll (2001)	Q	231, 232
	3.0×10^{-2}		Dunnivant et al. (1992)	Q	
	4.3×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,3-dichlorobiphenyl	4.3×10^{-2}	5800	Bamford et al. (2002)	M	
$C_{12}H_8Cl_2$	2.1×10^{-2}	5500	Paasivirta and Sinkkonen (2009)	V	
(PCB-5)	5.1×10^{-2}		Burkhard et al. (1985)	V	
[16605-91-7]	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
XOMKZKJEJBZBJJ-UHFFFAOYSA-N	7.1×10^{-2}		Duchowicz et al. (2020)	Q	185
	4.7×10^{-2}		Hilal et al. (2008)	Q	
	8.2×10^{-2}		Modarresi et al. (2007)	Q	68
	3.8×10^{-2}		Lee (2007)	Q	723
	4.1×10^{-2}		Lee (2007)	Q	724
		5000	Kühne et al. (2005)	Q	
	4.3×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
	3.5×10^{-2}		Sabljić and Güsten (1989)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.3×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		5800	Kühne et al. (2005)	?	
2,3'-dichlorobiphenyl	4.3×10^{-2}	5700	Bamford et al. (2002)	M	
$C_{12}H_8Cl_2$	3.9×10^{-2}		Brunner et al. (1990)	M	
(PCB-6)	3.2×10^{-2}		Murphy et al. (1987)	M	12
[25569-80-6]	4.7×10^{-2}		Murphy et al. (1983a)	M	24
ZHBBDTRJIVXKEX-UHFFFAOYSA-N	3.9×10^{-2}	5900	Paasivirta and Sinkkonen (2009)	V	
	2.5×10^{-2}		Shiu and Mackay (1986)	V	
	3.6×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.5×10^{-2}		Duchowicz et al. (2020)	Q	185
	5.6×10^{-2}		Hilal et al. (2008)	Q	
	7.2×10^{-2}		Modarresi et al. (2007)	Q	68
	3.4×10^{-2}		Lee (2007)	Q	723
	3.3×10^{-2}		Lee (2007)	Q	724
	4.3×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	3.0×10^{-2}		Dunnivant et al. (1992)	Q	
	2.5×10^{-2}		Sabljić and Güsten (1989)	Q	
	3.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,4-dichlorobiphenyl	3.7×10^{-2}	5200	Bamford et al. (2002)	M	
$C_{12}H_8Cl_2$	2.8×10^{-2}		Dunnivant and Elzerman (1988)	M	
(PCB-7)	2.7×10^{-2}		Murphy et al. (1987)	M	12
[33284-50-3]	3.0×10^{-2}	5700	Paasivirta and Sinkkonen (2009)	V	
WEJZHZJJXPXXMU-UHFFFAOYSA-N	2.2×10^{-2}		Mackay et al. (2006b)	V	
	2.2×10^{-2}		Mackay et al. (1992a)	V	
	2.2×10^{-2}		Shiu and Mackay (1986)	V	
	3.4×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	4.2×10^{-2}		Duchowicz et al. (2020)	Q	
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	8.6×10^{-2}		Modarresi et al. (2007)	Q	68
	2.2×10^{-2}		Lee (2007)	Q	723
	3.0×10^{-2}		Lee (2007)	Q	724
		4700	Kühne et al. (2005)	Q	
	3.4×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.6×10^{-2}		Dunnivant et al. (1992)	Q	
	3.5×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		5500	Kühne et al. (2005)	?	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4'-dichlorobiphenyl	3.8×10^{-2}	6000	Li et al. (2003)	L	368
$C_{12}H_8Cl_2$	4.4×10^{-2}	6300	Li et al. (2003)	L	369
(PCB-8)	2.6×10^{-2}		Lau et al. (2006)	M	721
[34883-43-7]	1.9×10^{-2}		Lau et al. (2006)	M	722
UFNIBRDIUNVOMX-UHFFFAOYSA-N	2.3×10^{-2}	5300	Charles and Destaillats (2005)	M	
	4.0×10^{-2}	5300	Bamford et al. (2000)	M	
	3.5×10^{-2}		Murphy et al. (1987)	M	12
	5.7×10^{-2}		Brownawell (1986)	M	295
	4.5×10^{-2}		Murphy et al. (1983a)	M	24
	1.0×10^{-2}		Atlas et al. (1982)	M	681
	2.2×10^{-2}	5600	Paasivirta and Sinkkonen (2009)	V	
	1.1×10^{-2}		Shiu and Mackay (1986)	V	
	4.0×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.5×10^{-2}		Duchowicz et al. (2020)	Q	300
	5.7×10^{-2}		Hilal et al. (2008)	Q	
	8.4×10^{-2}		Modarresi et al. (2007)	Q	68
	1.7×10^{-2}		Lee (2007)	Q	723
	3.4×10^{-2}		Lee (2007)	Q	724
		4700	Kühne et al. (2005)	Q	
	4.3×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	3.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.3×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		5600	Kühne et al. (2005)	?	
2,5-dichlorobiphenyl	2.3×10^{-2}	5700	ten Hulscher et al. (1992)	M	
$C_{12}H_8Cl_2$	2.5×10^{-2}		Dunnivant et al. (1988)	M	
(PCB-9)	2.5×10^{-2}		Dunnivant and Elzerman (1988)	M	725
[34883-39-1]	2.0×10^{-2}	5600	Paasivirta and Sinkkonen (2009)	V	
KKQWHYGECTYFIA-UHFFFAOYSA-N	5.0×10^{-2}		Mackay et al. (2006b)	V	
	5.0×10^{-2}		Mackay et al. (1992a)	V	
	5.0×10^{-2}		Shiu and Mackay (1986)	V	
	3.0×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	3.8×10^{-2}		Duchowicz et al. (2020)	Q	185
	4.1×10^{-2}		Hilal et al. (2008)	Q	
	7.0×10^{-2}		Modarresi et al. (2007)	Q	68
	3.1×10^{-2}		Lee (2007)	Q	723
	2.6×10^{-2}		Lee (2007)	Q	724
		4700	Kühne et al. (2005)	Q	
	3.4×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	3.0×10^{-2}		Dunnivant et al. (1992)	Q	
	3.5×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		5800	Kühne et al. (2005)	?	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,6-dichlorobiphenyl	1.2×10^{-2}	5700	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_8Cl_2$	2.1×10^{-2}		Burkhard et al. (1985)	V	
(PCB-10)	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
[33146-45-1]	4.2×10^{-2}		Duchowicz et al. (2020)	Q	300
IYZWUWBAFUBNCH-UHFFFAOYSA-N	3.0×10^{-2}		Hilal et al. (2008)	Q	
	5.8×10^{-2}		Modarresi et al. (2007)	Q	68
	1.9×10^{-2}		Lee (2007)	Q	723
	2.3×10^{-2}		Lee (2007)	Q	724
	4.3×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	2.3×10^{-2}		Dunnivant et al. (1992)	Q	
	2.1×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.3×10^{-2}		Duchowicz et al. (2020)	?	186, 21
3,3'-dichlorobiphenyl	4.2×10^{-2}		Dunnivant et al. (1988)	M	
$C_{12}H_8Cl_2$	4.2×10^{-2}		Dunnivant and Elzerman (1988)	M	725
(PCB-11)	3.4×10^{-2}	5700	Paasivirta and Sinkkonen (2009)	V	
[2050-67-1]	5.9×10^{-2}		Mackay et al. (2006b)	V	
KTXUOWUHFLBZPW-UHFFFAOYSA-N	5.8×10^{-2}		Mackay et al. (1992a)	V	
	7.4×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.5×10^{-2}		Duchowicz et al. (2020)	Q	185
	9.0×10^{-2}		Hilal et al. (2008)	Q	
	2.0×10^{-1}		Modarresi et al. (2007)	Q	68
	7.4×10^{-2}		Lee (2007)	Q	723
	4.3×10^{-2}		Lee (2007)	Q	724
	3.4×10^{-2}		Dunnivant et al. (1992)	Q	
	4.3×10^{-2}		Meylan and Howard (1991)	Q	
	4.2×10^{-2}		Duchowicz et al. (2020)	?	186, 21
3,4-dichlorobiphenyl	7.0×10^{-2}		Brunner et al. (1990)	M	
$C_{12}H_8Cl_2$	4.8×10^{-2}		Dunnivant et al. (1988)	M	
(PCB-12)	4.8×10^{-2}		Dunnivant and Elzerman (1988)	M	725
[2974-92-7]	2.0×10^{-2}	5300	Paasivirta and Sinkkonen (2009)	V	
ZGHQUYZPMWMLBM-UHFFFAOYSA-N	1.0×10^{-1}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	7.1×10^{-2}		Duchowicz et al. (2020)	Q	185
	7.7×10^{-2}		Hilal et al. (2008)	Q	
	1.1×10^{-1}		Modarresi et al. (2007)	Q	68
	4.8×10^{-2}		Lee (2007)	Q	723
	4.3×10^{-2}		Lee (2007)	Q	724
	7.3×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	4.2×10^{-2}		Dunnivant et al. (1992)	Q	
	7.0×10^{-2}		Duchowicz et al. (2020)	?	186, 21

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4'-dichlorobiphenyl	4.9×10^{-2}	6100	Bamford et al. (2002)	M	
$C_{12}H_8Cl_2$	8.5×10^{-2}	5900	Paasivirta and Sinkkonen (2009)	V	
(PCB-13)	8.1×10^{-2}		Burkhard et al. (1985)	V	
[2974-90-5]	9.5×10^{-2}		Hilal et al. (2008)	Q	
CJDNEKOMKXLSBN-UHFFFAOYSA-N	3.7×10^{-2}		Lee (2007)	Q	723
	4.4×10^{-2}		Lee (2007)	Q	724
	3.9×10^{-2}		Dunnivant et al. (1992)	Q	
	3.1×10^{-2}		Sabljić and Güsten (1989)	Q	
3,5-dichlorobiphenyl	2.7×10^{-2}	5500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_8Cl_2$	6.0×10^{-2}		Burkhard et al. (1985)	V	
(PCB-14)	5.0×10^{-2}		Hilal et al. (2008)	Q	
[34883-41-5]	9.4×10^{-2}		Modarresi et al. (2007)	Q	68
QHZSDTDMQZPUKC-UHFFFAOYSA-N	6.7×10^{-2}		Lee (2007)	Q	723
	3.2×10^{-2}		Lee (2007)	Q	724
	2.3×10^{-2}		Dunnivant et al. (1992)	Q	
	2.0×10^{-2}		Sabljić and Güsten (1989)	Q	
4,4'-dichlorobiphenyl	7.0×10^{-2}	6000	Li et al. (2003)	L	368
$C_{12}H_8Cl_2$	7.5×10^{-2}	6700	Li et al. (2003)	L	369
(PCB-15)	5.0×10^{-2}		Lau et al. (2006)	M	721
[2050-68-2]	3.3×10^{-2}		Lau et al. (2006)	M	722
YTBRNEUEFCNVHC-UHFFFAOYSA-N	3.5×10^{-2}	5300	Charles and Destaillats (2005)	M	33
	1.0×10^{-1}		Fendinger and Glotfelty (1990)	M	
	5.0×10^{-2}		Dunnivant et al. (1988)	M	
	5.0×10^{-2}		Dunnivant and Elzerman (1988)	M	725
	3.3×10^{-3}	4900	Paasivirta and Sinkkonen (2009)	V	
	5.6×10^{-2}		Mackay et al. (2006b)	V	
	5.9×10^{-2}		Mackay et al. (1992a)	V	
	5.9×10^{-2}		Shiu and Mackay (1986)	V	
	9.1×10^{-2}		Burkhard et al. (1985)	V	
	1.0×10^{-1}		Chiou et al. (1980)	V	
	3.3×10^{-2}		Murphy et al. (1983b)	X	726, 24
	6.8×10^{-2}		Dunnivant et al. (1988)	C	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.5×10^{-2}		Duchowicz et al. (2020)	Q	185
	9.7×10^{-2}		Hilal et al. (2008)	Q	
	1.8×10^{-1}		Modarresi et al. (2007)	Q	68
	2.1×10^{-2}		Lee (2007)	Q	723
	4.8×10^{-2}		Lee (2007)	Q	724
	4.4×10^{-2}		Dunnivant et al. (1992)	Q	
	4.3×10^{-2}		Meylan and Howard (1991)	Q	
	5.0×10^{-2}		Duchowicz et al. (2020)	?	186, 21

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3-trichlorobiphenyl	4.2×10^{-2}	5700	Bamford et al. (2002)	M	
$C_{12}H_7Cl_3$	4.1×10^{-2}		Murphy et al. (1987)	M	12
(PCB-16)	1.2×10^{-2}		Atlas et al. (1982)	M	681
[38444-78-9]	1.5×10^{-2}	5800	Paasivirta and Sinkkonen (2009)	V	
XVIZMMSINIOIQP-UHFFFAOYSA-N	1.3×10^{-2}		Shiu and Mackay (1986)	V	
	2.8×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	300
	5.6×10^{-2}		Hilal et al. (2008)	Q	
	6.9×10^{-2}		Modarresi et al. (2007)	Q	68
	6.1×10^{-2}		Lee (2007)	Q	723
	4.4×10^{-2}		Lee (2007)	Q	724
		4500	Kühne et al. (2005)	Q	
	3.9×10^{-2}		Dunnivant et al. (1992)	Q	
	3.6×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		4700	Kühne et al. (2005)	?	
2,2',4-trichlorobiphenyl	3.3×10^{-2}	4700	Bamford et al. (2002)	M	
$C_{12}H_7Cl_3$	3.0×10^{-2}		Murphy et al. (1987)	M	12
(PCB-17)	4.0×10^{-2}	6200	Paasivirta and Sinkkonen (2009)	V	
[37680-66-3]	1.9×10^{-2}		Burkhard et al. (1985)	V	
YKKYCYQDUUXNLN-UHFFFAOYSA-N	3.7×10^{-2}		Hilal et al. (2008)	Q	
	3.5×10^{-2}		Lee (2007)	Q	723
	3.2×10^{-2}		Lee (2007)	Q	724
	2.6×10^{-2}		Dunnivant et al. (1992)	Q	
	2.5×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',5-trichlorobiphenyl	2.9×10^{-1}		Bhangare et al. (2019)	M	727
$C_{12}H_7Cl_3$	9.0×10^{-2}		Bhangare et al. (2019)	M	728
(PCB-18)	3.9×10^{-2}	4200	Bamford et al. (2000)	M	
[37680-65-2]	3.9×10^{-2}		Brunner et al. (1990)	M	
DCMURXAZTZQAFB-UHFFFAOYSA-N	2.6×10^{-2}		Dunnivant and Elzerman (1988)	M	
	3.3×10^{-2}		Murphy et al. (1987)	M	12
	4.9×10^{-2}		Oliver (1985)	M	
	4.9×10^{-2}		Murphy et al. (1983a)	M	24
	9.9×10^{-3}		Atlas et al. (1982)	M	681
	9.8×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
	1.1×10^{-2}		Mackay et al. (2006b)	V	
	1.1×10^{-2}		Mackay et al. (1992a)	V	
	1.1×10^{-2}		Shiu and Mackay (1986)	V	
	1.7×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.5×10^{-2}		Duchowicz et al. (2020)	Q	300
	4.6×10^{-2}		Hilal et al. (2008)	Q	
	6.4×10^{-2}		Modarresi et al. (2007)	Q	68
	4.9×10^{-2}		Lee (2007)	Q	723

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.0×10^{-2}		Lee (2007)	Q	724
		4200	Kühne et al. (2005)	Q	
	5.8×10^{-2}		Yaffe et al. (2003)	Q	249, 273
	6.0×10^{-2}		English and Carroll (2001)	Q	231, 275
	3.1×10^{-2}		Dunnivant et al. (1992)	Q	
	3.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		4500	Kühne et al. (2005)	?	
2,2',6-trichlorobiphenyl	3.3×10^{-2}	4700	Bamford et al. (2002)	M	
$C_{12}H_7Cl_3$	4.3×10^{-2}		Brunner et al. (1990)	M	
(PCB-19)	3.3×10^{-2}		Murphy et al. (1987)	M	12
[38444-73-4]	4.7×10^{-2}		Murphy et al. (1983a)	M	24
MVXIJRBBCDLNLX-UHFFFAOYSA-N	2.5×10^{-3}	5400	Paasivirta and Sinkkonen (2009)	V	
	8.0×10^{-3}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	6.0×10^{-2}		Duchowicz et al. (2020)	Q	
	5.4×10^{-2}		Hilal et al. (2008)	Q	
	6.0×10^{-2}		Modarresi et al. (2007)	Q	68
	3.0×10^{-2}		Lee (2007)	Q	723
	2.4×10^{-2}		Lee (2007)	Q	724
		3600	Kühne et al. (2005)	Q	
	2.2×10^{-2}		Dunnivant et al. (1992)	Q	
	2.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.3×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		3100	Kühne et al. (2005)	?	
2,3,3'-trichlorobiphenyl	1.2×10^{-2}		Atlas et al. (1982)	M	681
$C_{12}H_7Cl_3$	2.0×10^{-2}	5800	Paasivirta and Sinkkonen (2009)	V	
(PCB-20)	1.2×10^{-2}		Shiu and Mackay (1986)	V	
[38444-84-7]	5.8×10^{-2}		Burkhard et al. (1985)	V	
SXHLTVKPNQVZGL-UHFFFAOYSA-N	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	300
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	8.4×10^{-2}		Modarresi et al. (2007)	Q	68
	7.6×10^{-2}		Lee (2007)	Q	723
	6.5×10^{-2}		Lee (2007)	Q	724
	4.5×10^{-2}		Dunnivant et al. (1992)	Q	
	3.3×10^{-2}		Sabljić and Güsten (1989)	Q	
	6.2×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,3,4-trichlorobiphenyl	4.3×10^{-3}	5200	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_7Cl_3$	6.8×10^{-2}		Burkhard et al. (1985)	V	
(PCB-21)	7.9×10^{-2}		Hilal et al. (2008)	Q	
[55702-46-0]	5.0×10^{-2}		Lee (2007)	Q	723
IUYHQGMDSZOPDZ-UHFFFAOYSA-N	5.9×10^{-2}		Lee (2007)	Q	724
	4.3×10^{-2}		Dunnivant et al. (1992)	Q	
	4.7×10^{-2}		Sabljić and Güsten (1989)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4'-trichlorobiphenyl	3.4×10^{-2}	4800	Bamford et al. (2002)	M	
$C_{12}H_7Cl_3$	5.0×10^{-2}		Murphy et al. (1987)	M	12
(PCB-22)	5.5×10^{-2}		Murphy et al. (1983a)	M	24
[38444-85-8]	1.3×10^{-2}	5600	Paasivirta and Sinkkonen (2009)	V	
ZMHWQAHZKUPENF-UHFFFAOYSA-N	6.5×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	1.0×10^{-1}		Modarresi et al. (2007)	Q	68
	3.8×10^{-2}		Lee (2007)	Q	723
	6.4×10^{-2}		Lee (2007)	Q	724
	5.2×10^{-2}		Dunnivant et al. (1992)	Q	
	4.4×10^{-2}		Sabljić and Güsten (1989)	Q	
	7.0×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,3,5-trichlorobiphenyl	1.5×10^{-2}	5700	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_7Cl_3$	3.9×10^{-2}		Burkhard et al. (1985)	V	
(PCB-23)	6.9×10^{-2}		Lee (2007)	Q	723
[55720-44-0]	4.7×10^{-2}		Lee (2007)	Q	724
GBUCDGDROYMOAN-UHFFFAOYSA-N	3.1×10^{-2}		Dunnivant et al. (1992)	Q	
	2.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,6-trichlorobiphenyl	3.3×10^{-2}	4700	Bamford et al. (2002)	M	
$C_{12}H_7Cl_3$	4.5×10^{-2}		Brunner et al. (1990)	M	
(PCB-24)	3.1×10^{-2}		Murphy et al. (1987)	M	12
[55702-45-9]	7.7×10^{-3}	5600	Paasivirta and Sinkkonen (2009)	V	
LVROLHVSYNLFBE-UHFFFAOYSA-N	2.3×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.3×10^{-2}		Duchowicz et al. (2020)	Q	300
	4.7×10^{-2}		Hilal et al. (2008)	Q	
	8.5×10^{-2}		Modarresi et al. (2007)	Q	68
	4.2×10^{-2}		Lee (2007)	Q	723
	4.4×10^{-2}		Lee (2007)	Q	724
		4500	Kühne et al. (2005)	Q	
	3.2×10^{-2}		Dunnivant et al. (1992)	Q	
	2.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.5×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		2800	Kühne et al. (2005)	?	
2,3',4-trichlorobiphenyl	3.3×10^{-2}	4700	Bamford et al. (2002)	M	
$C_{12}H_7Cl_3$	2.4×10^{-2}		Murphy et al. (1987)	M	12
(PCB-25)	6.2×10^{-2}		Murphy et al. (1983a)	M	24
[55712-37-3]	2.8×10^{-2}	5900	Paasivirta and Sinkkonen (2009)	V	
XBBZAULFUPBZSP-UHFFFAOYSA-N	3.9×10^{-2}		Burkhard et al. (1985)	V	
	4.4×10^{-2}		Lee (2007)	Q	723
	4.5×10^{-2}		Lee (2007)	Q	724
		4800	Kühne et al. (2005)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.1×10^{-2}		Dunnivant et al. (1992)	Q	
	2.3×10^{-2}		Sabljić and Güsten (1989)	Q	
		5700	Kühne et al. (2005)	?	
2,3',5-trichlorobiphenyl	3.5×10^{-2}	4900	Bamford et al. (2002)	M	
$C_{12}H_7Cl_3$	3.0×10^{-2}		Dunnivant et al. (1988)	M	
(PCB-26)	3.0×10^{-2}		Dunnivant and Elzerman (1988)	M	725
[38444-81-4]	2.9×10^{-2}		Murphy et al. (1987)	M	12
ONNCPBRWFSKDMQ-UHFFFAOYSA-N	2.2×10^{-2}	5900	Paasivirta and Sinkkonen (2009)	V	
	3.5×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.5×10^{-2}		Duchowicz et al. (2020)	Q	300
	9.9×10^{-2}		Hilal et al. (2008)	Q	
	7.3×10^{-2}		Modarresi et al. (2007)	Q	68
	6.1×10^{-2}		Lee (2007)	Q	723
	4.3×10^{-2}		Lee (2007)	Q	724
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	5.9×10^{-2}		Meylan and Howard (1991)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,3',6-trichlorobiphenyl	3.5×10^{-2}		Murphy et al. (1987)	M	12
$C_{12}H_7Cl_3$	3.1×10^{-2}	6100	Paasivirta and Sinkkonen (2009)	V	
(PCB-27)	2.4×10^{-2}		Burkhard et al. (1985)	V	
[38444-76-7]	3.7×10^{-2}		Lee (2007)	Q	723
VQOFJPFYTCHPTR-UHFFFAOYSA-N	4.2×10^{-2}		Lee (2007)	Q	724
	2.4×10^{-2}		Dunnivant et al. (1992)	Q	
	2.0×10^{-2}		Sabljić and Güsten (1989)	Q	
2,4,4'-trichlorobiphenyl	3.0×10^{-2}	6300	Li et al. (2003)	L	368
$C_{12}H_7Cl_3$	3.3×10^{-2}	6600	Li et al. (2003)	L	369
(PCB-28)	5.9×10^{-3}		Bhangare et al. (2019)	M	727
[7012-37-5]	5.0×10^{-2}		Bhangare et al. (2019)	M	728
BZTYNSQSZHARAZ-UHFFFAOYSA-N	2.3×10^{-2}		Lau et al. (2006)	M	721
	1.4×10^{-2}		Lau et al. (2006)	M	722
	1.8×10^{-2}	2300	Charles and Destaillats (2005)	M	33
	2.6×10^{-2}	3900	Bamford et al. (2000)	M	
	3.6×10^{-2}	6100	ten Hulscher et al. (1992)	M	
	4.9×10^{-2}		Brunner et al. (1990)	M	
	3.1×10^{-2}		Dunnivant and Elzerman (1988)	M	
	3.7×10^{-2}		Murphy et al. (1987)	M	12
	6.9×10^{-2}		Brownawell (1986)	M	295
	2.7×10^{-2}	5900	Paasivirta and Sinkkonen (2009)	V	
	4.4×10^{-2}		Burkhard et al. (1985)	V	
	2.7×10^{-2}	7100	Paasivirta et al. (1999)	T	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	6.0×10^{-2}		Duchowicz et al. (2020)	Q	
	1.0×10^{-1}		Hilal et al. (2008)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.9×10^{-2}		Modarresi et al. (2007)	Q	68
	2.2×10^{-2}		Lee (2007)	Q	723
	4.7×10^{-2}		Lee (2007)	Q	724
		4800	Kühne et al. (2005)	Q	
	5.2×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	3.5×10^{-2}		Dunnivant et al. (1992)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		4800	Kühne et al. (2005)	?	
2,4,5-trichlorobiphenyl	3.1×10^{-2}	6500	Schwardt et al. (2021)	L	1
$C_{12}H_7Cl_3$	3.1×10^{-2}	6300	Li et al. (2003)	L	368
(PCB-29)	3.3×10^{-2}	6700	Li et al. (2003)	L	369
[15862-07-4]	2.6×10^{-2}	4200	Bamford et al. (2000)	M	
VGVIKVCCUATMNG-UHFFFAOYSA-N	4.9×10^{-2}		Brunner et al. (1990)	M	
	7.7×10^{-3}	5500	Paasivirta and Sinkkonen (2009)	V	
	4.1×10^{-3}		Mackay et al. (2006b)	V	
	4.1×10^{-2}		Mackay et al. (1992a)	V	
	4.2×10^{-2}		Shiu and Mackay (1986)	V	
	3.9×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.3×10^{-2}		Duchowicz et al. (2020)	Q	
	4.5×10^{-2}		Bhangare et al. (2019)	Q	
	7.9×10^{-2}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	68
	4.0×10^{-2}		Lee (2007)	Q	723
	4.2×10^{-2}		Lee (2007)	Q	724
		5100	Kühne et al. (2005)	Q	
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	3.7×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		4500	Kühne et al. (2005)	?	
2,4,6-trichlorobiphenyl	1.5×10^{-2}		Dunnivant et al. (1988)	M	
$C_{12}H_7Cl_3$	1.5×10^{-2}		Dunnivant and Elzerman (1988)	M	725
(PCB-30)	1.0×10^{-2}		Duchowicz et al. (2020)	V	187
[35693-92-6]	8.5×10^{-3}	5600	Paasivirta and Sinkkonen (2009)	V	
MTLMVEWEYZFYTH-UHFFFAOYSA-N	2.0×10^{-2}		Mackay et al. (2006b)	V	
	2.0×10^{-2}		Mackay et al. (1992a)	V	
	2.0×10^{-2}		Shiu and Mackay (1986)	V	
	1.6×10^{-2}		Burkhard et al. (1985)	V	
	3.5×10^{-2}		Duchowicz et al. (2020)	Q	
	2.9×10^{-2}		Hilal et al. (2008)	Q	
	2.4×10^{-2}		Lee (2007)	Q	723
	2.5×10^{-2}		Lee (2007)	Q	724
	1.7×10^{-2}		Dunnivant et al. (1992)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4',5-trichlorobiphenyl	2.7×10^{-2}	6100	Li et al. (2003)	L	368
$C_{12}H_7Cl_3$	2.9×10^{-2}	6600	Li et al. (2003)	L	369
(PCB-31)	3.4×10^{-2}	4900	Bamford et al. (2002)	M	
[16606-02-3]	5.2×10^{-2}		Brunner et al. (1990)	M	
VAHKBZSAUKPEOV-UHFFFAOYSA-N	3.7×10^{-2}		Murphy et al. (1987)	M	12
	4.9×10^{-2}		Murphy et al. (1983a)	M	24
	1.1×10^{-2}		Atlas et al. (1982)	M	681
	1.3×10^{-2}	5700	Paasivirta and Sinkkonen (2009)	V	
	1.8×10^{-2}		Shiu and Mackay (1986)	V	
	3.9×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.5×10^{-2}		Duchowicz et al. (2020)	Q	
	1.0×10^{-1}		Hilal et al. (2008)	Q	
	9.1×10^{-2}		Modarresi et al. (2007)	Q	68
	3.0×10^{-2}		Lee (2007)	Q	723
	4.1×10^{-2}		Lee (2007)	Q	724
	3.6×10^{-2}		Dunnivant et al. (1992)	Q	
	3.5×10^{-2}		Sabljić and Güsten (1989)	Q	
	5.2×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,4',6-trichlorobiphenyl	1.2×10^{-2}	5700	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_7Cl_3$	2.7×10^{-2}		Burkhard et al. (1985)	V	
(PCB-32)	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
[38444-77-8]	6.0×10^{-2}		Duchowicz et al. (2020)	Q	300
IHIDFKLAWYPTKB-UHFFFAOYSA-N	7.5×10^{-2}		Hilal et al. (2008)	Q	
	6.9×10^{-2}		Modarresi et al. (2007)	Q	68
	1.8×10^{-2}		Lee (2007)	Q	723
	4.1×10^{-2}		Lee (2007)	Q	724
	2.5×10^{-2}		Dunnivant et al. (1992)	Q	
	2.4×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,3',4'-trichlorobiphenyl	3.6×10^{-2}	5100	Bamford et al. (2002)	M	
$C_{12}H_7Cl_3$	4.4×10^{-2}		Murphy et al. (1987)	M	12
(PCB-33)	6.6×10^{-2}		Murphy et al. (1983a)	M	24
[38444-86-9]	2.5×10^{-2}		Westcott et al. (1981)	M	
RIMXLXBUOQMDHV-UHFFFAOYSA-N	1.3×10^{-2}	5600	Paasivirta and Sinkkonen (2009)	V	
			Mackay et al. (2006b)	V	685
	2.3×10^{-2}		Mackay et al. (1992a)	V	
	2.3×10^{-2}		Shiu and Mackay (1986)	V	
	5.9×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	300
	1.1×10^{-1}		Hilal et al. (2008)	Q	
	7.0×10^{-2}		Modarresi et al. (2007)	Q	68
	7.7×10^{-2}		Lee (2007)	Q	723
	5.0×10^{-2}		Lee (2007)	Q	724

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
	4.5×10^{-2}		Sabljić and Güsten (1989)	Q	
	6.2×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,3',5'-trichlorobiphenyl	1.3×10^{-2}	5800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_7Cl_3$	3.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-34)	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
[37680-68-5]	6.0×10^{-2}		Duchowicz et al. (2020)	Q	185
GXVMAQACUOSFJF-UHFFFAOYSA-N	7.3×10^{-2}		Hilal et al. (2008)	Q	
	7.1×10^{-2}		Modarresi et al. (2007)	Q	68
	1.1×10^{-1}		Lee (2007)	Q	723
	3.9×10^{-2}		Lee (2007)	Q	724
	2.3×10^{-2}		Dunnivant et al. (1992)	Q	
	2.0×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
3,3',4-trichlorobiphenyl	1.8×10^{-2}	5600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_7Cl_3$	1.2×10^{-1}		Burkhard et al. (1985)	V	
(PCB-35)	9.5×10^{-2}		Lee (2007)	Q	723
[37680-69-6]	5.9×10^{-2}		Lee (2007)	Q	724
JHBVPKZLIBDTJR-UHFFFAOYSA-N	5.5×10^{-2}		Dunnivant et al. (1992)	Q	
	4.4×10^{-2}		Sabljić and Güsten (1989)	Q	
3,3',5-trichlorobiphenyl	5.8×10^{-2}		Brunner et al. (1990)	M	
$C_{12}H_7Cl_3$	1.3×10^{-2}	5600	Paasivirta and Sinkkonen (2009)	V	
(PCB-36)	7.2×10^{-2}		Burkhard et al. (1985)	V	
[38444-87-0]	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
RIBGNAJQTOXRDK-UHFFFAOYSA-N	6.0×10^{-2}		Duchowicz et al. (2020)	Q	300
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	8.8×10^{-2}		Modarresi et al. (2007)	Q	68
	1.3×10^{-1}		Lee (2007)	Q	723
	4.7×10^{-2}		Lee (2007)	Q	724
	5.8×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.9×10^{-2}		Dunnivant et al. (1992)	Q	
	1.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	5.8×10^{-2}		Duchowicz et al. (2020)	?	186, 21
3,4,4'-trichlorobiphenyl	9.9×10^{-2}		Brunner et al. (1990)	M	
$C_{12}H_7Cl_3$	6.5×10^{-2}		Murphy et al. (1987)	M	12
(PCB-37)	1.2×10^{-2}		Atlas et al. (1982)	M	681
[38444-90-5]	1.3×10^{-2}	5400	Paasivirta and Sinkkonen (2009)	V	
YZANRISAORXTHU-UHFFFAOYSA-N	1.2×10^{-2}		Shiu and Mackay (1986)	V	
	1.4×10^{-1}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	68
	4.8×10^{-2}		Lee (2007)	Q	723

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.1×10^{-2}		Lee (2007)	Q	724
	6.5×10^{-2}		Dunnivant et al. (1992)	Q	
	6.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	9.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
3,4,5-trichlorobiphenyl	1.2×10^{-2}	5400	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_7Cl_3$	1.3×10^{-1}		Burkhard et al. (1985)	V	
(PCB-38)	8.8×10^{-2}		Lee (2007)	Q	723
[53555-66-1]	5.2×10^{-2}		Lee (2007)	Q	724
BSFZSQRJGZHMMV-UHFFFAOYSA-N	4.2×10^{-2}		Dunnivant et al. (1992)	Q	
	4.8×10^{-2}		Sabljić and Güsten (1989)	Q	
3,4',5-trichlorobiphenyl	1.2×10^{-2}	5600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_7Cl_3$	8.0×10^{-2}		Burkhard et al. (1985)	V	
(PCB-39)	6.6×10^{-2}		Lee (2007)	Q	723
[38444-88-1]	4.4×10^{-2}		Lee (2007)	Q	724
SYSBNFJJSJLZMM-UHFFFAOYSA-N	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	2.3×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,3'-tetrachlorobiphenyl	3.6×10^{-2}	3600	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	9.9×10^{-2}		Brunner et al. (1990)	M	
(PCB-40)	4.9×10^{-2}		Dunnivant et al. (1988)	M	
[38444-93-8]	4.9×10^{-2}		Dunnivant and Elzerman (1988)	M	725
VTLYHLREPCPDKX-UHFFFAOYSA-N	6.1×10^{-2}		Murphy et al. (1987)	M	12
	8.2×10^{-2}		Oliver (1985)	M	
	1.8×10^{-3}	5300	Paasivirta and Sinkkonen (2009)	V	
	4.6×10^{-2}		Mackay et al. (2006b)	V	
	4.6×10^{-2}		Mackay et al. (1992a)	V	
	4.5×10^{-2}		Shiu and Mackay (1986)	V	
	4.9×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.9×10^{-1}		Duchowicz et al. (2020)	Q	300
	1.1×10^{-1}		Hilal et al. (2008)	Q	
	6.8×10^{-2}		Modarresi et al. (2007)	Q	68
	1.2×10^{-1}		Lee (2007)	Q	723
	9.7×10^{-2}		Lee (2007)	Q	724
	2.3×10^{-1}		Yaffe et al. (2003)	Q	249, 273
	6.5×10^{-2}		English and Carroll (2001)	Q	231, 232
	5.4×10^{-2}		Dunnivant et al. (1992)	Q	
	9.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,2',3,4-tetrachlorobiphenyl	4.9×10^{-2}		Murphy et al. (1987)	M	12
$C_{12}H_6Cl_4$	1.6×10^{-2}	6200	Paasivirta and Sinkkonen (2009)	V	
(PCB-41)	4.2×10^{-2}		Burkhard et al. (1985)	V	
[52663-59-9]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
SEWHDNLIHDBVDZ-UHFFFAOYSA-N	1.4×10^{-1}		Duchowicz et al. (2020)	Q	185
	6.9×10^{-2}		Hilal et al. (2008)	Q	
	8.7×10^{-2}		Modarresi et al. (2007)	Q	68

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.9×10^{-2}		Lee (2007)	Q	723
	7.1×10^{-2}		Lee (2007)	Q	724
	4.0×10^{-2}		Dunnivant et al. (1992)	Q	
	4.8×10^{-2}		Sabljić and Güsten (1989)	Q	
	7.0×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,2',3,4'-tetrachlorobiphenyl	2.8×10^{-2}	3100	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	5.0×10^{-2}		Murphy et al. (1987)	M	12
(PCB-42)	8.6×10^{-3}	5900	Paasivirta and Sinkkonen (2009)	V	
[36559-22-5]	3.4×10^{-2}		Burkhard et al. (1985)	V	
ALFHIHDQSYXSGP-UHFFFAOYSA-N	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	300
	7.2×10^{-2}		Hilal et al. (2008)	Q	
	8.1×10^{-2}		Modarresi et al. (2007)	Q	68
	6.0×10^{-2}		Lee (2007)	Q	723
	6.7×10^{-2}		Lee (2007)	Q	724
	3.9×10^{-2}		Dunnivant et al. (1992)	Q	
	3.1×10^{-2}		Sabljić and Güsten (1989)	Q	
	7.0×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,2',3,5-tetrachlorobiphenyl	1.3×10^{-2}	6300	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	2.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-43)	1.1×10^{-1}		Lee (2007)	Q	723
[70362-46-8]	6.1×10^{-2}		Lee (2007)	Q	724
NRBNBYFPJCCKTO-UHFFFAOYSA-N	2.9×10^{-2}		Dunnivant et al. (1992)	Q	
	2.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,5'-tetrachlorobiphenyl	5.4×10^{-3}		Bhangare et al. (2019)	M	727
$C_{12}H_6Cl_4$	3.4×10^{-2}		Bhangare et al. (2019)	M	728
(PCB-44)	3.6×10^{-2}	3100	Bamford et al. (2000)	M	
[41464-39-5]	5.2×10^{-2}		Murphy et al. (1987)	M	12
ALDJIKXAHSDLLB-UHFFFAOYSA-N	4.1×10^{-2}		Murphy et al. (1983a)	M	24
	1.3×10^{-2}		Atlas et al. (1982)	M	681
	1.1×10^{-2}	6000	Paasivirta and Sinkkonen (2009)	V	
	2.0×10^{-2}		Shiu and Mackay (1986)	V	
	3.0×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	185
	9.7×10^{-2}		Hilal et al. (2008)	Q	
	7.7×10^{-2}		Modarresi et al. (2007)	Q	68
	1.2×10^{-1}		Lee (2007)	Q	723
	6.7×10^{-2}		Lee (2007)	Q	724
		4600	Kühne et al. (2005)	Q	
	4.3×10^{-2}		Dunnivant et al. (1992)	Q	
	3.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	7.0×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		3400	Kühne et al. (2005)	?	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,6-tetrachlorobiphenyl	2.5×10^{-2}	2900	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	3.8×10^{-3}	6000	Paasivirta and Sinkkonen (2009)	V	
(PCB-45)	9.9×10^{-3}		Burkhard et al. (1985)	V	
[70362-45-7]	6.7×10^{-2}		Lee (2007)	Q	723
VHGHHZZTMJLTJX-UHFFFAOYSA-N	5.1×10^{-2}		Lee (2007)	Q	724
	2.8×10^{-2}		Dunnivant et al. (1992)	Q	
	3.1×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,6'-tetrachlorobiphenyl	3.0×10^{-2}	3400	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	3.8×10^{-2}		Murphy et al. (1987)	M	12
(PCB-46)	9.1×10^{-4}	5300	Paasivirta and Sinkkonen (2009)	V	
[41464-47-5]	1.4×10^{-2}		Burkhard et al. (1985)	V	
CUGLICQCTXWQNF-UHFFFAOYSA-N	6.7×10^{-2}		Lee (2007)	Q	723
	5.7×10^{-2}		Lee (2007)	Q	724
	2.9×10^{-2}		Dunnivant et al. (1992)	Q	
	2.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',4,4'-tetrachlorobiphenyl	2.1×10^{-1}		Lau et al. (2006)	M	721
$C_{12}H_6Cl_4$	9.1×10^{-3}		Lau et al. (2006)	M	722
(PCB-47)	1.8×10^{-1}	-6000	Charles and Destaillats (2005)	M	
[2437-79-8]	5.2×10^{-2}		Brunner et al. (1990)	M	
QORAVNMWUNPXAO-UHFFFAOYSA-N	2.0×10^{-2}	6200	Paasivirta and Sinkkonen (2009)	V	
	5.7×10^{-2}		Mackay et al. (2006b)	V	
	5.8×10^{-2}		Mackay et al. (1992a)	V	
	2.0×10^{-3}		Hwang et al. (1992)	V	
	5.9×10^{-2}		Shiu and Mackay (1986)	V	
	2.3×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	6.6×10^{-2}		Duchowicz et al. (2020)	Q	300
	5.0×10^{-2}		Hilal et al. (2008)	Q	
	8.2×10^{-2}		Modarresi et al. (2007)	Q	68
	3.5×10^{-2}		Lee (2007)	Q	723
	4.8×10^{-2}		Lee (2007)	Q	724
	2.7×10^{-2}		Dunnivant et al. (1992)	Q	
	2.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	5.2×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,2',4,5-tetrachlorobiphenyl	2.7×10^{-2}	3000	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	3.9×10^{-2}		Murphy et al. (1987)	M	12
(PCB-48)	6.1×10^{-3}	6100	Paasivirta and Sinkkonen (2009)	V	
[70362-47-9]	2.5×10^{-2}		Burkhard et al. (1985)	V	
XBTHILIDLBPRPM-UHFFFAOYSA-N	6.3×10^{-2}		Lee (2007)	Q	723
	5.3×10^{-2}		Lee (2007)	Q	724
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	3.8×10^{-2}		Sabljić and Güsten (1989)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',4,5'-tetrachlorobiphenyl	2.7×10^{-2}	3000	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	3.6×10^{-2}		Murphy et al. (1987)	M	12
(PCB-49)	4.9×10^{-2}		Murphy et al. (1983a)	M	24
[41464-40-8]	8.3×10^{-3}	5900	Paasivirta and Sinkkonen (2009)	V	
ZWPVHELAQPIZHO-UHFFFAOYSA-N	5.0×10^{-2}		Shiu and Mackay (1986)	V	
	2.1×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	6.1×10^{-2}		Duchowicz et al. (2020)	Q	300
	6.1×10^{-2}		Hilal et al. (2008)	Q	
	7.6×10^{-2}		Modarresi et al. (2007)	Q	68
	7.0×10^{-2}		Lee (2007)	Q	723
	4.5×10^{-2}		Lee (2007)	Q	724
	2.8×10^{-2}		Dunnivant et al. (1992)	Q	
	2.6×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.7×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,2',4,6-tetrachlorobiphenyl	1.6×10^{-2}	2900	Bamford et al. (2000)	M	
$C_{12}H_6Cl_4$	1.3×10^{-2}		Atlas et al. (1982)	M	681
(PCB-50)	9.9×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
[62796-65-0]	1.3×10^{-2}		Shiu and Mackay (1986)	V	
VLLVVZDKBSYMCG-UHFFFAOYSA-N	7.3×10^{-3}		Burkhard et al. (1985)	V	
	3.1×10^{-2}		Bhangare et al. (2019)	Q	
	3.9×10^{-2}		Lee (2007)	Q	723
	2.8×10^{-2}		Lee (2007)	Q	724
		3600	Kühne et al. (2005)	Q	
	1.6×10^{-2}		Dunnivant et al. (1992)	Q	
	1.7×10^{-2}		Sabljić and Güsten (1989)	Q	
		3100	Kühne et al. (2005)	?	
2,2',4,6'-tetrachlorobiphenyl	2.5×10^{-2}	6300	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	9.9×10^{-3}		Burkhard et al. (1985)	V	
(PCB-51)	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
[68194-04-7]	6.6×10^{-2}		Duchowicz et al. (2020)	Q	185
WVHNUGRFECMVLQ-UHFFFAOYSA-N	7.3×10^{-2}		Hilal et al. (2008)	Q	
	5.9×10^{-2}		Modarresi et al. (2007)	Q	68
	3.8×10^{-2}		Lee (2007)	Q	723
	4.0×10^{-2}		Lee (2007)	Q	724
	1.9×10^{-2}		Dunnivant et al. (1992)	Q	
	2.0×10^{-2}		Sabljić and Güsten (1989)	Q	
	7.0×10^{-2}		Duchowicz et al. (2020)	?	186, 21

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',5,5'-tetrachlorobiphenyl	3.5×10^{-2}	6600	Li et al. (2003)	L	368
$C_{12}H_6Cl_4$	4.0×10^{-2}	6800	Li et al. (2003)	L	369
(PCB-52)	4.9×10^{-3}		Bhangare et al. (2019)	M	727
[35693-99-3]	2.9×10^{-2}		Bhangare et al. (2019)	M	728
HCWZEPKLWVAEOV-UHFFFAOYSA-N	3.2×10^{-2}	3700	Bamford et al. (2000)	M	
	4.2×10^{-2}	6200	ten Hulscher et al. (1992)	M	
	4.9×10^{-2}		Brunner et al. (1990)	M	
	2.9×10^{-2}		Dunnivant et al. (1988)	M	
	2.9×10^{-2}		Dunnivant and Elzerman (1988)	M	725
	4.1×10^{-2}		Murphy et al. (1987)	M	12
	8.2×10^{-2}		Oliver (1985)	M	
	4.5×10^{-2}		Murphy et al. (1983a)	M	24
	1.1×10^{-2}		Atlas et al. (1982)	M	681
			Westcott et al. (1981)	M	729
	3.7×10^{-3}	5700	Paasivirta and Sinkkonen (2009)	V	
	2.1×10^{-2}		Mackay et al. (2006b)	V	
	2.1×10^{-2}		Mackay et al. (1992a)	V	
	1.2×10^{-1}		McLachlan et al. (1990)	V	375
	2.1×10^{-2}		Shiu and Mackay (1986)	V	
	1.9×10^{-2}		Burkhard et al. (1985)	V	
	1.2×10^{-2}	7700	Paasivirta et al. (1999)	T	
	3.8×10^{-2}		Murphy et al. (1983b)	X	726, 24
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	5.6×10^{-2}		Duchowicz et al. (2020)	Q	185
	7.9×10^{-2}		Hilal et al. (2008)	Q	
	6.5×10^{-2}		Modarresi et al. (2007)	Q	68
	9.7×10^{-2}		Lee (2007)	Q	723
	4.6×10^{-2}		Lee (2007)	Q	724
		4200	Kühne et al. (2005)	Q	
	3.1×10^{-2}		Dunnivant et al. (1992)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		4900	Kühne et al. (2005)	?	
2,2',5,6'-tetrachlorobiphenyl	2.4×10^{-2}		Dunnivant et al. (1988)	M	
$C_{12}H_6Cl_4$	2.4×10^{-2}		Dunnivant and Elzerman (1988)	M	725
(PCB-53)	3.5×10^{-2}		Murphy et al. (1987)	M	12
[41464-41-9]	3.3×10^{-2}		Murphy et al. (1983a)	M	24
SFTUSTXGTCCSHX-UHFFFAOYSA-N	5.4×10^{-2}		Duchowicz et al. (2020)	V	187
	1.6×10^{-3}	5500	Paasivirta and Sinkkonen (2009)	V	
	3.3×10^{-2}		Shiu and Mackay (1986)	V	
	8.9×10^{-3}		Burkhard et al. (1985)	V	
	6.1×10^{-2}		Duchowicz et al. (2020)	Q	
	8.8×10^{-2}		Hilal et al. (2008)	Q	
	5.9×10^{-2}		Modarresi et al. (2007)	Q	68
	5.3×10^{-2}		Lee (2007)	Q	723
	4.1×10^{-2}		Lee (2007)	Q	724

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.3×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',6,6'-tetrachlorobiphenyl	4.9×10^{-2}		Brunner et al. (1990)	M	
$C_{12}H_6Cl_4$	1.8×10^{-2}		Dunnivant et al. (1988)	M	
(PCB-54)	1.8×10^{-2}		Dunnivant and Elzerman (1988)	M	725
[15968-05-5]	1.0×10^{-4}	4800	Paasivirta and Sinkkonen (2009)	V	
PXAGFNRKXSYIHU-UHFFFAOYSA-N	5.3×10^{-3}		Burkhard et al. (1985)	V	
	6.7×10^{-2}		Dunnivant et al. (1988)	C	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	6.6×10^{-2}		Duchowicz et al. (2020)	Q	185
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	6.5×10^{-2}		Modarresi et al. (2007)	Q	68
	3.3×10^{-2}		Lee (2007)	Q	723
	2.7×10^{-2}		Lee (2007)	Q	724
	5.2×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.7×10^{-2}		Dunnivant et al. (1992)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,3,3',4-tetrachlorobiphenyl	9.6×10^{-3}	5900	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	8.7×10^{-2}		Burkhard et al. (1985)	V	
(PCB-55)	9.9×10^{-2}		Lee (2007)	Q	723
[74338-24-2]	9.3×10^{-2}		Lee (2007)	Q	724
ZKGSEEWIVLAUNH-UHFFFAOYSA-N	5.4×10^{-2}		Dunnivant et al. (1992)	Q	
	4.3×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',4'-tetrachlorobiphenyl	3.8×10^{-2}	3800	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	6.1×10^{-2}		Murphy et al. (1987)	M	12
(PCB-56)	4.9×10^{-3}	5400	Paasivirta and Sinkkonen (2009)	V	
[41464-43-1]	1.1×10^{-1}		Burkhard et al. (1985)	V	
UNCGJRRROFURDV-UHFFFAOYSA-N	7.5×10^{-2}		Lee (2007)	Q	723
	9.7×10^{-2}		Lee (2007)	Q	724
	6.5×10^{-2}		Dunnivant et al. (1992)	Q	
	7.5×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',5-tetrachlorobiphenyl	8.9×10^{-3}	6100	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	5.1×10^{-2}		Burkhard et al. (1985)	V	
(PCB-57)	1.4×10^{-1}		Lee (2007)	Q	723
[70424-67-8]	7.8×10^{-2}		Lee (2007)	Q	724
DHDBTLFALXRTLB-UHFFFAOYSA-N	3.6×10^{-2}		Dunnivant et al. (1992)	Q	
	2.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',5'-tetrachlorobiphenyl	2.3×10^{-3}	5400	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	6.2×10^{-2}		Burkhard et al. (1985)	V	
(PCB-58)	1.5×10^{-1}		Lee (2007)	Q	723
[41464-49-7]	8.1×10^{-2}		Lee (2007)	Q	724
IOPBNBSKOPJKEG-UHFFFAOYSA-N	3.9×10^{-2}		Dunnivant et al. (1992)	Q	
	2.4×10^{-2}		Sabljić and Güsten (1989)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',6-tetrachlorobiphenyl	4.4×10^{-2}	6600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	2.9×10^{-2}		Burkhard et al. (1985)	V	
(PCB-59)	8.3×10^{-2}		Lee (2007)	Q	723
[74472-33-6]	8.3×10^{-2}		Lee (2007)	Q	724
WZNAMGYIQPAXDH-UHFFFAOYSA-N	3.2×10^{-2}		Dunnivant et al. (1992)	Q	
	2.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,4,4'-tetrachlorobiphenyl	6.1×10^{-2}		Murphy et al. (1987)	M	12
$C_{12}H_6Cl_4$	1.2×10^{-2}		Atlas et al. (1982)	M	681
(PCB-60)	2.9×10^{-3}	5500	Paasivirta and Sinkkonen (2009)	V	
[33025-41-1]	9.7×10^{-2}		Burkhard et al. (1985)	V	
XLDBTRJKXLKYTC-UHFFFAOYSA-N	4.9×10^{-2}		Lee (2007)	Q	723
	9.2×10^{-2}		Lee (2007)	Q	724
	6.5×10^{-2}		Dunnivant et al. (1992)	Q	
	6.5×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,4,5-tetrachlorobiphenyl	4.9×10^{-2}	6600	Li et al. (2003)	L	368
$C_{12}H_6Cl_4$	5.0×10^{-2}	7200	Li et al. (2003)	L	369
(PCB-61)	9.6×10^{-3}		Duchowicz et al. (2020)	V	187
[33284-53-6]	4.9×10^{-3}	5600	Paasivirta and Sinkkonen (2009)	V	
HLQDGCWIOSOMDP-UHFFFAOYSA-N	8.7×10^{-2}		Burkhard et al. (1985)	V	
	9.6×10^{-2}		Duchowicz et al. (2020)	Q	
	9.0×10^{-2}		Lee (2007)	Q	723
	8.4×10^{-2}		Lee (2007)	Q	724
	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
	5.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,4,6-tetrachlorobiphenyl	4.7×10^{-2}		Brunner et al. (1990)	M	
$C_{12}H_6Cl_4$	7.1×10^{-3}	6000	Paasivirta and Sinkkonen (2009)	V	
(PCB-62)	3.3×10^{-2}		Burkhard et al. (1985)	V	
[54230-22-7]	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
HOBRTVXSIVSXIA-UHFFFAOYSA-N	5.7×10^{-2}		Duchowicz et al. (2020)	Q	300
	4.0×10^{-2}		Hilal et al. (2008)	Q	
	1.8×10^{-1}		Modarresi et al. (2007)	Q	68
	5.5×10^{-2}		Lee (2007)	Q	723
	6.4×10^{-2}		Lee (2007)	Q	724
	2.7×10^{-2}		Dunnivant et al. (1992)	Q	
	2.7×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.7×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,3,4',5-tetrachlorobiphenyl	2.5×10^{-2}	3000	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	3.4×10^{-2}		Murphy et al. (1987)	M	12
(PCB-63)	9.4×10^{-3}	6100	Paasivirta and Sinkkonen (2009)	V	
[74472-34-7]	5.6×10^{-2}		Burkhard et al. (1985)	V	
CITMYAMXIZQCJD-UHFFFAOYSA-N	6.8×10^{-2}		Lee (2007)	Q	723
	7.1×10^{-2}		Lee (2007)	Q	724
	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
	3.4×10^{-2}		Sabljić and Güsten (1989)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4',6-tetrachlorobiphenyl	2.5×10^{-2}	2900	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	5.8×10^{-2}		Murphy et al. (1987)	M	12
(PCB-64)	7.9×10^{-3}	6000	Paasivirta and Sinkkonen (2009)	V	
[52663-58-8]	3.2×10^{-2}		Burkhard et al. (1985)	V	
FXRXQYZZALWWGA-UHFFFAOYSA-N	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	7.7×10^{-2}		Duchowicz et al. (2020)	Q	300
	1.1×10^{-1}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	68
	4.2×10^{-2}		Lee (2007)	Q	723
	7.7×10^{-2}		Lee (2007)	Q	724
	3.6×10^{-2}		Dunnivant et al. (1992)	Q	
	3.5×10^{-2}		Sabljić and Güsten (1989)	Q	
	7.0×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,3,5,6-tetrachlorobiphenyl	4.9×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	3.7×10^{-2}		Burkhard et al. (1985)	V	
(PCB-65)	5.3×10^{-2}		Hilal et al. (2008)	Q	
[33284-54-7]	1.4×10^{-1}		Modarresi et al. (2007)	Q	68
BLAYIQLVUNIICD-UHFFFAOYSA-N	7.6×10^{-2}		Lee (2007)	Q	723
	9.9×10^{-2}		Lee (2007)	Q	724
	2.9×10^{-2}		Dunnivant et al. (1992)	Q	
	3.2×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3',4,4'-tetrachlorobiphenyl	2.7×10^{-2}	3500	Bamford et al. (2000)	M	
$C_{12}H_6Cl_4$	4.9×10^{-2}		Murphy et al. (1987)	M	12
(PCB-66)	3.0×10^{-3}	5300	Paasivirta and Sinkkonen (2009)	V	
[32598-10-0]	1.2×10^{-2}		Shiu and Mackay (1986)	V	
RKLLTEAEZIJBAU-UHFFFAOYSA-N	7.3×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	300
	2.9×10^{-2}		Bhangare et al. (2019)	Q	
	2.1×10^{-1}		Hilal et al. (2008)	Q	
	8.5×10^{-2}		Modarresi et al. (2007)	Q	68
	4.3×10^{-2}		Lee (2007)	Q	723
	6.8×10^{-2}		Lee (2007)	Q	724
		5200	Kühne et al. (2005)	Q	
	4.9×10^{-2}		Dunnivant et al. (1992)	Q	
	3.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	8.2×10^{-2}		Duchowicz et al. (2020)	?	186, 21
		3800	Kühne et al. (2005)	?	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3',4,5-tetrachlorobiphenyl	9.9×10^{-2}		Brunner et al. (1990)	M	
$C_{12}H_6Cl_4$	1.6×10^{-2}	6200	Paasivirta and Sinkkonen (2009)	V	
(PCB-67)	5.2×10^{-2}		Burkhard et al. (1985)	V	
[73575-53-8]	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
LQEGJNOKOZHBBZ-UHFFFAOYSA-N	7.7×10^{-2}		Duchowicz et al. (2020)	Q	300
	1.9×10^{-1}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	68
	7.9×10^{-2}		Lee (2007)	Q	723
	6.8×10^{-2}		Lee (2007)	Q	724
	4.2×10^{-2}		Dunnivant et al. (1992)	Q	
	3.4×10^{-2}		Sabljić and Güsten (1989)	Q	
	9.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,3',4,5'-tetrachlorobiphenyl	7.2×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	4.3×10^{-2}		Burkhard et al. (1985)	V	
(PCB-68)	8.7×10^{-2}		Lee (2007)	Q	723
[73575-52-7]	5.2×10^{-2}		Lee (2007)	Q	724
KTTXLLZIBIDUCR-UHFFFAOYSA-N	2.6×10^{-2}		Dunnivant et al. (1992)	Q	
	1.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3',4,6-tetrachlorobiphenyl	1.9×10^{-2}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	2.1×10^{-2}		Burkhard et al. (1985)	V	
(PCB-69)	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
[60233-24-1]	5.0×10^{-2}		Duchowicz et al. (2020)	Q	
CKUBKYSLNCKBOI-UHFFFAOYSA-N	7.9×10^{-2}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	68
	4.8×10^{-2}		Lee (2007)	Q	723
	4.5×10^{-2}		Lee (2007)	Q	724
	2.0×10^{-2}		Dunnivant et al. (1992)	Q	
	1.6×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.7×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,3',4',5-tetrachlorobiphenyl	3.3×10^{-2}	3500	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	9.9×10^{-2}		Brunner et al. (1990)	M	
(PCB-70)	5.2×10^{-2}		Murphy et al. (1987)	M	12
[32598-11-1]	1.1×10^{-1}		Brownawell (1986)	M	295
KENZYIHFBRWMOD-UHFFFAOYSA-N	4.9×10^{-2}		Murphy et al. (1983a)	M	24
	4.0×10^{-3}	5400	Paasivirta and Sinkkonen (2009)	V	
	5.0×10^{-2}		Shiu and Mackay (1986)	V	
	6.5×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	300
	2.0×10^{-1}		Hilal et al. (2008)	Q	
	7.2×10^{-2}		Modarresi et al. (2007)	Q	68
	6.0×10^{-2}		Lee (2007)	Q	723
	6.4×10^{-2}		Lee (2007)	Q	724
	4.9×10^{-2}		Dunnivant et al. (1992)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	9.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,3',4',6-tetrachlorobiphenyl	1.8×10^{-2}	6000	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	4.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-71)	3.6×10^{-2}		Lee (2007)	Q	723
[41464-46-4]	7.0×10^{-2}		Lee (2007)	Q	724
WYVBETQIUHPLFO-UHFFFAOYSA-N	3.1×10^{-2}		Dunnivant et al. (1992)	Q	
	3.1×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3',5,5'-tetrachlorobiphenyl	4.0×10^{-3}	5700	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	3.9×10^{-2}		Burkhard et al. (1985)	V	
(PCB-72)	1.2×10^{-1}		Lee (2007)	Q	723
[41464-42-0]	5.3×10^{-2}		Lee (2007)	Q	724
WBTMFEPLVQOWFI-UHFFFAOYSA-N	2.7×10^{-2}		Dunnivant et al. (1992)	Q	
	2.1×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3',5',6-tetrachlorobiphenyl	6.4×10^{-3}	5900	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	2.6×10^{-2}		Burkhard et al. (1985)	V	
(PCB-73)	7.4×10^{-2}		Lee (2007)	Q	723
[74338-23-1]	6.0×10^{-2}		Lee (2007)	Q	724
HDULUCZRGGWTMZ-UHFFFAOYSA-N	1.9×10^{-2}		Dunnivant et al. (1992)	Q	
	1.6×10^{-2}		Sabljić and Güsten (1989)	Q	
2,4,4',5-tetrachlorobiphenyl	2.6×10^{-2}	3000	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	9.9×10^{-2}		Brunner et al. (1990)	M	
(PCB-74)	4.7×10^{-2}		Murphy et al. (1987)	M	12
[32690-93-0]	4.8×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
TULCXSBAPHCWCF-UHFFFAOYSA-N	5.8×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	7.7×10^{-2}		Duchowicz et al. (2020)	Q	185
	2.0×10^{-1}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	68
	3.9×10^{-2}		Lee (2007)	Q	723
	6.5×10^{-2}		Lee (2007)	Q	724
	4.6×10^{-2}		Dunnivant et al. (1992)	Q	
	4.7×10^{-2}		Sabljić and Güsten (1989)	Q	
	9.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,4,4',6-tetrachlorobiphenyl	2.1×10^{-2}	6400	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	2.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-75)	2.4×10^{-2}		Lee (2007)	Q	723
[32598-12-2]	4.4×10^{-2}		Lee (2007)	Q	724
RZFZBHKDGHISSH-UHFFFAOYSA-N	2.1×10^{-2}		Dunnivant et al. (1992)	Q	
	1.8×10^{-2}		Sabljić and Güsten (1989)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3',4',5'-tetrachlorobiphenyl	7.7×10^{-2}		Murphy et al. (1987)	M	12
$C_{12}H_6Cl_4$	2.3×10^{-3}	5500	Paasivirta and Sinkkonen (2009)	V	
(PCB-76)	8.2×10^{-2}		Burkhard et al. (1985)	V	
[70362-48-0]	1.4×10^{-1}		Lee (2007)	Q	723
QILUYCYPNYWMIL-UHFFFAOYSA-N	7.0×10^{-2}		Lee (2007)	Q	724
	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
	4.4×10^{-2}		Sabljić and Güsten (1989)	Q	
3,3',4,4'-tetrachlorobiphenyl	1.2×10^{-2}		Bhangare et al. (2019)	M	727
$C_{12}H_6Cl_4$	7.1×10^{-2}		Bhangare et al. (2019)	M	728
(PCB-77)	3.1×10^{-2}		Lau et al. (2006)	M	721
[32598-13-3]	1.8×10^{-2}		Lau et al. (2006)	M	722
UQMGJOKDKOLIDP-UHFFFAOYSA-N	9.1×10^{-2}		Fang et al. (2006)	M	
	2.9×10^{-2}	13000	Charles and Destaillats (2005)	M	33
	6.2×10^{-2}	4800	Bamford et al. (2000)	M	
	1.0×10^{-1}		Dunnivant et al. (1988)	M	
	1.0×10^{-1}		Dunnivant and Elzerman (1988)	M	725
	6.0×10^{-4}	4600	Paasivirta and Sinkkonen (2009)	V	
	5.8×10^{-2}		Mackay et al. (2006b)	V	
	5.8×10^{-1}		Mackay et al. (1992a)	V	
	5.9×10^{-1}		Shiu and Mackay (1986)	V	
	2.3×10^{-1}		Burkhard et al. (1985)	V	
	8.3×10^{-3}	7400	Paasivirta et al. (1999)	T	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.9×10^{-1}		Duchowicz et al. (2020)	Q	
	3.6×10^{-1}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	68
	9.4×10^{-2}		Lee (2007)	Q	723
	8.0×10^{-2}		Lee (2007)	Q	724
		6100	Kühne et al. (2005)	Q	
	9.6×10^{-2}		Dunnivant et al. (1992)	Q	
	7.9×10^{-2}		Meylan and Howard (1991)	Q	
	1.0		Duchowicz et al. (2020)	?	186, 21
		5600	Kühne et al. (2005)	?	
3,3',4,5-tetrachlorobiphenyl	5.1×10^{-3}	5600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	1.7×10^{-1}		Burkhard et al. (1985)	V	
(PCB-78)	1.7×10^{-1}		Lee (2007)	Q	723
[70362-49-1]	7.5×10^{-2}		Lee (2007)	Q	724
SXFLURRQRFKBNN-UHFFFAOYSA-N	6.0×10^{-2}		Dunnivant et al. (1992)	Q	
	4.4×10^{-2}		Sabljić and Güsten (1989)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3',4,5'-tetrachlorobiphenyl	3.8×10^{-3}	5400	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	1.4×10^{-1}		Burkhard et al. (1985)	V	
(PCB-79)	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
[41464-48-6]	1.1×10^{-1}		Duchowicz et al. (2020)	Q	300
QLCTXEMDCZGPCG-UHFFFAOYSA-N	2.5×10^{-1}		Hilal et al. (2008)	Q	
	8.2×10^{-2}		Modarresi et al. (2007)	Q	68
	1.9×10^{-1}		Lee (2007)	Q	723
	6.3×10^{-2}		Lee (2007)	Q	724
	5.0×10^{-2}		Dunnivant et al. (1992)	Q	
	2.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	?	186, 21
3,3',5,5'-tetrachlorobiphenyl	9.4×10^{-4}	5100	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	8.0×10^{-2}		Burkhard et al. (1985)	V	
(PCB-80)	2.6×10^{-1}		Lee (2007)	Q	723
[33284-52-5]	5.2×10^{-2}		Lee (2007)	Q	724
UTMWFJSRHLYRPY-UHFFFAOYSA-N	2.6×10^{-2}		Dunnivant et al. (1992)	Q	
	1.6×10^{-2}		Sabljić and Güsten (1989)	Q	
3,4,4',5-tetrachlorobiphenyl	8.8×10^{-2}		Fang et al. (2006)	M	
$C_{12}H_6Cl_4$	4.1×10^{-2}	4000	Bamford et al. (2002)	M	
(PCB-81)	2.0×10^{-3}	5300	Paasivirta and Sinkkonen (2009)	V	
[70362-50-4]	1.9×10^{-1}		Burkhard et al. (1985)	V	
BHWVLZJTVIYLIV-UHFFFAOYSA-N	8.6×10^{-2}		Lee (2007)	Q	723
	7.2×10^{-2}		Lee (2007)	Q	724
	6.9×10^{-2}		Dunnivant et al. (1992)	Q	
	6.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,3',4-pentachlorobiphenyl	2.7×10^{-2}	5100	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	8.4×10^{-2}		Murphy et al. (1987)	M	12
(PCB-82)	4.9×10^{-2}		Murphy et al. (1983a)	M	24
[52663-62-4]	3.2×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
AUGNBQPSMWGAJE-UHFFFAOYSA-N	5.0×10^{-2}		Shiu and Mackay (1986)	V	
	8.0×10^{-2}		Burkhard et al. (1985)	V	
	1.6×10^{-1}		Lee (2007)	Q	723
	1.5×10^{-1}		Lee (2007)	Q	724
	6.7×10^{-2}		Dunnivant et al. (1992)	Q	
	8.1×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,3',5-pentachlorobiphenyl	2.3×10^{-2}	3600	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	6.0×10^{-2}		Murphy et al. (1987)	M	12
(PCB-83)	7.7×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
[60145-20-2]	4.7×10^{-2}		Burkhard et al. (1985)	V	
SUBRHHYLRGOTHL-UHFFFAOYSA-N	2.2×10^{-1}		Lee (2007)	Q	723
	1.4×10^{-1}		Lee (2007)	Q	724
	4.7×10^{-2}		Dunnivant et al. (1992)	Q	
	3.8×10^{-2}		Sabljić and Güsten (1989)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',6-pentachlorobiphenyl	5.7×10^{-2}		Murphy et al. (1987)	M	12
$C_{12}H_5Cl_5$	2.3×10^{-3}	6000	Paasivirta and Sinkkonen (2009)	V	
(PCB-84)	1.9×10^{-2}		Burkhard et al. (1985)	V	
[52663-60-2]	1.3×10^{-1}		Lee (2007)	Q	723
QVWUJLANSDKRAH-UHFFFAOYSA-N	1.2×10^{-1}		Lee (2007)	Q	724
	3.9×10^{-2}		Dunnivant et al. (1992)	Q	
	4.3×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4,4'-pentachlorobiphenyl	2.3×10^{-2}	3100	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	1.5×10^{-1}		Brunner et al. (1990)	M	
(PCB-85)	6.0×10^{-2}		Murphy et al. (1987)	M	12
[65510-45-4]	2.8×10^{-2}	6600	Paasivirta and Sinkkonen (2009)	V	
LACXVZHAJMVESG-UHFFFAOYSA-N	5.6×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.6×10^{-1}		Duchowicz et al. (2020)	Q	
	9.2×10^{-2}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	68
	7.8×10^{-2}		Lee (2007)	Q	723
	1.1×10^{-1}		Lee (2007)	Q	724
	5.1×10^{-2}		Dunnivant et al. (1992)	Q	
	4.0×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.5×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,4,5-pentachlorobiphenyl	3.2×10^{-3}		Duchowicz et al. (2020)	V	187
$C_{12}H_5Cl_5$	8.9×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
(PCB-86)	6.6×10^{-3}		Mackay et al. (2006b)	V	
[55312-69-1]	6.6×10^{-3}		Mackay et al. (1992a)	V	
AIURIRUDHVDRFQ-UHFFFAOYSA-N	6.6×10^{-3}		Shiu and Mackay (1986)	V	
	1.2×10^{-2}		Burkhard et al. (1985)	V	
	1.4×10^{-1}		Duchowicz et al. (2020)	Q	
	7.5×10^{-2}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Lee (2007)	Q	723
	1.2×10^{-1}		Lee (2007)	Q	724
	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
	5.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4,5'-pentachlorobiphenyl	2.7×10^{-2}	3900	Bamford et al. (2000)	M	
$C_{12}H_5Cl_5$	7.8×10^{-2}		Murphy et al. (1987)	M	12
(PCB-87)	1.4×10^{-1}		Brownawell (1986)	M	295
[38380-02-8]	3.0×10^{-2}		Murphy et al. (1983a)	M	24
OPKYDBFRKPQCBS-UHFFFAOYSA-N	4.1×10^{-3}	6000	Paasivirta and Sinkkonen (2009)	V	
	4.0×10^{-2}		Mackay et al. (2006b)	V	
	4.0×10^{-2}		Mackay et al. (1992a)	V	
	4.0×10^{-2}		Shiu and Mackay (1986)	V	
	5.0×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.5×10^{-1}		Duchowicz et al. (2020)	Q	300

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.3×10^{-2}		Bhangare et al. (2019)	Q	
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Lee (2007)	Q	723
	1.0×10^{-1}		Lee (2007)	Q	724
		5000	Kühne et al. (2005)	Q	
	5.4×10^{-2}		Dunnivant et al. (1992)	Q	
	5.5×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.3×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		4200	Kühne et al. (2005)	?	
2,2',3,4,6-pentachlorobiphenyl	9.6×10^{-3}	6800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	7.3×10^{-3}		Burkhard et al. (1985)	V	
(PCB-88)	1.2×10^{-1}		Lee (2007)	Q	723
[55215-17-3]	7.8×10^{-2}		Lee (2007)	Q	724
QGDKRLQRLFUJPP-UHFFFAOYSA-N	2.6×10^{-2}		Dunnivant et al. (1992)	Q	
	2.9×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4,6'-pentachlorobiphenyl	2.2×10^{-2}	2500	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	4.3×10^{-3}	6100	Paasivirta and Sinkkonen (2009)	V	
(PCB-89)	2.4×10^{-2}		Burkhard et al. (1985)	V	
[73575-57-2]	8.7×10^{-2}		Lee (2007)	Q	723
GLOOIONSKMZYQZ-UHFFFAOYSA-N	9.8×10^{-2}		Lee (2007)	Q	724
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	3.4×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4',5-pentachlorobiphenyl	2.1×10^{-2}	6600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	3.3×10^{-2}		Burkhard et al. (1985)	V	
(PCB-90)	1.1×10^{-1}		Lee (2007)	Q	723
[68194-07-0]	8.8×10^{-2}		Lee (2007)	Q	724
SUOAMBOBSWRMNQ-UHFFFAOYSA-N	3.4×10^{-2}		Dunnivant et al. (1992)	Q	
	2.6×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4',6-pentachlorobiphenyl	1.9×10^{-2}	1200	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	3.6×10^{-2}		Murphy et al. (1987)	M	12
(PCB-91)	1.1×10^{-2}	6500	Paasivirta and Sinkkonen (2009)	V	
[68194-05-8]	1.4×10^{-2}		Burkhard et al. (1985)	V	
CXKIGWXPPVZSQK-UHFFFAOYSA-N	6.6×10^{-2}		Lee (2007)	Q	723
	8.3×10^{-2}		Lee (2007)	Q	724
	2.9×10^{-2}		Dunnivant et al. (1992)	Q	
	2.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,5,5'-pentachlorobiphenyl	2.2×10^{-2}	2900	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	1.2×10^{-2}	6500	Paasivirta and Sinkkonen (2009)	V	
(PCB-92)	3.0×10^{-2}		Burkhard et al. (1985)	V	
[52663-61-3]	2.2×10^{-1}		Lee (2007)	Q	723
CRCBRZBVCDKPGA-UHFFFAOYSA-N	9.5×10^{-2}		Lee (2007)	Q	724
	3.8×10^{-2}		Dunnivant et al. (1992)	Q	
	3.1×10^{-2}		Sabljić and Güsten (1989)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,5,6-pentachlorobiphenyl	4.1×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	8.3×10^{-3}		Burkhard et al. (1985)	V	
(PCB-93)	1.2×10^{-1}		Lee (2007)	Q	723
[73575-56-1]	1.3×10^{-1}		Lee (2007)	Q	724
BMXRLHMJGHJGLR-UHFFFAOYSA-N	2.9×10^{-2}		Dunnivant et al. (1992)	Q	
	3.5×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,5,6'-pentachlorobiphenyl	4.5×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	1.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-94)	1.2×10^{-1}		Lee (2007)	Q	723
[73575-55-0]	9.1×10^{-2}		Lee (2007)	Q	724
FJUVPPYNSDTRQV-UHFFFAOYSA-N	2.5×10^{-2}		Dunnivant et al. (1992)	Q	
	2.3×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,5',6-pentachlorobiphenyl	2.1×10^{-2}	2500	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	5.0×10^{-2}		Murphy et al. (1987)	M	12
(PCB-95)	3.3×10^{-3}	6200	Paasivirta and Sinkkonen (2009)	V	
[38379-99-6]	1.2×10^{-2}		Burkhard et al. (1985)	V	
GXNNLIMMEXHBKV-UHFFFAOYSA-N	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	7.9×10^{-2}		Duchowicz et al. (2020)	Q	
	1.3×10^{-1}		Lee (2007)	Q	723
	9.0×10^{-2}		Lee (2007)	Q	724
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	3.4×10^{-2}		Sabljić and Güsten (1989)	Q	
	8.2×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,2',3,6,6'-pentachlorobiphenyl	8.7×10^{-4}	5800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	7.2×10^{-3}		Burkhard et al. (1985)	V	
(PCB-96)	7.4×10^{-2}		Lee (2007)	Q	723
[73575-54-9]	6.5×10^{-2}		Lee (2007)	Q	724
QQFGAXUIQVKBKU-UHFFFAOYSA-N	2.4×10^{-2}		Dunnivant et al. (1992)	Q	
	2.6×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4',5'-pentachlorobiphenyl	2.3×10^{-2}	3600	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	1.3×10^{-1}		Brunner et al. (1990)	M	
(PCB-97)	6.6×10^{-2}		Murphy et al. (1987)	M	12
[41464-51-1]	8.6×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
JTUSORDQZVOEAZ-UHFFFAOYSA-N	4.8×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.5×10^{-1}		Duchowicz et al. (2020)	Q	
	1.5×10^{-1}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Modarresi et al. (2007)	Q	68
	1.2×10^{-1}		Lee (2007)	Q	723
	1.1×10^{-1}		Lee (2007)	Q	724
	5.5×10^{-2}		Dunnivant et al. (1992)	Q	
	5.5×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.3×10^{-1}		Duchowicz et al. (2020)	?	186, 21

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4',6'-pentachlorobiphenyl	5.5×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	1.5×10^{-2}		Burkhard et al. (1985)	V	
(PCB-98)	7.6×10^{-2}		Lee (2007)	Q	723
[60233-25-2]	6.5×10^{-2}		Lee (2007)	Q	724
GOFFZTAPOOICFT-UHFFFAOYSA-N	2.5×10^{-2}		Dunnivant et al. (1992)	Q	
	2.0×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',4,4',5-pentachlorobiphenyl	2.2×10^{-2}		Lau et al. (2006)	M	721
$C_{12}H_5Cl_5$	4.2×10^{-3}		Lau et al. (2006)	M	722
(PCB-99)	8.8×10^{-3}	8700	Charles and Destaillats (2005)	M	33
[38380-01-7]	2.1×10^{-2}	1900	Bamford et al. (2002)	M	
LMQJBFRGXHMNOX-UHFFFAOYSA-N	1.3×10^{-1}		Brunner et al. (1990)	M	
	4.6×10^{-2}		Murphy et al. (1987)	M	12
	2.1×10^{-2}	6600	Paasivirta and Sinkkonen (2009)	V	
	3.4×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	8.6×10^{-2}		Duchowicz et al. (2020)	Q	300
	6.2×10^{-2}		Lee (2007)	Q	723
	7.9×10^{-2}		Lee (2007)	Q	724
	4.0×10^{-2}		Dunnivant et al. (1992)	Q	
	3.3×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.3×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',4,4',6-pentachlorobiphenyl	9.7×10^{-3}	6600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	1.0×10^{-2}		Burkhard et al. (1985)	V	
(PCB-100)	3.8×10^{-2}		Lee (2007)	Q	723
[39485-83-1]	4.6×10^{-2}		Lee (2007)	Q	724
RKUAZJIXKHPFRK-UHFFFAOYSA-N	1.8×10^{-2}		Dunnivant et al. (1992)	Q	
	1.6×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',4,5,5'-pentachlorobiphenyl	3.2×10^{-2}	6800	Li et al. (2003)	L	368
$C_{12}H_5Cl_5$	4.1×10^{-2}	7500	Li et al. (2003)	L	369
(PCB-101)	6.9×10^{-3}		Bhangare et al. (2019)	M	727
[37680-73-2]	2.0×10^{-2}		Bhangare et al. (2019)	M	728
LAHWLEDBADHJGA-UHFFFAOYSA-N	2.4×10^{-2}	3600	Bamford et al. (2000)	M	
	3.9×10^{-2}		Dunnivant et al. (1988)	M	
	3.9×10^{-2}		Dunnivant and Elzerman (1988)	M	725
	5.5×10^{-2}		Murphy et al. (1987)	M	12
	1.4×10^{-1}		Oliver (1985)	M	
			Westcott et al. (1981)	M	730
	8.9×10^{-3}	6400	Paasivirta and Sinkkonen (2009)	V	
	2.8×10^{-2}		Mackay et al. (2006b)	V	
	2.8×10^{-2}		Mackay et al. (1992a)	V	
	2.9×10^{-2}		Shiu and Mackay (1986)	V	
	3.1×10^{-2}		Burkhard et al. (1985)	V	
	2.0×10^{-2}	8100	Paasivirta et al. (1999)	T	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.9×10^{-2}		Duchowicz et al. (2020)	Q	185
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	68
	1.3×10^{-1}		Lee (2007)	Q	723
	7.9×10^{-2}		Lee (2007)	Q	724
		4600	Kühne et al. (2005)	Q	
	1.2×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	6.1×10^{-2}		English and Carroll (2001)	Q	231, 232
	4.0×10^{-2}		Dunnivant et al. (1992)	Q	
	1.1×10^{-1}		Meylan and Howard (1991)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		3900	Kühne et al. (2005)	?	
2,2',4,5,6'-pentachlorobiphenyl	1.1×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_5Cl_5$	6.3×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
(PCB-102)	1.5×10^{-2}		Burkhard et al. (1985)	V	
[68194-06-9]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
BWWVXHRLMPBDCK-UHFFFAOYSA-N	8.6×10^{-2}		Duchowicz et al. (2020)	Q	
	8.8×10^{-2}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	68
	6.9×10^{-2}		Lee (2007)	Q	723
	7.7×10^{-2}		Lee (2007)	Q	724
	2.7×10^{-2}		Dunnivant et al. (1992)	Q	
	2.8×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',4,5',6-pentachlorobiphenyl	8.1×10^{-3}	6600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	9.1×10^{-3}		Burkhard et al. (1985)	V	
(PCB-103)	7.7×10^{-2}		Lee (2007)	Q	723
[60145-21-3]	4.6×10^{-2}		Lee (2007)	Q	724
PQHZWWBJPCNNGI-UHFFFAOYSA-N	2.0×10^{-2}		Dunnivant et al. (1992)	Q	
	1.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',4,6,6'-pentachlorobiphenyl	1.5×10^{-2}	1700	Bamford et al. (2000)	M	
$C_{12}H_5Cl_5$	1.1×10^{-2}		Dunnivant et al. (1988)	M	
(PCB-104)	1.1×10^{-2}		Dunnivant and Elzerman (1988)	M	725
[56558-16-8]	2.8×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
MTCPZNVSDFCBBE-UHFFFAOYSA-N	4.3×10^{-2}		Mackay et al. (2006b)	V	
	7.2×10^{-2}		Mackay et al. (1992a)	V	
	5.4×10^{-3}		Burkhard et al. (1985)	V	
	2.0×10^{-2}		Bhangare et al. (2019)	Q	
	4.2×10^{-2}		Lee (2007)	Q	723
	3.4×10^{-2}		Lee (2007)	Q	724
		3100	Kühne et al. (2005)	Q	
	1.3×10^{-2}		Dunnivant et al. (1992)	Q	
		2000	Kühne et al. (2005)	?	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',4,4'-pentachlorobiphenyl	3.0×10^{-2}	6800	Li et al. (2003)	L	368
$C_{12}H_5Cl_5$	7.2×10^{-2}	7500	Li et al. (2003)	L	369
(PCB-105)	1.8×10^{-1}		Fang et al. (2006)	M	
[32598-14-4]	3.0×10^{-2}	9100	Bamford et al. (2000)	M	
WIDHRBRBACOVOY-UHFFFAOYSA-N	1.2×10^{-2}		Duchowicz et al. (2020)	V	187
	5.0×10^{-3}	5700	Paasivirta and Sinkkonen (2009)	V	
	1.8×10^{-1}		Burkhard et al. (1985)	V	
	2.9×10^{-2}	8300	Paasivirta et al. (1999)	T	
	2.7×10^{-1}		Duchowicz et al. (2020)	Q	
	2.0×10^{-2}		Bhangare et al. (2019)	Q	
	9.7×10^{-2}		Lee (2007)	Q	723
	1.4×10^{-1}		Lee (2007)	Q	724
	9.9×10^{-2}		Dunnivant et al. (1992)	Q	
	1.6×10^{-1}		Sabljić and Güsten (1989)	Q	
2,3,3',4,5-pentachlorobiphenyl	1.3×10^{-2}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	2.5×10^{-2}		Burkhard et al. (1985)	V	
(PCB-106)	1.8×10^{-1}		Lee (2007)	Q	723
[70424-69-0]	1.4×10^{-1}		Lee (2007)	Q	724
BQENMISTWGTJIJ-UHFFFAOYSA-N	6.0×10^{-2}		Dunnivant et al. (1992)	Q	
	5.1×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',4',5-pentachlorobiphenyl	4.3×10^{-2}	2200	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	1.7×10^{-1}		Murphy et al. (1987)	M	12
(PCB-107)	9.1×10^{-3}	6200	Paasivirta and Sinkkonen (2009)	V	
[70424-68-9]	1.0×10^{-1}		Burkhard et al. (1985)	V	
PVYBHVJTMRRXLG-UHFFFAOYSA-N	2.0×10^{-1}		Lee (2007)	Q	723
	1.2×10^{-1}		Lee (2007)	Q	724
	6.2×10^{-2}		Dunnivant et al. (1992)	Q	
	4.9×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',4,5'-pentachlorobiphenyl	4.1×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	1.0×10^{-1}		Burkhard et al. (1985)	V	
(PCB-108)	1.1×10^{-1}		Lee (2007)	Q	723
[70362-41-3]	1.1×10^{-1}		Lee (2007)	Q	724
MPCDNZSLJWJDNW-UHFFFAOYSA-N	5.6×10^{-2}		Dunnivant et al. (1992)	Q	
	2.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',4,6-pentachlorobiphenyl	1.5×10^{-2}	6600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	2.1×10^{-2}		Burkhard et al. (1985)	V	
(PCB-109)	1.4×10^{-1}		Lee (2007)	Q	723
[74472-35-8]	1.2×10^{-1}		Lee (2007)	Q	724
XGQBSVVYMVILEL-UHFFFAOYSA-N	3.5×10^{-2}		Dunnivant et al. (1992)	Q	
	2.5×10^{-2}		Sabljić and Güsten (1989)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',4',6-pentachlorobiphenyl	2.3×10^{-2}	5200	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	9.3×10^{-2}		Murphy et al. (1987)	M	12
(PCB-110)	2.7×10^{-2}		Murphy et al. (1983a)	M	24
[38380-03-9]	1.8×10^{-2}	6400	Paasivirta and Sinkkonen (2009)	V	
ARXHIJMGSIYYRZ-UHFFFAOYSA-N	5.8×10^{-2}		Burkhard et al. (1985)	V	
	8.3×10^{-2}		Lee (2007)	Q	723
	1.4×10^{-1}		Lee (2007)	Q	724
		5000	Kühne et al. (2005)	Q	
	5.0×10^{-2}		Dunnivant et al. (1992)	Q	
	5.2×10^{-2}		Sabljić and Güsten (1989)	Q	
		4300	Kühne et al. (2005)	?	
2,3,3',5,5'-pentachlorobiphenyl	6.5×10^{-3}	6200	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	6.2×10^{-2}		Burkhard et al. (1985)	V	
(PCB-111)	2.7×10^{-1}		Lee (2007)	Q	723
[39635-32-0]	7.8×10^{-2}		Lee (2007)	Q	724
QMUDLTGWHILKHH-UHFFFAOYSA-N	3.7×10^{-2}		Dunnivant et al. (1992)	Q	
	2.0×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',5,6-pentachlorobiphenyl	7.8×10^{-3}	6600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	2.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-112)	1.5×10^{-1}		Lee (2007)	Q	723
[74472-36-9]	2.0×10^{-1}		Lee (2007)	Q	724
NTKSJAPQYKCFPP-UHFFFAOYSA-N	3.7×10^{-2}		Dunnivant et al. (1992)	Q	
	3.0×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',5',6-pentachlorobiphenyl	1.5×10^{-2}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	3.5×10^{-2}		Burkhard et al. (1985)	V	
(PCB-113)	1.7×10^{-1}		Lee (2007)	Q	723
[68194-10-5]	1.2×10^{-1}		Lee (2007)	Q	724
YDGFMDPEJCJZEV-UHFFFAOYSA-N	3.0×10^{-2}		Dunnivant et al. (1992)	Q	
	2.1×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,4,4',5-pentachlorobiphenyl	5.3×10^{-2}		Fang et al. (2006)	M	
$C_{12}H_5Cl_5$	1.4×10^{-1}		Murphy et al. (1987)	M	12
(PCB-114)	1.2×10^{-2}	6400	Paasivirta and Sinkkonen (2009)	V	
[74472-37-0]	2.8×10^{-2}		Burkhard et al. (1985)	V	
SXZSFWHOSHAKMN-UHFFFAOYSA-N	8.9×10^{-2}		Lee (2007)	Q	723
	1.3×10^{-1}		Lee (2007)	Q	724
	6.9×10^{-2}		Dunnivant et al. (1992)	Q	
	8.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,4,4',6-pentachlorobiphenyl	2.6×10^{-2}	6900	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	2.3×10^{-2}		Burkhard et al. (1985)	V	
(PCB-115)	5.4×10^{-2}		Lee (2007)	Q	723
[74472-38-1]	1.1×10^{-1}		Lee (2007)	Q	724
IOVARPVVZDOPGQ-UHFFFAOYSA-N	4.0×10^{-2}		Dunnivant et al. (1992)	Q	
	3.2×10^{-2}		Sabljić and Güsten (1989)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4,5,6-pentachlorobiphenyl	4.3×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	5.5×10^{-2}		Burkhard et al. (1985)	V	
(PCB-116)	9.9×10^{-2}		Lee (2007)	Q	723
[18259-05-7]	1.8×10^{-1}		Lee (2007)	Q	724
GGMPTLAAIUQMIE-UHFFFAOYSA-N	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	4.3×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,4',5,6-pentachlorobiphenyl	1.5×10^{-3}	5900	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	2.7×10^{-2}		Burkhard et al. (1985)	V	
(PCB-117)	7.5×10^{-2}		Lee (2007)	Q	723
[68194-11-6]	1.7×10^{-1}		Lee (2007)	Q	724
ZDDZPDTVCZLFFC-UHFFFAOYSA-N	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
	4.0×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3',4,4',5-pentachlorobiphenyl	3.1×10^{-2}	6800	Li et al. (2003)	L	368
$C_{12}H_5Cl_5$	6.9×10^{-2}	7600	Li et al. (2003)	L	369
(PCB-118)	4.6×10^{-3}		Bhangare et al. (2019)	M	727
[31508-00-6]	1.9×10^{-2}		Bhangare et al. (2019)	M	728
IUTPYMGCWINGEY-UHFFFAOYSA-N	1.1×10^{-2}		Lau et al. (2006)	M	721
	5.6×10^{-3}		Lau et al. (2006)	M	722
	5.7×10^{-2}		Fang et al. (2006)	M	
	1.8×10^{-2}	14000	Charles and Destaillats (2005)	M	33
	2.8×10^{-2}	6000	Bamford et al. (2000)	M	
	1.2×10^{-1}		Murphy et al. (1987)	M	12
	2.5×10^{-2}		Murphy et al. (1983a)	M	24
	3.4×10^{-2}		Duchowicz et al. (2020)	V	187
	6.6×10^{-3}	6000	Paasivirta and Sinkkonen (2009)	V	
	1.1×10^{-1}		Burkhard et al. (1985)	V	
	2.6×10^{-2}	8100	Paasivirta et al. (1999)	T	
	1.5×10^{-1}		Duchowicz et al. (2020)	Q	
	7.8×10^{-2}		Lee (2007)	Q	723
	1.0×10^{-1}		Lee (2007)	Q	724
		5600	Kühne et al. (2005)	Q	
	7.9×10^{-2}		Dunnivant et al. (1992)	Q	
	8.5×10^{-2}		Sabljić and Güsten (1989)	Q	
		6300	Kühne et al. (2005)	?	
2,3',4,4',6-pentachlorobiphenyl	1.5×10^{-2}	4600	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	1.5×10^{-2}	6500	Paasivirta and Sinkkonen (2009)	V	
(PCB-119)	4.4×10^{-2}		Burkhard et al. (1985)	V	
[56558-17-9]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
OAEQTHQGPZKTQP-UHFFFAOYSA-N	9.4×10^{-2}		Duchowicz et al. (2020)	Q	185
	1.6×10^{-1}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Modarresi et al. (2007)	Q	68
	4.7×10^{-2}		Lee (2007)	Q	723
	7.4×10^{-2}		Lee (2007)	Q	724
	3.2×10^{-2}		Dunnivant et al. (1992)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.3×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,3',4,5,5'-pentachlorobiphenyl	1.8×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_5Cl_5$	3.9×10^{-3}	6000	Paasivirta and Sinkkonen (2009)	V	
(PCB-120)	6.4×10^{-2}		Burkhard et al. (1985)	V	
[68194-12-7]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
ZLGYJAIAVPVCNF-UHFFFAOYSA-N	8.6×10^{-2}		Duchowicz et al. (2020)	Q	300
	2.5×10^{-1}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	68
	1.6×10^{-1}		Lee (2007)	Q	723
	8.3×10^{-2}		Lee (2007)	Q	724
	4.0×10^{-2}		Dunnivant et al. (1992)	Q	
	2.4×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.8×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,3',4,5',6-pentachlorobiphenyl	8.5×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	2.6×10^{-2}		Burkhard et al. (1985)	V	
(PCB-121)	9.6×10^{-2}		Lee (2007)	Q	723
[56558-18-0]	6.2×10^{-2}		Lee (2007)	Q	724
XBVSGJGMWSKAKL-UHFFFAOYSA-N	1.8×10^{-2}		Dunnivant et al. (1992)	Q	
	1.3×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',4',5'-pentachlorobiphenyl	1.6×10^{-1}		Murphy et al. (1987)	M	12
$C_{12}H_5Cl_5$	4.3×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
(PCB-122)	1.6×10^{-1}		Burkhard et al. (1985)	V	
[76842-07-4]	2.8×10^{-1}		Lee (2007)	Q	723
GWOWBISZHLPYEK-UHFFFAOYSA-N	1.4×10^{-1}		Lee (2007)	Q	724
	7.9×10^{-2}		Dunnivant et al. (1992)	Q	
	7.2×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3',4,4',5'-pentachlorobiphenyl	4.6×10^{-2}		Fang et al. (2006)	M	
$C_{12}H_5Cl_5$	3.7×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
(PCB-123)	1.1×10^{-1}		Burkhard et al. (1985)	V	
[65510-44-3]	1.4×10^{-1}		Lee (2007)	Q	723
YAHNWSSFXMVPOU-UHFFFAOYSA-N	9.3×10^{-2}		Lee (2007)	Q	724
	5.7×10^{-2}		Dunnivant et al. (1992)	Q	
	3.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3',4',5,5'-pentachlorobiphenyl	1.9×10^{-1}		Murphy et al. (1987)	M	12
$C_{12}H_5Cl_5$	4.5×10^{-3}	5900	Paasivirta and Sinkkonen (2009)	V	
(PCB-124)	1.0×10^{-1}		Burkhard et al. (1985)	V	
[70424-70-3]	2.8×10^{-1}		Lee (2007)	Q	723
PIVBPZFQXKMHBD-UHFFFAOYSA-N	9.4×10^{-2}		Lee (2007)	Q	724
	5.8×10^{-2}		Dunnivant et al. (1992)	Q	
	5.1×10^{-2}		Sabljić and Güsten (1989)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3',4',5',6-pentachlorobiphenyl	2.3×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	6.7×10^{-2}		Burkhard et al. (1985)	V	
(PCB-125)	1.5×10^{-1}		Lee (2007)	Q	723
[74472-39-2]	1.1×10^{-1}		Lee (2007)	Q	724
WAZUWHGJMMZVHH-UHFFFAOYSA-N	3.4×10^{-2}		Dunnivant et al. (1992)	Q	
	3.0×10^{-2}		Sabljić and Güsten (1989)	Q	
3,3',4,4',5-pentachlorobiphenyl	1.0×10^{-1}		Fang et al. (2006)	M	
$C_{12}H_5Cl_5$	4.8×10^{-2}	12000	Bamford et al. (2000)	M	
(PCB-126)	1.6×10^{-3}	5400	Paasivirta and Sinkkonen (2009)	V	
[57465-28-8]	3.6×10^{-1}		Burkhard et al. (1985)	V	
REHONNLQRWTIFF-UHFFFAOYSA-N	6.5×10^{-2}	8800	Paasivirta et al. (1999)	T	
	1.8×10^{-2}		Bhangare et al. (2019)	Q	
	1.7×10^{-1}		Lee (2007)	Q	723
	1.0×10^{-1}		Lee (2007)	Q	724
	1.2×10^{-1}		Dunnivant et al. (1992)	Q	
	1.8×10^{-1}		Sabljić and Güsten (1989)	Q	
3,3',4,5,5'-pentachlorobiphenyl	2.2×10^{-3}	5600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	2.2×10^{-1}		Burkhard et al. (1985)	V	
(PCB-127)	3.4×10^{-1}		Lee (2007)	Q	723
[39635-33-1]	8.4×10^{-2}		Lee (2007)	Q	724
MXVAYAXIPRGORY-UHFFFAOYSA-N	6.3×10^{-2}		Dunnivant et al. (1992)	Q	
	2.9×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,3',4,4'-hexachlorobiphenyl	2.8×10^{-2}	14000	Bamford et al. (2000)	M	
$C_{12}H_4Cl_6$	7.6×10^{-1}		Brunner et al. (1990)	M	
(PCB-128)	3.3×10^{-1}		Dunnivant et al. (1988)	M	
[38380-07-3]	3.3×10^{-1}		Dunnivant and Elzerman (1988)	M	725
BTAGRXWGMYTPBY-UHFFFAOYSA-N	1.7×10^{-1}		Murphy et al. (1987)	M	12
	2.0×10^{-2}		Murphy et al. (1983a)	M	24
	6.9×10^{-3}	6100	Paasivirta and Sinkkonen (2009)	V	
	8.4×10^{-2}		Mackay et al. (2006b)	V	
	8.4×10^{-2}		Mackay et al. (1992a)	V	
	8.3×10^{-2}		Shiu and Mackay (1986)	V	
	1.5×10^{-1}		Burkhard et al. (1985)	V	
	2.0×10^{-2}		Murphy et al. (1983b)	X	726, 24
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	3.8×10^{-1}		Duchowicz et al. (2020)	Q	300
	1.5×10^{-2}		Bhangare et al. (2019)	Q	
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	68
	1.5×10^{-1}		Lee (2007)	Q	723
	2.4×10^{-1}		Lee (2007)	Q	724
	1.2×10^{-1}		English and Carroll (2001)	Q	231, 232
	9.5×10^{-2}		Dunnivant et al. (1992)	Q	
	7.6×10^{-1}		Duchowicz et al. (2020)	?	186, 21

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,5-hexachlorobiphenyl	3.4×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_4Cl_6$	6.4×10^{-3}	6400	Paasivirta and Sinkkonen (2009)	V	
(PCB-129)	2.5×10^{-2}		Burkhard et al. (1985)	V	
[55215-18-4]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
VQQKIXKPMJTUMP-UHFFFAOYSA-N	2.7×10^{-1}		Duchowicz et al. (2020)	Q	
	1.6×10^{-1}		Hilal et al. (2008)	Q	
	2.2×10^{-1}		Modarresi et al. (2007)	Q	68
	2.9×10^{-1}		Lee (2007)	Q	723
	2.6×10^{-1}		Lee (2007)	Q	724
	7.1×10^{-2}		Dunnivant et al. (1992)	Q	
	1.2×10^{-1}		Sabljić and Güsten (1989)	Q	
	3.4×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,3',4,5'-hexachlorobiphenyl	2.7×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_4Cl_6$	9.2×10^{-2}		Murphy et al. (1987)	M	12
(PCB-130)	5.9×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
[52663-66-8]	8.7×10^{-2}		Burkhard et al. (1985)	V	
YFSLABAYQDPWPF-UHFFFAOYSA-N	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	
	1.9×10^{-1}		Hilal et al. (2008)	Q	
	2.0×10^{-1}		Modarresi et al. (2007)	Q	68
	3.1×10^{-1}		Lee (2007)	Q	723
	2.1×10^{-1}		Lee (2007)	Q	724
	6.5×10^{-2}		Dunnivant et al. (1992)	Q	
	5.1×10^{-2}		Sabljić and Güsten (1989)	Q	
	2.7×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,3',4,6-hexachlorobiphenyl	1.5×10^{-1}		Murphy et al. (1987)	M	12
$C_{12}H_4Cl_6$	3.0×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
(PCB-131)	1.6×10^{-2}		Burkhard et al. (1985)	V	
[61798-70-7]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
WDLTVNWWEZJMPF-UHFFFAOYSA-N	1.6×10^{-1}		Duchowicz et al. (2020)	Q	300
	1.6×10^{-1}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	68
	1.7×10^{-1}		Lee (2007)	Q	723
	1.9×10^{-1}		Lee (2007)	Q	724
	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
	3.8×10^{-2}		Sabljić and Güsten (1989)	Q	
	2.5×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,3',4,6'-hexachlorobiphenyl	4.0×10^{-2}	2400	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	2.2×10^{-1}		Brunner et al. (1990)	M	
(PCB-132)	4.1×10^{-3}	6400	Paasivirta and Sinkkonen (2009)	V	
[38380-05-1]	3.6×10^{-2}		Burkhard et al. (1985)	V	
OKBJVIVEFXPEOU-UHFFFAOYSA-N	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	300
	2.2×10^{-1}		Hilal et al. (2008)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{-1}		Modarresi et al. (2007)	Q	68
	1.7×10^{-1}		Lee (2007)	Q	723
	2.1×10^{-1}		Lee (2007)	Q	724
	2.3×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	4.9×10^{-2}		Dunnivant et al. (1992)	Q	
	6.1×10^{-2}		Sabljić and Güsten (1989)	Q	
	2.2×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,3',5,5'-hexachlorobiphenyl	4.1×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	5.2×10^{-2}		Burkhard et al. (1985)	V	
(PCB-133)	1.8×10^{-1}		Hilal et al. (2008)	Q	
[35694-04-3]	4.3×10^{-1}		Lee (2007)	Q	723
AJKLKINFZLWHQE-UHFFFAOYSA-N	2.0×10^{-1}		Lee (2007)	Q	724
	4.8×10^{-2}		Dunnivant et al. (1992)	Q	
	3.0×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,3',5,6-hexachlorobiphenyl	1.2×10^{-2}	7300	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	2.0×10^{-1}		Brunner et al. (1990)	M	
(PCB-134)	1.0×10^{-1}		Murphy et al. (1987)	M	12
[52704-70-8]	1.7×10^{-2}		Murphy et al. (1983a)	M	24
RVWLHPJFOKUPNM-UHFFFAOYSA-N	2.8×10^{-3}	6400	Paasivirta and Sinkkonen (2009)	V	
	1.8×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.5×10^{-1}		Duchowicz et al. (2020)	Q	300
	2.0×10^{-1}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	68
	2.4×10^{-1}		Lee (2007)	Q	723
	3.2×10^{-1}		Lee (2007)	Q	724
	4.3×10^{-2}		Dunnivant et al. (1992)	Q	
	4.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	2.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,3',5,6'-hexachlorobiphenyl	1.5×10^{-2}	5500	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	1.8×10^{-1}		Brunner et al. (1990)	M	
(PCB-135)	7.0×10^{-2}		Murphy et al. (1987)	M	12
[52744-13-5]	4.8×10^{-3}	6600	Paasivirta and Sinkkonen (2009)	V	
UUTNFLRSJBQQJM-UHFFFAOYSA-N	2.1×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	185
	2.3×10^{-1}		Hilal et al. (2008)	Q	
	1.9×10^{-1}		Modarresi et al. (2007)	Q	68
	2.4×10^{-1}		Lee (2007)	Q	723
	2.1×10^{-1}		Lee (2007)	Q	724
	3.7×10^{-2}		Dunnivant et al. (1992)	Q	
	3.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.8×10^{-1}		Duchowicz et al. (2020)	?	186, 21

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',6,6'-hexachlorobiphenyl	9.0×10^{-3}	5400	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	1.1×10^{-1}		Brunner et al. (1990)	M	
(PCB-136)	4.4×10^{-2}		Murphy et al. (1987)	M	12
[38411-22-2]	1.6×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
FZFUUSROAHKTTF-UHFFFAOYSA-N	1.1×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	300
	2.7×10^{-1}		Hilal et al. (2008)	Q	
	1.5×10^{-1}		Modarresi et al. (2007)	Q	68
	1.4×10^{-1}		Lee (2007)	Q	723
	1.6×10^{-1}		Lee (2007)	Q	724
	3.1×10^{-2}		Dunnivant et al. (1992)	Q	
	3.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,4,4',5-hexachlorobiphenyl	4.5×10^{-2}	3200	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	1.5×10^{-1}		Murphy et al. (1987)	M	12
(PCB-137)	2.1×10^{-2}		Murphy et al. (1983a)	M	24
[35694-06-5]	1.8×10^{-2}	6800	Paasivirta and Sinkkonen (2009)	V	
CKLLRBPBZLTGDJ-UHFFFAOYSA-N	1.8×10^{-2}		Burkhard et al. (1985)	V	
	1.4×10^{-1}		Lee (2007)	Q	723
	1.7×10^{-1}		Lee (2007)	Q	724
	5.3×10^{-2}		Dunnivant et al. (1992)	Q	
	4.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4,4',5'-hexachlorobiphenyl	2.5×10^{-2}	7100	Li et al. (2003)	L	368
$C_{12}H_4Cl_6$	3.3×10^{-2}	7700	Li et al. (2003)	L	369
(PCB-138)	2.2×10^{-2}	10000	Bamford et al. (2000)	M	
[35065-28-2]	4.7×10^{-1}		Brunner et al. (1990)	M	
RPUMZMSNLZHIGZ-UHFFFAOYSA-N	1.3×10^{-1}		Murphy et al. (1987)	M	12
	1.4×10^{-1}		Brownawell (1986)	M	295
	2.1×10^{-2}		Murphy et al. (1983a)	M	24
	1.8×10^{-2}	6800	Paasivirta and Sinkkonen (2009)	V	
	1.2×10^{-2}		Shiu and Mackay (1986)	V	
	9.1×10^{-2}		Burkhard et al. (1985)	V	
	4.7×10^{-2}	8700	Paasivirta et al. (1999)	T	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.5×10^{-2}		Bhangare et al. (2019)	Q	
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	2.2×10^{-1}		Modarresi et al. (2007)	Q	68
	1.6×10^{-1}		Lee (2007)	Q	723
	1.8×10^{-1}		Lee (2007)	Q	724
	5.2×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	7.6×10^{-2}		Dunnivant et al. (1992)	Q	
	9.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.7×10^{-1}		Duchowicz et al. (2020)	?	186, 21

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,4',6-hexachlorobiphenyl	1.4×10^{-2}	6900	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	1.1×10^{-2}		Burkhard et al. (1985)	V	
(PCB-139)	8.6×10^{-2}		Lee (2007)	Q	723
[56030-56-9]	1.3×10^{-1}		Lee (2007)	Q	724
SPOPSCCFZQFGDL-UHFFFAOYSA-N	3.0×10^{-2}		Dunnivant et al. (1992)	Q	
	2.6×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4,4',6'-hexachlorobiphenyl	1.7×10^{-2}	7000	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	2.7×10^{-2}		Burkhard et al. (1985)	V	
(PCB-140)	8.5×10^{-2}		Lee (2007)	Q	723
[59291-64-4]	1.1×10^{-1}		Lee (2007)	Q	724
XBBRGUHRZBZMPP-UHFFFAOYSA-N	3.2×10^{-2}		Dunnivant et al. (1992)	Q	
	2.3×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4,5,5'-hexachlorobiphenyl	2.0×10^{-2}	8400	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	4.3×10^{-1}		Brunner et al. (1990)	M	
(PCB-141)	1.0×10^{-1}		Murphy et al. (1987)	M	12
[52712-04-6]	2.5×10^{-2}		Murphy et al. (1983a)	M	24
UCLKLGIYGBLTSM-UHFFFAOYSA-N	1.0×10^{-2}	6700	Paasivirta and Sinkkonen (2009)	V	
	2.5×10^{-2}		Shiu and Mackay (1986)	V	
	1.6×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.5×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.3×10^{-1}		Hilal et al. (2008)	Q	
	2.0×10^{-1}		Modarresi et al. (2007)	Q	68
	2.9×10^{-1}		Lee (2007)	Q	723
	1.8×10^{-1}		Lee (2007)	Q	724
	5.7×10^{-2}		Dunnivant et al. (1992)	Q	
	6.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.3×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,4,5,6-hexachlorobiphenyl	4.0×10^{-3}	6900	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	1.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-142)	1.6×10^{-1}		Lee (2007)	Q	723
[41411-61-4]	2.4×10^{-1}		Lee (2007)	Q	724
RUEIBQJFGMERJD-UHFFFAOYSA-N	3.1×10^{-2}		Dunnivant et al. (1992)	Q	
	4.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4,5,6'-hexachlorobiphenyl	6.5×10^{-3}	6600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	7.8×10^{-3}		Burkhard et al. (1985)	V	
(PCB-143)	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
[68194-15-0]	1.6×10^{-1}		Duchowicz et al. (2020)	Q	185
UQPQKLGBEKEZBV-UHFFFAOYSA-N	1.6×10^{-1}		Hilal et al. (2008)	Q	
	1.7×10^{-1}		Modarresi et al. (2007)	Q	68
	1.6×10^{-1}		Lee (2007)	Q	723
	1.9×10^{-1}		Lee (2007)	Q	724
	3.4×10^{-2}		Dunnivant et al. (1992)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	2.5×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,4,5',6-hexachlorobiphenyl	7.0×10^{-2}		Murphy et al. (1987)	M	12
$C_{12}H_4Cl_6$	1.6×10^{-2}		Murphy et al. (1983a)	M	24
(PCB-144)	1.2×10^{-2}	7000	Paasivirta and Sinkkonen (2009)	V	
[68194-14-9]	1.7×10^{-2}		Shiu and Mackay (1986)	V	
CXXRQFOKRZJAJA-UHFFFAOYSA-N	1.0×10^{-2}		Burkhard et al. (1985)	V	
	1.8×10^{-1}		Lee (2007)	Q	723
	1.4×10^{-1}		Lee (2007)	Q	724
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	3.1×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4,6,6'-hexachlorobiphenyl	1.5×10^{-3}	6400	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	5.9×10^{-3}		Burkhard et al. (1985)	V	
(PCB-145)	9.6×10^{-2}		Lee (2007)	Q	723
[74472-40-5]	1.1×10^{-1}		Lee (2007)	Q	724
JZFZCLFEPXCRCA-UHFFFAOYSA-N	2.1×10^{-2}		Dunnivant et al. (1992)	Q	
	2.4×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4',5,5'-hexachlorobiphenyl	1.7×10^{-2}	7100	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	3.9×10^{-1}		Brunner et al. (1990)	M	
(PCB-146)	1.1×10^{-1}		Murphy et al. (1987)	M	12
[51908-16-8]	1.2×10^{-2}	6800	Paasivirta and Sinkkonen (2009)	V	
BQHCQAQLTCQFJZ-UHFFFAOYSA-N	5.4×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	185
	2.0×10^{-1}		Hilal et al. (2008)	Q	
	2.2×10^{-1}		Modarresi et al. (2007)	Q	68
	2.2×10^{-1}		Lee (2007)	Q	723
	1.6×10^{-1}		Lee (2007)	Q	724
	5.3×10^{-2}		Dunnivant et al. (1992)	Q	
	4.0×10^{-2}		Sabljić and Güsten (1989)	Q	
	3.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,4',5,6-hexachlorobiphenyl	1.9×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_4Cl_6$	3.1×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
(PCB-147)	1.3×10^{-2}		Burkhard et al. (1985)	V	
[68194-13-8]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
AQONCPKMJSBHQT-UHFFFAOYSA-N	8.7×10^{-2}		Duchowicz et al. (2020)	Q	300
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	68
	1.2×10^{-1}		Lee (2007)	Q	723
	2.1×10^{-1}		Lee (2007)	Q	724
	3.1×10^{-2}		Dunnivant et al. (1992)	Q	
	3.1×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4',5,6'-hexachlorobiphenyl	1.2×10^{-2}	7000	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	1.6×10^{-2}		Burkhard et al. (1985)	V	
(PCB-148)	1.2×10^{-1}		Lee (2007)	Q	723
[74472-41-6]	1.0×10^{-1}		Lee (2007)	Q	724
CTVRBEKNQHJPLX-UHFFFAOYSA-N	2.3×10^{-2}		Dunnivant et al. (1992)	Q	
	1.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4',5',6-hexachlorobiphenyl	1.5×10^{-2}	5500	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	6.7×10^{-2}		Murphy et al. (1987)	M	12
(PCB-149)	3.3×10^{-2}		Murphy et al. (1983a)	M	24
[38380-04-0]	7.2×10^{-3}		Duchowicz et al. (2020)	V	187
LKHLFUVHHXCNJH-UHFFFAOYSA-N	1.0×10^{-2}	6800	Paasivirta and Sinkkonen (2009)	V	
	3.3×10^{-2}		Shiu and Mackay (1986)	V	
	2.2×10^{-2}		Burkhard et al. (1985)	V	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	
	1.3×10^{-1}		Lee (2007)	Q	723
	1.7×10^{-1}		Lee (2007)	Q	724
	2.1×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	4.2×10^{-2}		Dunnivant et al. (1992)	Q	
	4.5×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4',6,6'-hexachlorobiphenyl	6.5×10^{-3}	6900	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	8.2×10^{-3}		Burkhard et al. (1985)	V	
(PCB-150)	7.2×10^{-2}		Lee (2007)	Q	723
[68194-08-1]	8.0×10^{-2}		Lee (2007)	Q	724
RPPNJBZNXQNKNM-UHFFFAOYSA-N	2.0×10^{-2}		Dunnivant et al. (1992)	Q	
	1.9×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,5,5',6-hexachlorobiphenyl	1.4×10^{-2}	4500	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	1.7×10^{-1}		Brunner et al. (1990)	M	
(PCB-151)	6.3×10^{-2}		Murphy et al. (1987)	M	12
[52663-63-5]	3.3×10^{-2}		Murphy et al. (1983a)	M	24
UHCLFIWDCYOTOL-UHFFFAOYSA-N	5.2×10^{-3}	6700	Paasivirta and Sinkkonen (2009)	V	
	3.3×10^{-2}		Shiu and Mackay (1986)	V	
	1.2×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	7.9×10^{-2}		Duchowicz et al. (2020)	Q	
	1.6×10^{-1}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	68
	2.4×10^{-1}		Lee (2007)	Q	723
	2.4×10^{-1}		Lee (2007)	Q	724
	3.5×10^{-2}		Dunnivant et al. (1992)	Q	
	3.8×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.7×10^{-1}		Duchowicz et al. (2020)	?	186, 21

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,5,6,6'-hexachlorobiphenyl	1.3×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	6.8×10^{-3}		Burkhard et al. (1985)	V	
(PCB-152)	1.3×10^{-1}		Lee (2007)	Q	723
[68194-09-2]	1.9×10^{-1}		Lee (2007)	Q	724
CLODVDBWNVQLGO-UHFFFAOYSA-N	2.3×10^{-2}		Dunnivant et al. (1992)	Q	
	2.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',4,4',5,5'-hexachlorobiphenyl	4.0×10^{-2}	7100	Li et al. (2003)	L	368
$C_{12}H_4Cl_6$	5.1×10^{-2}	7900	Li et al. (2003)	L	369
(PCB-153)	1.9×10^{-2}	8000	Bamford et al. (2000)	M	
[35065-27-1]	4.3×10^{-1}		Brunner et al. (1990)	M	
MVWHGTYKUMDIHL-UHFFFAOYSA-N	7.5×10^{-2}		Dunnivant et al. (1988)	M	
	7.5×10^{-2}		Dunnivant and Elzerman (1988)	M	725
	1.0×10^{-1}		Murphy et al. (1987)	M	12
	1.6×10^{-1}		Oliver (1985)	M	
	2.8×10^{-2}		Murphy et al. (1983a)	M	24
	1.1×10^{-2}	6700	Paasivirta and Sinkkonen (2009)	V	
	2.3×10^{-2}		Mackay et al. (2006b)	V	
	2.3×10^{-2}		Mackay et al. (1992a)	V	
	2.3×10^{-2}		Shiu and Mackay (1986)	V	
	5.6×10^{-2}		Burkhard et al. (1985)	V	
	1.7×10^{-2}	8400	Paasivirta et al. (1999)	T	
	2.8×10^{-2}		Murphy et al. (1983b)	X	726, 24
	8.0×10^{-2}		Dunnivant et al. (1988)	C	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	300
	1.7×10^{-2}		Bhangare et al. (2019)	Q	
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	2.4×10^{-1}		Modarresi et al. (2007)	Q	68
	1.2×10^{-1}		Lee (2007)	Q	723
	1.4×10^{-1}		Lee (2007)	Q	724
	2.9×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	6.0×10^{-2}		Dunnivant et al. (1992)	Q	
	4.3×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',4,4',5,6'-hexachlorobiphenyl	1.3×10^{-2}	5600	Bamford et al. (2000)	M	
$C_{12}H_4Cl_6$	1.7×10^{-2}	7100	Paasivirta and Sinkkonen (2009)	V	
(PCB-154)	1.7×10^{-2}		Burkhard et al. (1985)	V	
[60145-22-4]	1.8×10^{-2}		Bhangare et al. (2019)	Q	
QXZHEJWDLVUFFB-UHFFFAOYSA-N	6.8×10^{-2}		Lee (2007)	Q	723
	8.7×10^{-2}		Lee (2007)	Q	724
	2.6×10^{-2}		Dunnivant et al. (1992)	Q	
	2.0×10^{-2}		Sabljić and Güsten (1989)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',4,4',6,6'-hexachlorobiphenyl	1.3×10^{-2}	7100	Li et al. (2003)	L	368
$C_{12}H_4Cl_6$	1.1×10^{-2}	7600	Li et al. (2003)	L	369
(PCB-155)	1.3×10^{-2}		Dunnivant et al. (1988)	M	
[33979-03-2]	1.3×10^{-2}		Dunnivant and Elzerman (1988)	M	725
ICOAEPDGFWLUTI-UHFFFAOYSA-N	3.9×10^{-3}		Duchowicz et al. (2020)	V	187
	4.6×10^{-3}	6900	Paasivirta and Sinkkonen (2009)	V	
	1.2×10^{-2}		Mackay et al. (2006b)	V	
	1.2×10^{-2}		Mackay et al. (1992a)	V	
	1.2×10^{-3}		Shiu and Mackay (1986)	V	
	6.4×10^{-3}		Burkhard et al. (1985)	V	
	8.6×10^{-2}		Dunnivant et al. (1988)	C	
	4.8×10^{-2}		Duchowicz et al. (2020)	Q	
	4.2×10^{-2}		Lee (2007)	Q	723
	4.2×10^{-2}		Lee (2007)	Q	724
	1.2×10^{-2}		Dunnivant et al. (1992)	Q	
2,3,3',4,4',5-hexachlorobiphenyl	6.8×10^{-2}		Fang et al. (2006)	M	
$C_{12}H_4Cl_6$	2.9×10^{-2}	13000	Bamford et al. (2002)	M	
(PCB-156)	1.1×10^{-2}		Murphy et al. (1983a)	M	24
[38380-08-4]	6.9×10^{-2}		Duchowicz et al. (2020)	V	187
LCXMEXLGMKFLQO-UHFFFAOYSA-N	5.9×10^{-3}	6200	Paasivirta and Sinkkonen (2009)	V	
	1.1×10^{-2}		Shiu and Mackay (1986)	V	
	5.7×10^{-2}		Burkhard et al. (1985)	V	
	2.7×10^{-1}		Duchowicz et al. (2020)	Q	
	1.8×10^{-1}		Lee (2007)	Q	723
	2.0×10^{-1}		Lee (2007)	Q	724
	1.1×10^{-1}		Dunnivant et al. (1992)	Q	
	4.5×10^{-1}		Sabljić and Güsten (1989)	Q	
2,3,3',4,4',5'-hexachlorobiphenyl	6.0×10^{-2}		Fang et al. (2006)	M	
$C_{12}H_4Cl_6$	3.4×10^{-2}	16000	Bamford et al. (2002)	M	
(PCB-157)	1.7×10^{-2}		Murphy et al. (1983a)	M	24
[69782-90-7]	2.3×10^{-3}	5900	Paasivirta and Sinkkonen (2009)	V	
YTWXDQVNPCIEOX-UHFFFAOYSA-N	1.7×10^{-2}		Shiu and Mackay (1986)	V	
	3.0×10^{-1}		Burkhard et al. (1985)	V	
	1.9×10^{-1}		Lee (2007)	Q	723
	2.0×10^{-1}		Lee (2007)	Q	724
		6300	Kühne et al. (2005)	Q	
	1.2×10^{-1}		Dunnivant et al. (1992)	Q	
	1.5×10^{-1}		Sabljić and Güsten (1989)	Q	
		5100	Kühne et al. (2005)	?	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',4,4',6-hexachlorobiphenyl	2.1×10^{-2}	9600	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	2.3×10^{-1}		Murphy et al. (1987)	M	12
(PCB-158)	1.5×10^{-2}		Murphy et al. (1983a)	M	24
[74472-42-7]	9.2×10^{-3}	6600	Paasivirta and Sinkkonen (2009)	V	
ZQUPQXINXTWCQR-UHFFFAOYSA-N	1.5×10^{-2}		Shiu and Mackay (1986)	V	
	4.8×10^{-2}		Burkhard et al. (1985)	V	
	1.1×10^{-1}		Lee (2007)	Q	723
	1.9×10^{-1}		Lee (2007)	Q	724
	6.0×10^{-2}		Dunnivant et al. (1992)	Q	
	4.6×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',4,5,5'-hexachlorobiphenyl	4.9×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_4Cl_6$	2.9×10^{-3}	6100	Paasivirta and Sinkkonen (2009)	V	
(PCB-159)	3.4×10^{-2}		Burkhard et al. (1985)	V	
[39635-35-3]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
YZKLGRAIIIGOHB-UHFFFAOYSA-N	1.6×10^{-1}		Duchowicz et al. (2020)	Q	185
	2.6×10^{-1}		Hilal et al. (2008)	Q	
	1.9×10^{-1}		Modarresi et al. (2007)	Q	68
	3.6×10^{-1}		Lee (2007)	Q	723
	1.8×10^{-1}		Lee (2007)	Q	724
	6.3×10^{-2}		Dunnivant et al. (1992)	Q	
	3.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,3,3',4,5,6-hexachlorobiphenyl	4.9×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_4Cl_6$	7.9×10^{-3}	7100	Paasivirta and Sinkkonen (2009)	V	
(PCB-160)	4.0×10^{-2}		Burkhard et al. (1985)	V	
[41411-62-5]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
JHJMZCXLJXRCHK-UHFFFAOYSA-N	1.1×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	3.8×10^{-1}		Modarresi et al. (2007)	Q	68
	2.0×10^{-1}		Lee (2007)	Q	723
	3.3×10^{-1}		Lee (2007)	Q	724
	4.6×10^{-2}		Dunnivant et al. (1992)	Q	
	3.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,3,3',4,5',6-hexachlorobiphenyl	9.2×10^{-3}	6800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	2.9×10^{-2}		Burkhard et al. (1985)	V	
(PCB-161)	2.2×10^{-1}		Lee (2007)	Q	723
[74472-43-8]	1.7×10^{-1}		Lee (2007)	Q	724
UNPTZXSJGZTGJJ-UHFFFAOYSA-N	3.5×10^{-2}		Dunnivant et al. (1992)	Q	
	2.0×10^{-2}		Sabljić and Güsten (1989)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',4',5,5'-hexachlorobiphenyl	3.7×10^{-3}	6200	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	1.8×10^{-1}		Burkhard et al. (1985)	V	
(PCB-162)	2.7×10^{-1}		Lee (2007)	Q	723
[39635-34-2]	1.8×10^{-1}		Lee (2007)	Q	724
AHZUOPSGLWYCNF-UHFFFAOYSA-N	7.5×10^{-2}		Dunnivant et al. (1992)	Q	
	4.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',4',5,6-hexachlorobiphenyl	2.1×10^{-2}	9700	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	6.6×10^{-1}		Brunner et al. (1990)	M	
(PCB-163)	4.9×10^{-3}	6400	Paasivirta and Sinkkonen (2009)	V	
[74472-44-9]	5.4×10^{-2}		Burkhard et al. (1985)	V	
ZAGRQXMWMRUYRB-UHFFFAOYSA-N	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.5×10^{-1}		Duchowicz et al. (2020)	Q	300
	2.5×10^{-1}		Hilal et al. (2008)	Q	
	2.6×10^{-1}		Modarresi et al. (2007)	Q	68
	1.5×10^{-1}		Lee (2007)	Q	723
	3.1×10^{-1}		Lee (2007)	Q	724
	6.0×10^{-2}		Dunnivant et al. (1992)	Q	
	6.3×10^{-2}		Sabljić and Güsten (1989)	Q	
	6.6×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,3,3',4',5',6-hexachlorobiphenyl	9.5×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	1.0×10^{-1}		Burkhard et al. (1985)	V	
(PCB-164)	1.6×10^{-1}		Lee (2007)	Q	723
[74472-45-0]	2.3×10^{-1}		Lee (2007)	Q	724
HAZQOLYHFUUJJN-UHFFFAOYSA-N	5.6×10^{-2}		Dunnivant et al. (1992)	Q	
	5.0×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',5,5',6-hexachlorobiphenyl	3.4×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_4Cl_6$	2.5×10^{-3}	6400	Paasivirta and Sinkkonen (2009)	V	
(PCB-165)	3.2×10^{-2}		Burkhard et al. (1985)	V	
[74472-46-1]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
ZEATXTCWXKQPHO-UHFFFAOYSA-N	8.7×10^{-2}		Duchowicz et al. (2020)	Q	
	1.6×10^{-1}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	68
	3.0×10^{-1}		Lee (2007)	Q	723
	2.9×10^{-1}		Lee (2007)	Q	724
	3.6×10^{-2}		Dunnivant et al. (1992)	Q	
	2.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	3.4×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,3,4,4',5,6-hexachlorobiphenyl	3.5×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	4.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-166)	1.2×10^{-1}		Hilal et al. (2008)	Q	
[41411-63-6]	3.1×10^{-1}		Modarresi et al. (2007)	Q	68
BTOCFTAWZMMTNB-UHFFFAOYSA-N	9.8×10^{-2}		Lee (2007)	Q	723
	2.9×10^{-1}		Lee (2007)	Q	724
		4100	Kühne et al. (2005)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.4×10^{-2}		Dunnivant et al. (1992)	Q	
	5.7×10^{-2}		Sabljić and Güsten (1989)	Q	
		5800	Kühne et al. (2005)	?	
2,3',4,4',5,5'-hexachlorobiphenyl	7.8×10^{-2}		Fang et al. (2006)	M	
$C_{12}H_4Cl_6$	2.7×10^{-2}	13000	Bamford et al. (2002)	M	
(PCB-167)	7.3×10^{-3}	6400	Paasivirta and Sinkkonen (2009)	V	
[52663-72-6]	1.9×10^{-1}		Burkhard et al. (1985)	V	
AZXHAWRMEPZSSV-UHFFFAOYSA-N	1.6×10^{-1}		Lee (2007)	Q	723
	1.4×10^{-1}		Lee (2007)	Q	724
	9.0×10^{-2}		Dunnivant et al. (1992)	Q	
	8.0×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3',4,4',5',6-hexachlorobiphenyl	1.1×10^{-2}	6700	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	7.7×10^{-2}		Burkhard et al. (1985)	V	
(PCB-168)	9.4×10^{-2}		Lee (2007)	Q	723
[59291-65-5]	1.2×10^{-1}		Lee (2007)	Q	724
PITHIPNORFGJPI-UHFFFAOYSA-N	3.6×10^{-2}		Dunnivant et al. (1992)	Q	
	2.1×10^{-2}		Sabljić and Güsten (1989)	Q	
3,3',4,4',5,5'-hexachlorobiphenyl	8.1×10^{-2}		Fang et al. (2006)	M	
$C_{12}H_4Cl_6$	4.7×10^{-2}	19000	Bamford et al. (2002)	M	
(PCB-169)	4.0×10^{-4}	5100	Paasivirta and Sinkkonen (2009)	V	
[32774-16-6]	6.4×10^{-1}		Burkhard et al. (1985)	V	
ZHLICBPIXDOFFG-UHFFFAOYSA-N	2.3×10^{-2}	9000	Paasivirta et al. (1999)	T	
	3.4×10^{-1}		Lee (2007)	Q	723
	1.3×10^{-1}		Lee (2007)	Q	724
	1.5×10^{-1}		Dunnivant et al. (1992)	Q	
	1.7×10^{-1}		Sabljić and Güsten (1989)	Q	
2,2',3,3',4,4',5-heptachlorobiphenyl	4.8×10^{-2}	20000	Bamford et al. (2000)	M	
$C_{12}H_3Cl_7$	1.1		Brunner et al. (1990)	M	
(PCB-170)	6.6×10^{-1}		Murphy et al. (1987)	M	12
[35065-30-6]	7.8×10^{-3}	6600	Paasivirta and Sinkkonen (2009)	V	
RMPWIIKNWPVWNG-UHFFFAOYSA-N	5.2×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	3.9×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.5×10^{-2}		Bhangare et al. (2019)	Q	
	2.1×10^{-1}		Hilal et al. (2008)	Q	
	3.2×10^{-1}		Modarresi et al. (2007)	Q	68
	2.8×10^{-1}		Lee (2007)	Q	723
	4.0×10^{-1}		Lee (2007)	Q	724
	1.1×10^{-1}		Dunnivant et al. (1992)	Q	
	1.1		Duchowicz et al. (2020)	?	186, 21

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,4',6-heptachlorobiphenyl	2.9×10^{-2}		Duchowicz et al. (2020)	V	187
$C_{12}H_3Cl_7$	1.3×10^{-2}	7100	Paasivirta and Sinkkonen (2009)	V	
(PCB-171)	1.9×10^{-1}		Mackay et al. (2006b)	V	
[52663-71-5]	1.9×10^{-1}		Mackay et al. (1992a)	V	
TZMHVHLTPWKZCI-UHFFFAOYSA-N	1.9×10^{-1}		Shiu and Mackay (1986)	V	
	3.4×10^{-2}		Burkhard et al. (1985)	V	
	2.3×10^{-1}		Duchowicz et al. (2020)	Q	
	2.1×10^{-1}		Hilal et al. (2008)	Q	
	2.8×10^{-1}		Modarresi et al. (2007)	Q	68
	1.7×10^{-1}		Lee (2007)	Q	723
	3.1×10^{-1}		Lee (2007)	Q	724
	5.7×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,3',4,5,5'-heptachlorobiphenyl	7.6×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_3Cl_7$	8.3×10^{-3}	6800	Paasivirta and Sinkkonen (2009)	V	
(PCB-172)	3.1×10^{-2}		Burkhard et al. (1985)	V	
[52663-74-8]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
HOPMUCXYRNOABF-UHFFFAOYSA-N	2.1×10^{-1}		Duchowicz et al. (2020)	Q	185
	3.2×10^{-1}		Modarresi et al. (2007)	Q	68
	5.6×10^{-1}		Lee (2007)	Q	723
	3.8×10^{-1}		Lee (2007)	Q	724
	8.3×10^{-2}		Dunnivant et al. (1992)	Q	
	7.6		Duchowicz et al. (2020)	?	186, 21
2,2',3,3',4,5,6-heptachlorobiphenyl	7.0×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_3Cl_7$	1.3×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
(PCB-173)	3.3×10^{-2}		Burkhard et al. (1985)	V	
[68194-16-1]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
PAYFWJAKKLILIT-UHFFFAOYSA-N	2.1×10^{-1}		Duchowicz et al. (2020)	Q	
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	3.5×10^{-1}		Modarresi et al. (2007)	Q	68
	3.1×10^{-1}		Lee (2007)	Q	723
	5.9×10^{-1}		Lee (2007)	Q	724
	5.4×10^{-2}		Dunnivant et al. (1992)	Q	
	7.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,3',4,5,6'-heptachlorobiphenyl	2.2×10^{-2}	14000	Bamford et al. (2002)	M	
$C_{12}H_3Cl_7$	7.0×10^{-1}		Brunner et al. (1990)	M	
(PCB-174)	2.0×10^{-1}		Murphy et al. (1987)	M	12
[38411-25-5]	5.4×10^{-3}	6700	Paasivirta and Sinkkonen (2009)	V	
ZDLMBNHYTPHDLF-UHFFFAOYSA-N	1.3×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	300
	2.6×10^{-1}		Hilal et al. (2008)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.3×10^{-1}		Modarresi et al. (2007)	Q	68
	3.1×10^{-1}		Lee (2007)	Q	723
	4.3×10^{-1}		Lee (2007)	Q	724
	5.8×10^{-2}		Dunnivant et al. (1992)	Q	
	7.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,3',4,5',6- heptachlorobiphenyl	1.0×10^{-2}	7200	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_3Cl_7$	2.0×10^{-2}		Burkhard et al. (1985)	V	
(PCB-175)	3.4×10^{-1}		Lee (2007)	Q	723
[40186-70-7]	3.0×10^{-1}		Lee (2007)	Q	724
KJBDZJFSYQUNJT-UHFFFAOYSA-N	4.4×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,3',4,6,6'- heptachlorobiphenyl	1.1×10^{-1}		Murphy et al. (1987)	M	12
$C_{12}H_3Cl_7$	8.5×10^{-3}	7200	Paasivirta and Sinkkonen (2009)	V	
(PCB-176)	1.0×10^{-2}		Burkhard et al. (1985)	V	
[52663-65-7]	1.9×10^{-1}		Lee (2007)	Q	723
HGMYRFJAJNYBRX-UHFFFAOYSA-N	2.6×10^{-1}		Lee (2007)	Q	724
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,3',4,5',6'- heptachlorobiphenyl	2.1×10^{-2}	13000	Bamford et al. (2002)	M	
$C_{12}H_3Cl_7$	3.0×10^{-1}		Murphy et al. (1987)	M	12
(PCB-177)	4.5×10^{-3}		Murphy et al. (1983a)	M	24
[52663-70-4]	3.4×10^{-3}	6600	Paasivirta and Sinkkonen (2009)	V	
CXOYNJAHPUASHN-UHFFFAOYSA-N	3.8×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Lee (2007)	Q	723
	5.3×10^{-1}		Lee (2007)	Q	724
	6.0×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,3',5,5',6- heptachlorobiphenyl	1.5×10^{-2}	11000	Bamford et al. (2002)	M	
$C_{12}H_3Cl_7$	4.3×10^{-1}		Brunner et al. (1990)	M	
(PCB-178)	1.5×10^{-1}		Murphy et al. (1987)	M	12
[52663-67-9]	1.0×10^{-2}	7200	Paasivirta and Sinkkonen (2009)	V	
WCIBKXHMIXUQHK-UHFFFAOYSA-N	2.3×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.2×10^{-1}		Duchowicz et al. (2020)	Q	185
	2.7×10^{-1}		Hilal et al. (2008)	Q	
	3.0×10^{-1}		Modarresi et al. (2007)	Q	68
	4.8×10^{-1}		Lee (2007)	Q	723
	5.6×10^{-1}		Lee (2007)	Q	724
	4.6×10^{-2}		Dunnivant et al. (1992)	Q	
	4.3×10^{-1}		Duchowicz et al. (2020)	?	186, 21

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',5,6,6'- heptachlorobiphenyl	4.1×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_3Cl_7$	4.2×10^{-3}	7000	Paasivirta and Sinkkonen (2009)	V	
(PCB-179)	1.1×10^{-2}		Burkhard et al. (1985)	V	
[52663-64-6]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
XYHVYEUZLSYHDP-UHFFFAOYSA-N	1.2×10^{-1}		Duchowicz et al. (2020)	Q	300
	3.1×10^{-1}		Hilal et al. (2008)	Q	
	3.1×10^{-1}		Modarresi et al. (2007)	Q	68
	2.6×10^{-1}		Lee (2007)	Q	723
	4.8×10^{-1}		Lee (2007)	Q	724
	3.6×10^{-2}		Dunnivant et al. (1992)	Q	
	4.1×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,4,4',5,5'- heptachlorobiphenyl	1.7×10^{-1}	7300	Li et al. (2003)	L	368
$C_{12}H_3Cl_7$	1.2×10^{-1}	7900	Li et al. (2003)	L	369
(PCB-180)	2.7×10^{-2}	17000	Bamford et al. (2000)	M	
[35065-29-3]	9.9×10^{-1}		Brunner et al. (1990)	M	
WBHQEUPUMONIKF-UHFFFAOYSA-N	3.1×10^{-1}		Murphy et al. (1987)	M	12
	1.5×10^{-2}	6900	Paasivirta and Sinkkonen (2009)	V	
	3.3×10^{-2}		Burkhard et al. (1985)	V	
	2.5×10^{-2}	9000	Paasivirta et al. (1999)	T	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	300
	1.4×10^{-2}		Bhangare et al. (2019)	Q	
	2.1×10^{-1}		Hilal et al. (2008)	Q	
	3.5×10^{-1}		Modarresi et al. (2007)	Q	68
	2.8×10^{-1}		Lee (2007)	Q	723
	3.0×10^{-1}		Lee (2007)	Q	724
	9.2×10^{-2}		Dunnivant et al. (1992)	Q	
	9.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,4,4',5,6-heptachlorobiphenyl	1.2×10^{-2}	7200	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_3Cl_7$	2.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-181)	1.6×10^{-1}		Lee (2007)	Q	723
[74472-47-2]	3.8×10^{-1}		Lee (2007)	Q	724
DJEUXBQAKBLKPO-UHFFFAOYSA-N	4.3×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,4,4',5,6'- heptachlorobiphenyl	1.7×10^{-2}	12000	Bamford et al. (2002)	M	
$C_{12}H_3Cl_7$	1.7×10^{-2}	7200	Paasivirta and Sinkkonen (2009)	V	
(PCB-182)	1.0×10^{-2}		Burkhard et al. (1985)	V	
[60145-23-5]	1.5×10^{-1}		Lee (2007)	Q	723
RXRLRYZUMSYVLS-UHFFFAOYSA-N	2.1×10^{-1}		Lee (2007)	Q	724
	3.8×10^{-2}		Dunnivant et al. (1992)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,4',5',6-heptachlorobiphenyl	1.7×10^{-2}	12000	Bamford et al. (2002)	M	
$C_{12}H_3Cl_7$	1.5×10^{-1}		Murphy et al. (1987)	M	12
(PCB-183)	1.6×10^{-2}		Murphy et al. (1983a)	M	24
[52663-69-1]	2.4×10^{-2}	7400	Paasivirta and Sinkkonen (2009)	V	
KQBFUDNJKCZEDQ-UHFFFAOYSA-N	2.1×10^{-2}		Burkhard et al. (1985)	V	
	1.7×10^{-1}		Lee (2007)	Q	723
	2.5×10^{-1}		Lee (2007)	Q	724
	4.9×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,4,4',6,6'-heptachlorobiphenyl	8.1×10^{-3}	7200	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_3Cl_7$	7.9×10^{-3}		Burkhard et al. (1985)	V	
(PCB-184)	9.4×10^{-2}		Lee (2007)	Q	723
[74472-48-3]	1.3×10^{-1}		Lee (2007)	Q	724
OBIUJJSQKPGKME-UHFFFAOYSA-N	2.2×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,4,5,5',6-heptachlorobiphenyl	6.2×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_3Cl_7$	4.9×10^{-3}	7000	Paasivirta and Sinkkonen (2009)	V	
(PCB-185)	2.2×10^{-2}		Burkhard et al. (1985)	V	
[52712-05-7]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
PYZHTHZEHQHHEN-UHFFFAOYSA-N	1.1×10^{-1}		Duchowicz et al. (2020)	Q	300
	1.5×10^{-1}		Hilal et al. (2008)	Q	
	3.4×10^{-1}		Modarresi et al. (2007)	Q	68
	3.1×10^{-1}		Lee (2007)	Q	723
	4.3×10^{-1}		Lee (2007)	Q	724
	4.6×10^{-2}		Dunnivant et al. (1992)	Q	
	6.2×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,4,5,6,6'-heptachlorobiphenyl	9.6×10^{-4}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_3Cl_7$	1.3×10^{-2}		Burkhard et al. (1985)	V	
(PCB-186)	1.7×10^{-1}		Lee (2007)	Q	723
[74472-49-4]	3.7×10^{-1}		Lee (2007)	Q	724
FGDPOTMRBQHPJK-UHFFFAOYSA-N	2.7×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,4',5,5',6-heptachlorobiphenyl	1.6×10^{-2}	12000	Bamford et al. (2000)	M	
$C_{12}H_3Cl_7$	1.2×10^{-1}		Murphy et al. (1987)	M	12
(PCB-187)	1.3×10^{-2}	7200	Paasivirta and Sinkkonen (2009)	V	
[52663-68-0]	2.4×10^{-2}		Burkhard et al. (1985)	V	
UDMZPLROONOSEF-UHFFFAOYSA-N	2.4×10^{-1}		Lee (2007)	Q	723
	4.3×10^{-1}		Lee (2007)	Q	724
	4.9×10^{-2}		Dunnivant et al. (1992)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4',5,6,6'- heptachlorobiphenyl	8.8×10^{-3}	7500	Bamford et al. (2000)	M	
$C_{12}H_3Cl_7$	4.8×10^{-3}	7100	Paasivirta and Sinkkonen (2009)	V	
(PCB-188)	8.8×10^{-3}		Burkhard et al. (1985)	V	
[74487-85-7]	1.6×10^{-2}		Bhangare et al. (2019)	Q	
MMTJWDQKGUNSDK-UHFFFAOYSA-N	1.3×10^{-1}		Lee (2007)	Q	723
	2.3×10^{-1}		Lee (2007)	Q	724
	2.2×10^{-2}		Dunnivant et al. (1992)	Q	
2,3,3',4,4',5,5'- heptachlorobiphenyl	8.4×10^{-2}		Fang et al. (2006)	M	
$C_{12}H_3Cl_7$	4.1×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
(PCB-189)	1.1×10^{-1}		Burkhard et al. (1985)	V	
[39635-31-9]	3.4×10^{-1}		Lee (2007)	Q	723
XUAWBXBYHDRROL-UHFFFAOYSA-N	3.0×10^{-1}		Lee (2007)	Q	724
	1.5×10^{-1}		Dunnivant et al. (1992)	Q	
2,3,3',4,4',5,6-heptachlorobiphenyl	1.5×10^{-2}	7000	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_3Cl_7$	9.9×10^{-2}		Burkhard et al. (1985)	V	
(PCB-190)	1.9×10^{-1}		Lee (2007)	Q	723
[41411-64-7]	5.3×10^{-1}		Lee (2007)	Q	724
TYEDCFVCFDKSBK-UHFFFAOYSA-N	8.8×10^{-2}		Dunnivant et al. (1992)	Q	
2,3,3',4,4',5',6- heptachlorobiphenyl	2.1×10^{-2}	7200	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_3Cl_7$	5.8×10^{-2}		Burkhard et al. (1985)	V	
(PCB-191)	2.1×10^{-1}		Lee (2007)	Q	723
[74472-50-7]	3.2×10^{-1}		Lee (2007)	Q	724
TVFXBXWAXIMLAQ-UHFFFAOYSA-N	7.4×10^{-2}		Dunnivant et al. (1992)	Q	
2,3,3',4,5,5',6-heptachlorobiphenyl	4.9×10^{-3}	6900	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_3Cl_7$	6.1×10^{-2}		Burkhard et al. (1985)	V	
(PCB-192)	3.8×10^{-1}		Lee (2007)	Q	723
[74472-51-8]	5.0×10^{-1}		Lee (2007)	Q	724
ZUTDUGMNROUBOX-UHFFFAOYSA-N	5.2×10^{-2}		Dunnivant et al. (1992)	Q	
2,3,3',4',5,5',6- heptachlorobiphenyl	3.2×10^{-2}	17000	Bamford et al. (2002)	M	
$C_{12}H_3Cl_7$	7.5×10^{-3}	6800	Paasivirta and Sinkkonen (2009)	V	
(PCB-193)	1.0×10^{-1}		Burkhard et al. (1985)	V	
[69782-91-8]	2.9×10^{-1}		Lee (2007)	Q	723
SSTJUBQGYXNFFP-UHFFFAOYSA-N	5.6×10^{-1}		Lee (2007)	Q	724
	7.3×10^{-2}		Dunnivant et al. (1992)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,4',5,5'- octachlorobiphenyl	1.5×10^{-1}	7500	Li et al. (2003)	L	368
$C_{12}H_2Cl_8$	2.3×10^{-1}	8200	Li et al. (2003)	L	369
(PCB-194)	1.0×10^{-1}	20000	Bamford et al. (2002)	M	
[35694-08-7]	9.9×10^{-1}		Brunner et al. (1990)	M	
DTMRKGRREZAYAP-UHFFFAOYSA-N	8.0×10^{-3}	6900	Paasivirta and Sinkkonen (2009)	V	
	2.1×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	4.0×10^{-1}		Duchowicz et al. (2020)	Q	185
	2.3×10^{-1}		Hilal et al. (2008)	Q	
	4.8×10^{-1}		Modarresi et al. (2007)	Q	68
	5.6×10^{-1}		Lee (2007)	Q	723
	7.1×10^{-1}		Lee (2007)	Q	724
		6500	Kühne et al. (2005)	Q	
	1.5×10^{-1}		Dunnivant et al. (1992)	Q	
	9.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		6600	Kühne et al. (2005)	?	
2,2',3,3',4,4',5,6- octachlorobiphenyl	7.1×10^{-2}	20000	Bamford et al. (2000)	M	
$C_{12}H_2Cl_8$	9.0×10^{-1}		Brunner et al. (1990)	M	
(PCB-195)	7.1×10^{-3}	7100	Paasivirta and Sinkkonen (2009)	V	
[52663-78-2]	7.8×10^{-2}		Burkhard et al. (1985)	V	
JAHJITLFJSDRCG-UHFFFAOYSA-N	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	3.1×10^{-1}		Duchowicz et al. (2020)	Q	300
	2.4×10^{-1}		Hilal et al. (2008)	Q	
	4.5×10^{-1}		Modarresi et al. (2007)	Q	68
	3.1×10^{-1}		Lee (2007)	Q	723
	1.0		Lee (2007)	Q	724
	8.3×10^{-2}		Dunnivant et al. (1992)	Q	
	9.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,3',4,4',5,6'- octachlorobiphenyl	9.9×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_2Cl_8$	1.8×10^{-2}	7400	Paasivirta and Sinkkonen (2009)	V	
(PCB-196)	1.4×10^{-2}		Burkhard et al. (1985)	V	
[42740-50-1]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
BQFCCUSDZLKBJG-UHFFFAOYSA-N	2.4×10^{-1}		Duchowicz et al. (2020)	Q	
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	5.0×10^{-1}		Modarresi et al. (2007)	Q	68
	3.4×10^{-1}		Lee (2007)	Q	723
	6.2×10^{-1}		Lee (2007)	Q	724
	7.6×10^{-2}		Dunnivant et al. (1992)	Q	
	9.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,4',6,6'- octachlorobiphenyl	1.3×10^{-2}	7600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_2Cl_8$	1.1×10^{-2}		Burkhard et al. (1985)	V	
(PCB-197)	1.9×10^{-1}		Lee (2007)	Q	723
[33091-17-7]	4.2×10^{-1}		Lee (2007)	Q	724
YPDBBDKYNWRFMF-UHFFFAOYSA-N	3.9×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,3',4,5,5',6- octachlorobiphenyl	7.0×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_2Cl_8$	3.5×10^{-3}	7000	Paasivirta and Sinkkonen (2009)	V	
(PCB-198)	4.8×10^{-2}		Burkhard et al. (1985)	V	
[68194-17-2]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
PJHBSPRZHUOIAS-UHFFFAOYSA-N	1.7×10^{-1}		Duchowicz et al. (2020)	Q	300
	2.5×10^{-1}		Hilal et al. (2008)	Q	
	4.5×10^{-1}		Modarresi et al. (2007)	Q	68
	6.2×10^{-1}		Lee (2007)	Q	723
	1.0		Lee (2007)	Q	724
	6.4×10^{-2}		Dunnivant et al. (1992)	Q	
	7.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,3',4,5,5',6'- octachlorobiphenyl	9.9×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_2Cl_8$	3.4×10^{-3}	7000	Paasivirta and Sinkkonen (2009)	V	
(PCB-199)	2.3×10^{-2}		Burkhard et al. (1985)	V	
[52663-75-9]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
HJBYDWKNARZTMJ-UHFFFAOYSA-N	2.2×10^{-1}		Duchowicz et al. (2020)	Q	300
	2.7×10^{-1}		Hilal et al. (2008)	Q	
	4.7×10^{-1}		Modarresi et al. (2007)	Q	68
	6.2×10^{-1}		Lee (2007)	Q	723
	9.1×10^{-1}		Lee (2007)	Q	724
	4.3×10^{-2}		Dunnivant et al. (1992)	Q	
	9.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,3',4,5,6,6'- octachlorobiphenyl	7.6×10^{-3}	7200	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_2Cl_8$	1.5×10^{-2}		Burkhard et al. (1985)	V	
(PCB-200)	3.4×10^{-1}		Lee (2007)	Q	723
[52663-73-7]	7.7×10^{-1}		Lee (2007)	Q	724
HHXNVASVVVNNDG-UHFFFAOYSA-N	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,3',4,5',6,6'- octachlorobiphenyl	1.0×10^{-2}	17000	Bamford et al. (2000)	M	
$C_{12}H_2Cl_8$	5.8×10^{-1}		Brunner et al. (1990)	M	
(PCB-201)	1.2×10^{-2}	7500	Paasivirta and Sinkkonen (2009)	V	
[40186-71-8]	1.5×10^{-2}		Burkhard et al. (1985)	V	
LJQOBQLZTUSEJA-UHFFFAOYSA-N	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.3×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.3×10^{-2}		Bhangare et al. (2019)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.9×10^{-1}		Hilal et al. (2008)	Q	
	5.1×10^{-1}		Modarresi et al. (2007)	Q	68
	3.7×10^{-1}		Lee (2007)	Q	723
	1.1		Lee (2007)	Q	724
	7.6×10^{-2}		Dunnivant et al. (1992)	Q	
	5.8×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,2',3,3',5,5',6,6'- octachlorobiphenyl	5.5×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_2Cl_8$	5.0×10^{-3}	7300	Paasivirta and Sinkkonen (2009)	V	
(PCB-202)	2.6×10^{-2}		Mackay et al. (2006b)	V	
[2136-99-4]	2.6×10^{-2}		Mackay et al. (1992a)	V	
JPOPEORRMSDUIP-UHFFFAOYSA-N	2.7×10^{-2}		Shiu and Mackay (1986)	V	
	1.3×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.2×10^{-1}		Duchowicz et al. (2020)	Q	
	3.7×10^{-1}		Hilal et al. (2008)	Q	
	5.5×10^{-1}		Modarresi et al. (2007)	Q	68
	5.3×10^{-1}		Lee (2007)	Q	723
	1.4		Lee (2007)	Q	724
		4700	Kühne et al. (2005)	Q	
	4.4×10^{-2}		Dunnivant et al. (1992)	Q	
	5.5×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		5000	Kühne et al. (2005)	?	
2,2',3,4,4',5,5',6- octachlorobiphenyl	3.2×10^{-2}	7800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_2Cl_8$	5.0×10^{-2}		Burkhard et al. (1985)	V	
(PCB-203)	1.3×10^{-2}		Bhangare et al. (2019)	Q	
[52663-76-0]	3.1×10^{-1}		Lee (2007)	Q	723
DCPDZFRGNJDWPP-UHFFFAOYSA-N	7.7×10^{-1}		Lee (2007)	Q	724
	7.0×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,4,4',5,6,6'- octachlorobiphenyl	1.1×10^{-2}	7800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_2Cl_8$	1.9×10^{-2}		Burkhard et al. (1985)	V	
(PCB-204)	1.3×10^{-2}		Bhangare et al. (2019)	Q	
[74472-52-9]	1.7×10^{-1}		Lee (2007)	Q	723
JDZUWXRNKHXZFE-UHFFFAOYSA-N	4.5×10^{-1}		Lee (2007)	Q	724
	2.9×10^{-2}		Dunnivant et al. (1992)	Q	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',4,4',5,5',6- octachlorobiphenyl	4.4×10^{-3}	6800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_2Cl_8$	2.1×10^{-1}		Burkhard et al. (1985)	V	
(PCB-205)	1.2×10^{-2}		Bhangare et al. (2019)	Q	
[74472-53-0]	3.8×10^{-1}		Lee (2007)	Q	723
VXXBCDUYUQKWCK-UHFFFAOYSA-N	9.1×10^{-1}		Lee (2007)	Q	724
	1.1×10^{-1}		Dunnivant et al. (1992)	Q	
2,2',3,3',4,4',5,5',6- nonachlorobiphenyl	2.1×10^{-3}	7300	Paasivirta and Sinkkonen (2009)	V	
$C_{12}HCl_9$	1.2		Mackay et al. (2006b)	V	
(PCB-206)	1.2×10^{-2}		Mackay et al. (1992a)	V	
[40186-72-9]	3.6×10^{-2}		Burkhard et al. (1985)	V	
JFIMDKGRGPNPRQ-UHFFFAOYSA-N	1.1×10^{-2}		Bhangare et al. (2019)	Q	
	6.2×10^{-1}		Lee (2007)	Q	723
	2.0		Lee (2007)	Q	724
	1.1×10^{-1}		Dunnivant et al. (1992)	Q	
2,2',3,3',4,4',5,6,6'- nonachlorobiphenyl	1.8×10^{-3}	7500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}HCl_9$	2.8×10^{-2}		Burkhard et al. (1985)	V	
(PCB-207)	1.1×10^{-2}		Bhangare et al. (2019)	Q	
[52663-79-3]	3.3×10^{-1}		Lee (2007)	Q	723
YGDPIDTZOQGPAX-UHFFFAOYSA-N	1.4		Lee (2007)	Q	724
	5.8×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,3',4,5,5',6,6'- nonachlorobiphenyl	3.0×10^{-3}	7700	Paasivirta and Sinkkonen (2009)	V	
$C_{12}HCl_9$	3.1×10^{-2}		Burkhard et al. (1985)	V	
(PCB-208)	1.2×10^{-2}		Bhangare et al. (2019)	Q	
[52663-77-1]	6.7×10^{-1}		Lee (2007)	Q	723
XIFFTDRFWYFAPO-UHFFFAOYSA-N	2.5		Lee (2007)	Q	724
	5.9×10^{-2}		Dunnivant et al. (1992)	Q	
decachlorobiphenyl	1.0×10^{-3}		Duchowicz et al. (2020)	V	187
$C_{12}Cl_{10}$	6.7×10^{-4}	7200	Paasivirta and Sinkkonen (2009)	V	
(PCB-209)			Mackay et al. (2006b)	V	685
[2051-24-3]	4.8×10^{-2}		Mackay et al. (1992a)	V	
ONXPZLFXDMAPRO-UHFFFAOYSA-N	4.8×10^{-2}		Shiu and Mackay (1986)	V	
	8.0×10^{-2}		Burkhard et al. (1985)	V	
	2.6×10^{-1}		Duchowicz et al. (2020)	Q	
	1.0×10^{-2}		Bhangare et al. (2019)	Q	
	3.1×10^{-1}		Hilal et al. (2008)	Q	
	6.7×10^{-1}		Lee (2007)	Q	723
	5.0		Lee (2007)	Q	724
		6100	Kühne et al. (2005)	Q	
	8.8×10^{-2}		Dunnivant et al. (1992)	Q	
		7300	Kühne et al. (2005)	?	

Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note

A6.4 Oxygenated chlorocarbons (C, H, O, Cl)

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
phosgene	5.9×10^{-4}	3800	De Bruyn et al. (1995a)	M	
CCl_2O	6.8×10^{-4}	4200	Manogue and Pigford (1960)	M	
[75-44-5]	7.0×10^{-4}		Yaws (2003)	X	238
YGYAWVDWMABLBF-UHFFFAOYSA-N	5.3×10^{-4}		Hayer et al. (2022)	Q	20
	8.8×10^{-3}		Keshavarz et al. (2022)	Q	
	6.1×10^{-2}		Duchowicz et al. (2020)	Q	
	3.7×10^{-1}		Wang et al. (2017)	Q	81, 239
	1.4×10^{-2}		Wang et al. (2017)	Q	81, 240
	1.1×10^{-4}		Wang et al. (2017)	Q	81, 241
	6.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
	5.9×10^{-4}		Duchowicz et al. (2020)	?	186, 21
	7.1×10^{-4}		Yaws (1999)	?	21
MCM:CCL3OOH	2.1×10^{1}		Wang et al. (2017)	Q	81, 239
CHO_2Cl_3	4.9		Wang et al. (2017)	Q	81, 240
DUBMHDTUZCIGCY-UHFFFAOYSA-N	3.8		Wang et al. (2017)	Q	81, 241
MCM:CH2CLOOH	1.8×10^{1}		Wang et al. (2017)	Q	81, 239
CH_3O_2Cl	6.2×10^{1}		Wang et al. (2017)	Q	81, 240
DUNYOPWYTOSXOC-UHFFFAOYSA-N	1.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CHCL2OOH	4.7×10^{1}		Wang et al. (2017)	Q	81, 239
$CH_2O_2Cl_2$	1.3×10^{2}		Wang et al. (2017)	Q	81, 240
TUIYYMKEIGYDJB-UHFFFAOYSA-N	5.6		Wang et al. (2017)	Q	81, 241
MCM:CCL3OH	4.7		Wang et al. (2017)	Q	81, 239
$CHOCl_3$	8.1×10^{-1}		Wang et al. (2017)	Q	81, 240
GYLIOGDFGLKMOL-UHFFFAOYSA-N	4.0×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CH2CLOH	1.9		Wang et al. (2017)	Q	81, 239
CH_3OCl	1.9×10^{1}		Wang et al. (2017)	Q	81, 240
BCUPGIHTCQJCSI-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CHCL2OH	6.6		Wang et al. (2017)	Q	81, 239
CH_2OCl_2	1.2×10^{1}		Wang et al. (2017)	Q	81, 240
GJYVZUKSNFSLCL-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CHOCL	2.2×10^{-1}		Wang et al. (2017)	Q	81, 239
CHOCl	2.0×10^{-2}		Wang et al. (2017)	Q	81, 240
GFAUNYMRSKVDJL-UHFFFAOYSA-N	3.0×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:CLCO2H	3.2×10^{1}		Wang et al. (2017)	Q	81, 239
CHO_2Cl	8.5		Wang et al. (2017)	Q	81, 240
AOGYCOYQMAVAFD-UHFFFAOYSA-N	9.1×10^{1}		Wang et al. (2017)	Q	81, 241

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dichloroacetaldehyde	4.7×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_2H_2Cl_2O$	7.4×10^{-1}		Wang et al. (2017)	Q	81, 240
[79-02-7]	1.1×10^{-2}		Wang et al. (2017)	Q	81, 241
NWQWQKUXRJYXFH-UHFFFAOYSA-N	1.2		HSDB (2015)	Q	100
chloroacetyl chloride	2.9×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_2H_2Cl_2O$	1.3×10^{-1}		Wang et al. (2017)	Q	81, 240
[79-04-9]	4.3×10^{-2}		Wang et al. (2017)	Q	81, 241
VGCXGMAHQTYDJK-UHFFFAOYSA-N	4.3×10^{-2}		HSDB (2015)	Q	100
chloral hydrate $C_2H_3Cl_3O_2$ [302-17-0] RNFNDJAIBTYOQL-UHFFFAOYSA-N	2.4×10^{3}		HSDB (2015)	V	
chloroacetaldehyde	1.9×10^{-1}		Wang et al. (2017)	Q	81, 239
C_2H_3ClO	2.3		Wang et al. (2017)	Q	81, 240
[107-20-0]	3.5		Wang et al. (2017)	Q	81, 241
QSKPIOLLBIHNAC-UHFFFAOYSA-N	4.1×10^{-1}		HSDB (2015)	Q	100
2-chloroethanol	1.3×10^{1}		Duchowicz et al. (2020)	V	187
C_2H_5ClO	3.3		Duchowicz et al. (2020)	Q	
[107-07-3]	1.1		Wang et al. (2017)	Q	81, 239
SZIFAVKTNFCBPC-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	81, 240
	4.7		Wang et al. (2017)	Q	81, 241
	9.5×10^{1}		HSDB (2015)	Q	100
	2.8×10^{1}		Modarresi et al. (2007)	Q	68
	1.4×10^{1}		Yaffe et al. (2003)	Q	249, 250
	1.7×10^{1}		Katritzky et al. (1998)	Q	
2,2-dichloroethanol	3.7×10^{-1}		Burkholder et al. (2019)	L	
$C_2H_4Cl_2O$	3.7×10^{-1}		Burkholder et al. (2015)	L	
[598-38-9]	3.7×10^{-1}		O'Farrell and Waghorne (2010)	M	
IDJOCJAIQSKSOP-UHFFFAOYSA-N	3.2		Wang et al. (2017)	Q	81, 239
	2.6×10^{1}		Wang et al. (2017)	Q	81, 240
	6.9		Wang et al. (2017)	Q	81, 241
2-chloroethanol-d4 ClC_2D_4OH [117067-62-6] SZIFAVKTNFCBPC-LNLMKGTHSA-N	5.0	8700	Hiatt (2013)	M	
MCM:CCL2CL2OOH	3.9×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_2O_2Cl_4$	7.1×10^{1}		Wang et al. (2017)	Q	81, 240
SWNDCAXLXSSRFN-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CCL3CH2OOH	1.7×10^{1}		Wang et al. (2017)	Q	81, 239
$C_2H_3O_2Cl_3$	1.8×10^{1}		Wang et al. (2017)	Q	81, 240
RJIYMCLTECJZCN-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	81, 241

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CCL3CO3H	2.6×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2HO_3Cl_3$	5.9		Wang et al. (2017)	Q	81, 240
DRTNVNKYVPOWCY-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	81, 241
MCM:CH2CL3OOH	1.2×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_3O_2Cl_3$	3.8×10^{1}		Wang et al. (2017)	Q	81, 240
CHVIFDTZRLKJET-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CH2CLCOOH	1.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_2H_5O_2Cl$	6.3×10^{1}		Wang et al. (2017)	Q	81, 240
PIXGNJBYAUTOCI-UHFFFAOYSA-N	5.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CH3CCL2OOH	1.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_2H_4O_2Cl_2$	1.0×10^{1}		Wang et al. (2017)	Q	81, 240
YUVMNUKOYYKKNS-UHFFFAOYSA-N	8.9		Wang et al. (2017)	Q	81, 241
MCM:CH3CHCLOOH	1.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_2H_5O_2Cl$	2.0×10^{1}		Wang et al. (2017)	Q	81, 240
MCYQTMMYWIXRIL-UHFFFAOYSA-N	5.6		Wang et al. (2017)	Q	81, 241
MCM:CHCL2CO3H	5.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_2O_3Cl_2$	4.3×10^{1}		Wang et al. (2017)	Q	81, 240
VWNSYHZUZUFFDM-UHFFFAOYSA-N	8.9		Wang et al. (2017)	Q	81, 241
MCM:CHCL2COOH	3.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_2H_4O_2Cl_2$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
GJBKLBBJOKITMY-UHFFFAOYSA-N	2.7×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CHCL3OOH	4.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_3O_2Cl_3$	1.2×10^{2}		Wang et al. (2017)	Q	81, 240
AMASFZACKVPSTN-UHFFFAOYSA-N	4.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CLETO3H	2.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_3O_3Cl$	5.5×10^{1}		Wang et al. (2017)	Q	81, 240
JSQPGNJFQUOEPA-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DICLETO2H	1.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_4O_2Cl_2$	7.3×10^{1}		Wang et al. (2017)	Q	81, 240
UPXDMONURWDHKL-UHFFFAOYSA-N	4.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:C2CL2OH2	1.4×10^{5}		Wang et al. (2017)	Q	81, 239
$C_2H_4O_2Cl_2$	1.3×10^{4}		Wang et al. (2017)	Q	81, 240
HHQQTVXFKGIICR-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:C2CL2OHOOH	2.8×10^{6}		Wang et al. (2017)	Q	81, 239
$C_2H_4O_3Cl_2$	1.7×10^{4}		Wang et al. (2017)	Q	81, 240
NCBKAYIJWMIXBU-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:C2CL32OH	1.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_2H_3O_2Cl_3$	5.1×10^{3}		Wang et al. (2017)	Q	81, 240
MYDJEUINZIFHKK-UHFFFAOYSA-N	2.8×10^{7}		Wang et al. (2017)	Q	81, 241

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C2CL3HOOOH	3.1×10^{6}		Wang et al. (2017)	Q	81, 239
$C_2H_3O_3Cl_3$	1.0×10^{4}		Wang et al. (2017)	Q	81, 240
KHLAQOPQQHOMKQ-UHFFFAOYSA-N	4.3×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:C2CL3OHOOH	2.6×10^{6}		Wang et al. (2017)	Q	81, 239
$C_2H_3O_3Cl_3$	1.1×10^{4}		Wang et al. (2017)	Q	81, 240
CEKNFZNLLTXCLL-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	81, 241
trichloroethanol	1.7		Wang et al. (2017)	Q	81, 239
$C_2H_3OCl_3$	3.9		Wang et al. (2017)	Q	81, 240
[115-20-8]	3.2		Wang et al. (2017)	Q	81, 241
KPWDGTGXUYRARH-UHFFFAOYSA-N					
MCM:CCLOHCOOH	1.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_2H_5O_3Cl$	9.6×10^{3}		Wang et al. (2017)	Q	81, 240
MIFGQALJBIDZDW-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	81, 241
MCM:CH2CL3OH	2.9×10^{1}		Wang et al. (2017)	Q	81, 239
$C_2H_3OCl_3$	1.3×10^{1}		Wang et al. (2017)	Q	81, 240
HYCHPIPDVAXCCJ-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CH2OHCCLOH	4.2×10^{3}		Wang et al. (2017)	Q	81, 239
$C_2H_5O_2Cl$	4.2×10^{3}		Wang et al. (2017)	Q	81, 240
VVKFXODVPQSIHU-UHFFFAOYSA-N	9.3×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CH3CCL2OH	1.6		Wang et al. (2017)	Q	81, 239
$C_2H_4OCl_2$	2.4		Wang et al. (2017)	Q	81, 240
DNBABSPIEDTPHK-UHFFFAOYSA-N	8.1		Wang et al. (2017)	Q	81, 241
MCM:CH3CHCLOH	1.8		Wang et al. (2017)	Q	81, 239
C_2H_5OCl	8.1		Wang et al. (2017)	Q	81, 240
KJESGYZFVCIMDE-UHFFFAOYSA-N	4.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CHCL2CL2OH	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_2OCl_4$	2.2×10^{1}		Wang et al. (2017)	Q	81, 240
LQINPQOSBLVJBS-UHFFFAOYSA-N	3.7×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CHCL3OH	9.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_2H_3OCl_3$	5.6×10^{1}		Wang et al. (2017)	Q	81, 240
NIBKDWIGIKUFKL-UHFFFAOYSA-N	3.4×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CL2OHCH2OH	4.5×10^{3}		Wang et al. (2017)	Q	81, 239
$C_2H_4O_2Cl_2$	1.6×10^{3}		Wang et al. (2017)	Q	81, 240
ZOZPDNLNQWCVSW-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:CL2OHCO3H	9.3×10^{4}		Wang et al. (2017)	Q	81, 239
$C_2H_2O_4Cl_2$	4.7		Wang et al. (2017)	Q	81, 240
MACSTFWYVGNISK-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	81, 241
MCM:CL2OHOOH	1.7×10^{5}		Wang et al. (2017)	Q	81, 239
$C_2H_4O_3Cl_2$	4.0×10^{3}		Wang et al. (2017)	Q	81, 240
WOJAYLCSWSBEJV-UHFFFAOYSA-N	4.1×10^{5}		Wang et al. (2017)	Q	81, 241

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CLOHCO3H	1.0×10^{5}		Wang et al. (2017)	Q	81, 239
$C_2H_3O_4Cl$	2.5×10^{2}		Wang et al. (2017)	Q	81, 240
IODLIDNNOHQSDW-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:COHCCLOOH	1.2×10^{5}		Wang et al. (2017)	Q	81, 239
$C_2H_5O_3Cl$	5.0×10^{3}		Wang et al. (2017)	Q	81, 240
WXPZQCJQULOKCY-UHFFFAOYSA-N	4.4×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:DICLETOH	2.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_2H_4OCl_2$	3.8×10^{1}		Wang et al. (2017)	Q	81, 240
QXBDFCZHAAOUBY-UHFFFAOYSA-N	3.1×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:TCE2OH	2.9×10^{5}		Wang et al. (2017)	Q	81, 239
$C_2H_2O_2Cl_4$	2.0×10^{3}		Wang et al. (2017)	Q	81, 240
BVBMRJKFECUARX-UHFFFAOYSA-N	4.2×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:TCEOHOOH	3.4×10^{6}		Wang et al. (2017)	Q	81, 239
$C_2H_2O_3Cl_4$	4.3×10^{3}		Wang et al. (2017)	Q	81, 240
YKIXQGIQZGTABG-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	81, 241
MCM:CCLOHCHO	8.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_2H_3O_2Cl$	8.9×10^{1}		Wang et al. (2017)	Q	81, 240
RYRGLFUQPWFXSD-UHFFFAOYSA-N	4.4		Wang et al. (2017)	Q	81, 241
MCM:CL2OHCHO	7.6×10^{1}		Wang et al. (2017)	Q	81, 239
$C_2H_2O_2Cl_2$	1.0		Wang et al. (2017)	Q	81, 240
LCOUNIIIIIWZOM-UHFFFAOYSA-N	6.0×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:CH3COCL	1.5×10^{-1}		Wang et al. (2017)	Q	81, 239
C_2H_3OCl	2.6×10^{-2}		Wang et al. (2017)	Q	81, 240
WETWJCDKMRHUPV-UHFFFAOYSA-N	8.7×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:CHCL2COCL	6.8×10^{-1}		Wang et al. (2017)	Q	81, 239
C_2HOCl_3	6.6×10^{-2}		Wang et al. (2017)	Q	81, 240
FBCCMZVIWNDFMO-UHFFFAOYSA-N	3.6×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:CLCOCH2OOH	1.1×10^{4}		Wang et al. (2017)	Q	81, 239
$C_2H_3O_3Cl$	2.1×10^{2}		Wang et al. (2017)	Q	81, 240
ARKKUYXZQNWAAF-UHFFFAOYSA-N	8.0		Wang et al. (2017)	Q	81, 241
MCM:CLCOCL2OOH	1.6×10^{4}		Wang et al. (2017)	Q	81, 239
$C_2HO_3Cl_3$	3.1×10^{1}		Wang et al. (2017)	Q	81, 240
FXUYMCPKRPYDCU-UHFFFAOYSA-N	2.1		Wang et al. (2017)	Q	81, 241
MCM:CLCOCLOOH	2.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_2H_2O_3Cl_2$	3.9×10^{2}		Wang et al. (2017)	Q	81, 240
WROSSTYSMNZXTC-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CLGLYOX	2.2×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2O_2Cl_2$	1.3×10^{-1}		Wang et al. (2017)	Q	81, 240
CTSLXHKWHWQRSH-UHFFFAOYSA-N	3.6×10^{-4}		Wang et al. (2017)	Q	81, 241

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CCL2OHCOCL	1.3×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2HO_2Cl_3$	1.2		Wang et al. (2017)	Q	81, 240
WBBOIYQGQVKNEO-UHFFFAOYSA-N	1.7×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:CCLOHCOCL	1.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_2O_2Cl_2$	5.6×10^{1}		Wang et al. (2017)	Q	81, 240
NABBVDLPPITPRF-UHFFFAOYSA-N	3.5		Wang et al. (2017)	Q	81, 241
MCM:CH2OHCOCL	2.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_2H_3O_2Cl$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
LCIMJULVQOQTEZ-UHFFFAOYSA-N	4.2×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CL1GLYOX	1.4×10^{2}		Wang et al. (2017)	Q	81, 239
C_2HO_2Cl	1.5		Wang et al. (2017)	Q	81, 240
ZNBGBHISQKMEPA-UHFFFAOYSA-N	4.2×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:CLOHCO2H	8.5×10^{4}		Wang et al. (2017)	Q	81, 239
$C_2H_3O_3Cl$	3.6×10^{4}		Wang et al. (2017)	Q	81, 240
SORBEIKZIPTJRS-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	81, 241
1,1,1-trichloro-2-propanone $C_3H_3Cl_3O$ [918-00-3] SMZHKGXSEAGRTI-UHFFFAOYSA-N	4.5		HSDB (2015)	Q	100
1,1-dichloro-2-propanone	3.3×10^{-1}		Burkholder et al. (2019)	L	
$C_3H_4Cl_2O$	3.3×10^{-1}		Burkholder et al. (2015)	L	
(1,1-dichloroacetone)	3.3×10^{-1}		O'Farrell and Waghorne (2010)	M	
[513-88-2]	1.6		HSDB (2015)	Q	100
CSVFWMMPUJDVKH-UHFFFAOYSA-N					
carbonochloridic acid, 2-chloroethyl ester $C_3H_4Cl_2O_2$ (chloroethyl chloroformate) [627-11-2] SVDDJQGVOFZBNX-UHFFFAOYSA-N	9.0×10^{-3}		HSDB (2015)	Q	100
carbonochloridic acid, ethyl ester $C_3H_5ClO_2$ (ethyl chloroformate) [541-41-3] RIFGWPKJUGCATF-UHFFFAOYSA-N	3.2×10^{-3}		HSDB (2015)	Q	100
2-chloropropanoic acid $C_3H_5ClO_2$ [598-78-7] GAWAYYRQGQZKCR-UHFFFAOYSA-N	3.8×10^{1}		HSDB (2015)	Q	100

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-dichloro-1-propanol	7.8		Wang et al. (2017)	Q	81, 239
$C_3H_6Cl_2O$	6.9×10^{1}		Wang et al. (2017)	Q	81, 240
[616-23-9]	1.3×10^{1}		Wang et al. (2017)	Q	81, 241
ZXCYIJGIGSDJQQ-UHFFFAOYSA-N	3.3×10^{3}		HSDB (2015)	Q	100
1,3-dichloro-2-propanol	5.8		Meylan and Howard (1991)	V	
$C_3H_6Cl_2O$	1.6×10^{1}		HSDB (2015)	Q	100
[96-23-1]	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	272, 244
DEWLEGDTCGBNGU-UHFFFAOYSA-N	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	246
	2.6×10^{1}		Hilal et al. (2008)	Q	
	3.0×10^{1}		Modarresi et al. (2007)	Q	68
	1.7×10^{1}		Meylan and Howard (1991)	Q	
3-chloro-1,2-propanediol $C_3H_7ClO_2$ [96-24-2] SSZWWUDQMAHNAQ-UHFFFAOYSA-N	1.6×10^{2}		HSDB (2015)	Q	100
1-chloro-2-propanol C_3H_7ClO [127-00-4] YYTSGNJTASLUOY-UHFFFAOYSA-N	5.8		HSDB (2015)	Q	100
2-chloro-1-propanol C_3H_7ClO [78-89-7] VZIQXGLTRZLBEX-UHFFFAOYSA-N	5.8		HSDB (2015)	Q	100
3-chloro-1-propanol C_3H_7ClO [627-30-5] LAMUXTNQCICZQX-UHFFFAOYSA-N	1.3×10^{1}		Ebert et al. (2023)	?	317
trichloroethanal	3.4×10^{3}	3500	Burkholder et al. (2019)	L	462
CCl_3CHO	3.4×10^{3}	3500	Burkholder et al. (2015)	L	462
(trichloroacetaldehyde; chloral)	3.4×10^{3}	3500	Betterton and Hoffmann (1988)	M	462
[75-87-6]	2.2×10^{3}		Keshavarz et al. (2022)	Q	
HFFLGKNGCAIQMO-UHFFFAOYSA-N	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
	2.1×10^{-1}		Wang et al. (2017)	Q	81, 239
	1.6×10^{-2}		Wang et al. (2017)	Q	81, 240
	3.2×10^{-3}		Wang et al. (2017)	Q	81, 241
	1.2×10^{3}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{2}		Raventos-Duran et al. (2010)	Q	245
	3.1		Raventos-Duran et al. (2010)	Q	246
		1700	Kühne et al. (2005)	Q	
	1.7×10^{3}		Meylan and Howard (1991)	Q	
	3.4×10^{3}		Duchowicz et al. (2020)	?	186, 21
		3500	Kühne et al. (2005)	?	

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chloro-2-propanone	5.8×10^{-1}	5400	Burkholder et al. (2019)	L	
$CH_2ClCOCH_3$	5.8×10^{-1}	5400	Burkholder et al. (2015)	L	
(chloroacetone)	5.8×10^{-1}	5400	Sander et al. (2011)	L	
[78-95-5]	5.8×10^{-1}	5400	Betterton (1991)	M	
BULLHNJGPPOUOX-UHFFFAOYSA-N	1.2×10^{-1}		Keshavarz et al. (2022)	Q	
	8.8×10^{-2}		Duchowicz et al. (2020)	Q	300
	1.3×10^{-1}		Wang et al. (2017)	Q	81, 239
	2.0		Wang et al. (2017)	Q	81, 240
	1.2		Wang et al. (2017)	Q	81, 241
	1.6		Raventos-Duran et al. (2010)	Q	272, 244
	1.2		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	246
	8.8×10^{-1}		Hilal et al. (2008)	Q	
	6.8×10^{-1}		Modarresi et al. (2007)	Q	68
		4400	Kühne et al. (2005)	Q	
	6.0×10^{-1}		Duchowicz et al. (2020)	?	186, 21
		5500	Kühne et al. (2005)	?	
chloroethanoic acid	1.1×10^{3}	9700	Burkholder et al. (2019)	L	
$CH_2ClCOOH$	1.1×10^{3}	9700	Burkholder et al. (2015)	L	
(chloroacetic acid)	1.1×10^{3}	9700	Sander et al. (2011)	L	
[79-11-8]	1.1×10^{3}	9700	Bowden et al. (1998a)	M	
FOCAUTSVDIKZOP-UHFFFAOYSA-N	1.1×10^{3}		Keshavarz et al. (2022)	Q	
	1.3×10^{2}		Duchowicz et al. (2020)	Q	
	2.0×10^{2}		Wang et al. (2017)	Q	81, 239
	3.6×10^{3}		Wang et al. (2017)	Q	81, 240
	1.1×10^{3}		Wang et al. (2017)	Q	81, 241
	1.2×10^{3}		Raventos-Duran et al. (2010)	Q	272, 244
	1.6×10^{3}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	246
	8.8×10^{2}		Hilal et al. (2008)	Q	
	3.1×10^{2}		Modarresi et al. (2007)	Q	68
		8100	Kühne et al. (2005)	Q	
	1.1×10^{3}		Duchowicz et al. (2020)	?	186, 21
		9400	Kühne et al. (2005)	?	
dichloroethanoic acid	1.2×10^{3}	8000	Burkholder et al. (2019)	L	
$CHCl_2COOH$	1.2×10^{3}	8000	Burkholder et al. (2015)	L	
(dichloroacetic acid)	1.2×10^{3}	8000	Sander et al. (2011)	L	
[79-43-6]	1.2×10^{3}	8000	Bowden et al. (1998a)	M	
JXTHNDFMNIQAHM-UHFFFAOYSA-N	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	3.9×10^{2}		Duchowicz et al. (2020)	Q	300
	6.6×10^{2}		Wang et al. (2017)	Q	81, 239
	1.4×10^{3}		Wang et al. (2017)	Q	81, 240
	3.8×10^{2}		Wang et al. (2017)	Q	81, 241
	2.5×10^{3}		Raventos-Duran et al. (2010)	Q	272, 244
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	245

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	246
	3.9×10^{2}		Hilal et al. (2008)	Q	
	8.5×10^{2}		Modarresi et al. (2007)	Q	68
		8400	Kühne et al. (2005)	Q	
	2.6×10^{1}		Katritzky et al. (1998)	Q	
	1.2×10^{3}		Duchowicz et al. (2020)	?	186, 21
		8000	Kühne et al. (2005)	?	
trichloroethanoic acid	7.3×10^{2}	8700	Burkholder et al. (2019)	L	
CCl_3COOH	7.3×10^{2}	8700	Burkholder et al. (2015)	L	
(trichloroacetic acid)	7.3×10^{2}	8700	Sander et al. (2011)	L	
[76-03-9]	7.3×10^{2}	8700	Bowden et al. (1998b)	M	
YNJBWRMUSHSURL-UHFFFAOYSA-N	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	2.3×10^{2}		Duchowicz et al. (2020)	Q	
	9.9×10^{2}		Raventos-Duran et al. (2010)	Q	272, 244
	3.9		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{2}		Raventos-Duran et al. (2010)	Q	246
	4.7		Hilal et al. (2008)	Q	
	7.6×10^{2}		Modarresi et al. (2007)	Q	68
		8800	Kühne et al. (2005)	Q	
	7.3×10^{2}		Duchowicz et al. (2020)	?	186, 21
		8600	Kühne et al. (2005)	?	
2,2-dichloro-propanoic acid	1.7×10^{2}		Duchowicz et al. (2020)	V	187
$C_3H_4Cl_2O_2$	3.5×10^{8}		Mackay et al. (2006d)	V	
[75-99-0]	1.8×10^{2}		Duchowicz et al. (2020)	Q	
NDUPDOJHUQKPAG-UHFFFAOYSA-N					
trichloroacetylchloride	2.0×10^{-2}		Mirabel et al. (1996)	M	
CCl_3COCl	2.0×10^{-2}		De Bruyn et al. (1995a)	M	451
[76-02-8]	2.0×10^{-2}		George et al. (1994a)	M	
PVFOMCVHYWHZJE-UHFFFAOYSA-N	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	7.3×10^{-2}		Duchowicz et al. (2020)	Q	185
	3.4×10^{-1}		HSDB (2015)	Q	100
	1.9×10^{-2}		Duchowicz et al. (2020)	?	186, 21
hexachloroacetone	1.0×10^{2}		Zhang et al. (2010)	Q	288, 289
C_3Cl_6O	9.0×10^{-4}		Zhang et al. (2010)	Q	288, 290
[116-16-5]	6.2×10^{-2}		Zhang et al. (2010)	Q	288, 291
DOJXGHGHTWFZHK-UHFFFAOYSA-N	1.8×10^{-1}		Zhang et al. (2010)	Q	288, 292
(chloromethyl)-oxirane	2.9×10^{-1}		Welke et al. (1998)	M	
C_3H_5ClO	3.2×10^{-1}		Duchowicz et al. (2020)	V	187
(epichlorohydrin)	3.3×10^{-1}		HSDB (2015)	V	
[106-89-8]	3.0×10^{-1}		Mackay et al. (2006c)	V	
BRLQWZUYTZBJKN-UHFFFAOYSA-N	3.0×10^{-1}		Mackay et al. (1993)	V	
	2.8×10^{-1}		Goldstein (1982)	X	448
	2.8×10^{-1}	3700	Goldstein (1982)	X	299

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
	9.9×10^{-2}		Hilal et al. (2008)	Q	
	1.7×10^{-1}		Modarresi et al. (2007)	Q	68
methyl chloroethanoate	4.9×10^{-1}	5600	Brockbank (2013)	L	1
$C_3H_5ClO_2$	4.2×10^{-1}		Duchowicz et al. (2020)	V	187
[96-34-4]	4.1×10^{-2}		HSDB (2015)	V	
QABLOFMHHSOFRJ-UHFFFAOYSA-N	3.3×10^{-1}		Duchowicz et al. (2020)	Q	
	2.3×10^{-1}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	68
MCM:CL12CO3H	1.6×10^{3}		Wang et al. (2017)	Q	81, 239
$C_3H_4O_3Cl_2$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
VMJCNPRTZBGZGF-UHFFFAOYSA-N	2.3		Wang et al. (2017)	Q	81, 241
MCM:CL12PRAOOH	1.0×10^{2}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_2Cl_2$	2.5×10^{2}		Wang et al. (2017)	Q	81, 240
WGVINOMLJVZPKZ-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CL12PRBOOH	7.1×10^{1}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_2Cl_2$	1.8×10^{1}		Wang et al. (2017)	Q	81, 240
OMIMXWULHYQJIC-UHFFFAOYSA-N	9.3		Wang et al. (2017)	Q	81, 241
MCM:CL12PRCOOH	1.2×10^{2}		Wang et al. (2017)	Q	81, 239
$C_3H_6O_2Cl_2$	3.8×10^{1}		Wang et al. (2017)	Q	81, 240
ULSSYZYIMOSSQB-UHFFFAOYSA-N	3.8×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CL12PRBOH	1.4×10^{1}		Wang et al. (2017)	Q	81, 239
$C_3H_6OCl_2$	1.5×10^{1}		Wang et al. (2017)	Q	81, 240
QEZDCTNHTRSNMD-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CL12PRCOH	2.3×10^{1}		Wang et al. (2017)	Q	81, 239
$C_3H_6OCl_2$	1.8×10^{1}		Wang et al. (2017)	Q	81, 240
FLTSEOGWHPJWRV-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:CL12PRCHO	1.3		Wang et al. (2017)	Q	81, 239
$C_3H_4OCl_2$	3.5		Wang et al. (2017)	Q	81, 240
IZRKUJREXIKAQM-UHFFFAOYSA-N	5.5×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:CH3CLCOCL	2.7×10^{-1}		Wang et al. (2017)	Q	81, 239
$C_3H_4OCl_2$	3.8×10^{-2}		Wang et al. (2017)	Q	81, 240
JEQDSBVHLKBEIZ-UHFFFAOYSA-N	1.1×10^{-2}		Wang et al. (2017)	Q	81, 241
MCM:CH3COCLOOH	1.0×10^{4}		Wang et al. (2017)	Q	81, 239
$C_3H_5O_3Cl$	3.5×10^{2}		Wang et al. (2017)	Q	81, 240
HLLYIZVQRAGDFF-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	81, 241
MCM:CLCOCLMOOH	1.4×10^{4}		Wang et al. (2017)	Q	81, 239
$C_3H_4O_3Cl_2$	6.0×10^{1}		Wang et al. (2017)	Q	81, 240
RUPGTCZALLJKQM-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	81, 241

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CL12CO2H $C_3H_4O_2Cl_2$ GKFWNPPZHDYVLI-UHFFFAOYSA-N	1.3×10^{3} 3.5×10^{3} 8.1×10^{2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
3-chloro-2-butanone C_4H_7ClO [4091-39-8] OIMRLHCSLQUXLL-UHFFFAOYSA-N	9.5×10^{-2}		Ebert et al. (2023)	?	317
ethyl chloroethanoate $C_4H_7ClO_2$ [105-39-5] VEUUMBGHMNQHGO-UHFFFAOYSA-N	2.6×10^{-1} 2.4×10^{-1} 1.5×10^{-1} 1.2×10^{-1} 1.1×10^{-1} 1.1×10^{-1} 2.4×10^{-1}	6100	Brockbank (2013) Duchowicz et al. (2020) Duchowicz et al. (2020) HSDB (2015) Hilal et al. (2008) Modarresi et al. (2007) Bartelt-Hunt et al. (2008)	L V Q Q Q Q ?	1 187 100 68 21
carbonochloridic acid, 1-methylethyl ester $C_4H_7ClO_2$ [108-23-6] IVRIRQXJSNCSPQ-UHFFFAOYSA-N	2.4×10^{-3}		HSDB (2015)	Q	100
chloroacetic acid anhydride $C_4H_4Cl_2O_3$ [541-88-8] PNVPNXKRAUBJGW-UHFFFAOYSA-N	2.2		HSDB (2015)	Q	100
chlorobutanol C_4H_9ClO [1320-66-7] OSASVXMJTNOKOY-UHFFFAOYSA-N	4.5		HSDB (2015)	Q	100
methyl 2-chloroacetoacetate $C_5H_7ClO_3$ [4755-81-1] GYQRIAVRKLRQKP-UHFFFAOYSA-N	2.3		Ebert et al. (2023)	?	319
3-chloro-4-(dichloromethyl)-2-(5H)-furanone $C_5H_3Cl_3O_2$ [122551-89-7] WNQKLIFDPFSPIZ-UHFFFAOYSA-N	1.5		HSDB (2015)	Q	100
3-chloro-4-(dichloromethyl)-5-hydroxy-2-(5H)-furanone $C_5H_3Cl_3O_3$ [77439-76-0] WNTRMRXAGJOLCU-UHFFFAOYSA-N	3.9×10^{4}		HSDB (2015)	Q	100

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,4-trichloro-2-methyl-3-pentanone	1.9		Zhang et al. (2010)	Q	288, 289
$C_6H_9Cl_3O$	1.9		Zhang et al. (2010)	Q	288, 290
[145556-04-3]	1.1×10^{2}		Zhang et al. (2010)	Q	288, 291
KAUWEMQJFDRELR-UHFFFAOYSA-N	4.1×10^{-1}		Zhang et al. (2010)	Q	288, 292
bis(2-chloroisopropyl) ether	3.0×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_6H_{12}Cl_2O$	3.3×10^{-4}		Zhang et al. (2010)	Q	288, 290
[39638-32-9]	9.5×10^{-1}		Zhang et al. (2010)	Q	288, 291
BULHJTXRZFEUDQ-UHFFFAOYSA-N	1.6×10^{-3}		Zhang et al. (2010)	Q	288, 292
butyl 2,2,3,4,4-pentachloro-3-butenoate	3.9×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_8H_9Cl_5O_2$	3.9×10^{-2}		Zhang et al. (2010)	Q	288, 290
[75147-20-5]	7.9×10^{-2}		Zhang et al. (2010)	Q	288, 291
JZJILZTVTMMGAR-UHFFFAOYSA-N	1.8×10^{-1}		Zhang et al. (2010)	Q	288, 292
3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropane carbonyl chloride	1.6×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_8H_9Cl_3O$	9.7×10^{-3}		Zhang et al. (2010)	Q	288, 290
[52314-67-7]	1.6×10^{-1}		Zhang et al. (2010)	Q	288, 291
CHLAOFANYRDCPD-UHFFFAOYSA-N	8.8×10^{-1}		Zhang et al. (2010)	Q	288, 292
3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropane carboxylic acid	1.9×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_8H_{10}Cl_2O_2$	9.0×10^{1}		Zhang et al. (2010)	Q	288, 290
[55701-05-8]	6.1×10^{4}		Zhang et al. (2010)	Q	288, 291
LLMLSUSAKZVFOA-UHFFFAOYSA-N	6.1×10^{1}		Zhang et al. (2010)	Q	288, 292
hexanoic acid, 3,3-dimethyl-4,6,6,6-tetrachloro, methyl ester	6.7×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_9H_{14}Cl_4O_2$	2.7×10^{-1}		Zhang et al. (2010)	Q	288, 290
[64667-33-0]	6.1×10^{2}		Zhang et al. (2010)	Q	288, 291
POFHGKISWXYKLB-UHFFFAOYSA-N	1.8×10^{-2}		Zhang et al. (2010)	Q	288, 292
methyl 3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate	6.1×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_9H_{12}Cl_2O_2$	5.2×10^{-2}		Zhang et al. (2010)	Q	288, 290
[61898-95-1]	1.3×10^{-1}		Zhang et al. (2010)	Q	288, 291
QJOOIMSFFIUFKX-UHFFFAOYSA-N	1.7×10^{-1}		Zhang et al. (2010)	Q	288, 292
oxychlordane	6.0×10^{-2}	4300	Paasivirta et al. (1999)	T	
$C_{10}H_4Cl_8O$	1.1×10^{2}		HSDB (2015)	Q	100
[27304-13-8]					
VWGNQYSIWFHEQU-UHFFFAOYSA-N					

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
kepone	1.8×10^{2}		Duchowicz et al. (2020)	V	187
$C_{10}Cl_{10}O$	1.8×10^{2}		HSDB (2015)	V	
[143-50-0]	2.0×10^{2}		Mackay et al. (2006d)	V	
LHHGDZSESBACKH-UHFFFAOYSA-N	1.5×10^{2}		Duchowicz et al. (2020)	Q	
bis-(chloromethyl) ether	2.3×10^{-3}		Duchowicz et al. (2020)	V	187
$C_2H_4Cl_2O$	4.8×10^{-2}		Mackay et al. (2006c)	V	
[542-88-1]	4.8×10^{-2}		Mackay et al. (1993)	V	
HRQGCQVOJVTVLU-UHFFFAOYSA-N	4.7×10^{-3}		Ryan et al. (1988)	C	
	1.9×10^{-2}		Duchowicz et al. (2020)	Q	
	4.3×10^{-2}		Modarresi et al. (2007)	Q	68
1,5-dichloro-3-oxapentane	4.8×10^{-1}	6200	Brockbank (2013)	L	1
$C_4H_8Cl_2O$	5.8×10^{-1}		Duchowicz et al. (2020)	V	187
(bis-(2-chloroethyl)-ether)	3.4×10^{-1}		HSDB (2015)	V	
[111-44-4]	3.5×10^{-1}		Mackay et al. (2006c)	V	
ZNSMNVMLTJELDZ-UHFFFAOYSA-N	3.4×10^{-2}		Lide and Frederikse (1995)	V	
	3.5×10^{-1}		Mackay et al. (1993)	V	
	4.6×10^{-1}		Goldstein (1982)	X	448
	4.7×10^{-1}	4100	Goldstein (1982)	X	299
	3.7×10^{-1}		Harrison et al. (1993)	C	
	8.6		Ryan et al. (1988)	C	
	3.4×10^{-2}		Duchowicz et al. (2020)	Q	
	5.2×10^{-2}		Zhang et al. (2010)	Q	288, 289
	2.8×10^{-1}		Zhang et al. (2010)	Q	288, 290
	4.4×10^{-2}		Zhang et al. (2010)	Q	288, 291
	4.6×10^{-3}		Zhang et al. (2010)	Q	288, 292
	2.9×10^{-1}		Hilal et al. (2008)	Q	
	3.7×10^{-1}		Modarresi et al. (2007)	Q	68
		6000	Kühne et al. (2005)	Q	
		6000	Kühne et al. (2005)	?	
2-chloro-1,1-dimethoxyethane $C_4H_9ClO_2$ [97-97-2] CRZJPEIBPQWDGJ-UHFFFAOYSA-N	3.2×10^{-1}		Ebert et al. (2023)	?	319
(2-chloroethoxy)-ethene	1.1×10^{-3}		Duchowicz et al. (2020)	V	187
C_4H_7ClO	1.1×10^{-3}		HSDB (2015)	V	
(2-chloroethylvinylether)	3.9×10^{-2}		Mackay et al. (2006c)	V	
[110-75-8]	3.9×10^{-2}		Mackay et al. (1993)	V	
DNJRKFKAFWSXSE-UHFFFAOYSA-N	1.1×10^{-3}		Goldstein (1982)	X	448
	3.1×10^{-2}	2500	Goldstein (1982)	X	299
	4.0×10^{-2}		Ryan et al. (1988)	C	
	4.9×10^{-2}		Duchowicz et al. (2020)	Q	
	2.3×10^{-3}		Hilal et al. (2008)	Q	
	2.1×10^{-2}		Modarresi et al. (2007)	Q	68

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bis-(2-chloroethoxy)-methane	2.6		Duchowicz et al. (2020)	V	187
$C_5H_{10}Cl_2O_2$	2.5		HSDB (2015)	V	
[111-91-1]	2.2×10^{1}		Mackay et al. (2006c)	V	
NLXGURFLBLRZRO-UHFFFAOYSA-N	2.2		Mackay et al. (1993)	V	
	8.8		Goldstein (1982)	X	448
	2.6×10^{1}	5500	Goldstein (1982)	X	299
	3.7×10^{1}		Ryan et al. (1988)	C	
	2.9×10^{-1}		Duchowicz et al. (2020)	Q	
	3.4		Hilal et al. (2008)	Q	
bis-(2-chloroisopropyl) ether	4.2×10^{-1}		Kawamoto and Urano (1989)	M	
$C_6H_{12}Cl_2O$	1.3×10^{-1}		HSDB (2015)	V	
(DCIP)	9.6×10^{-2}		Mackay et al. (2006c)	V	
[108-60-1]	9.6×10^{-2}		Mackay et al. (1993)	V	
QCFYJCYNJLBDRT-UHFFFAOYSA-N	6.5×10^{-2}		Goldstein (1982)	X	448
	6.4×10^{-2}	2800	Goldstein (1982)	X	299
	8.6×10^{-3}		Ryan et al. (1988)	C	
	7.2×10^{-2}		Hilal et al. (2008)	Q	
	2.9×10^{-1}		Modarresi et al. (2007)	Q	68
1,2-bis(2-chloroethoxy)ethane	1.3×10^{1}		HSDB (2015)	V	
$C_6H_{12}Cl_2O_2$	4.7		Modarresi et al. (2007)	Q	68
[112-26-5]					
AGYUOJIYYGGHKV-UHFFFAOYSA-N					
2-hydroxychlorobenzene	1.5		Sheikheldin et al. (2001)	M	12
C_6H_5ClO	3.6	5700	Tabai et al. (1997)	M	11
(*o*-chlorophenol)	1.5		Mackay et al. (2006c)	V	
[95-57-8]	1.2		Fogg and Sangster (2003)	V	731
ISPYQTSUDJAMAB-UHFFFAOYSA-N	1.8×10^{1}		Lide and Frederikse (1995)	V	
	1.5		Mackay et al. (1995)	V	
	1.5		Shiu et al. (1994)	V	
	8.8×10^{-1}		Abraham et al. (1994a)	R	
	1.2		Goldstein (1982)	X	448
	1.2	4600	Goldstein (1982)	X	299
	1.8×10^{1}		Howard (1989)	X	420
	2.1		Ryan et al. (1988)	C	
	2.2		Keshavarz et al. (2022)	Q	
	8.2		Duchowicz et al. (2020)	Q	300
	4.2		Hilal et al. (2008)	Q	
	4.6		Modarresi et al. (2007)	Q	68
		6200	Kühne et al. (2005)	Q	
	9.2×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	1.8×10^{2}		Nirmalakhandan et al. (1997)	Q	
	8.8×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	8.8×10^{-1}		HSDB (2015)	?	421
		5600	Kühne et al. (2005)	?	
	2.6×10^{-1}		Yaws (1999)	?	21

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.0		Chiou et al. (1980)	?	80
3-hydroxychlorobenzene	7.2		Chao et al. (2017)	M	
C_6H_5ClO	3.4×10^1	6400	Tabai et al. (1997)	M	11
(*m*-chlorophenol)	4.9		Mackay et al. (2006c)	V	
[108-43-0]	7.3		Fogg and Sangster (2003)	V	
HORNXRXVQWOLPJ-UHFFFAOYSA-N	1.8×10^1		Lide and Frederikse (1995)	V	
	4.9		Mackay et al. (1995)	V	
	4.9		Shiu et al. (1994)	V	
	2.9×10^1		Abraham et al. (1994a)	R	
	1.8×10^1		Howard (1989)	X	420
	4.3		Keshavarz et al. (2022)	Q	
	9.9×10^1		Duchowicz et al. (2020)	Q	300
	1.6×10^1		Hilal et al. (2008)	Q	
	2.5×10^1		Modarresi et al. (2007)	Q	68
		6200	Kühne et al. (2005)	Q	
	3.0×10^1		Yaffe et al. (2003)	Q	249, 250
	1.3×10^1		English and Carroll (2001)	Q	231, 232
	2.4×10^1		Katritzky et al. (1998)	Q	
	1.8×10^2		Nirmalakhandan et al. (1997)	Q	
	2.9×10^1		Duchowicz et al. (2020)	?	186, 21
	2.9×10^1		HSDB (2015)	?	421
		6100	Kühne et al. (2005)	?	
	4.8		Yaws (1999)	?	21, 12
4-hydroxychlorobenzene	6.7		Chao et al. (2017)	M	
C_6H_5ClO	1.4×10^3	11000	Tabai et al. (1997)	M	11
(*p*-chlorophenol)	1.6×10^1		HSDB (2015)	V	
[106-48-9]	1.1×10^1		Mackay et al. (2006c)	V	
WXNZTHHGJRFXKQ-UHFFFAOYSA-N	1.2×10^1		Fogg and Sangster (2003)	V	
	1.8×10^1		Lide and Frederikse (1995)	V	
	1.1×10^1		Mackay et al. (1995)	V	
	1.1×10^1		Shiu et al. (1994)	V	
	5.8×10^1		Abraham et al. (1994a)	R	
	1.8×10^1		Howard (1989)	X	420
	4.3		Keshavarz et al. (2022)	Q	
	1.5×10^2		Duchowicz et al. (2020)	Q	185
	2.4×10^1		Li et al. (2014)	Q	242
	1.3×10^1		Hilal et al. (2008)	Q	
	9.8		Modarresi et al. (2007)	Q	68
		6200	Kühne et al. (2005)	Q	
	5.8×10^1		Yaffe et al. (2003)	Q	249, 250
	3.4×10^1		Yao et al. (2002)	Q	230
	2.3×10^1		English and Carroll (2001)	Q	231, 261
	3.0×10^1		Katritzky et al. (1998)	Q	
	1.8×10^2		Nirmalakhandan et al. (1997)	Q	
	1.6×10^1		Duchowicz et al. (2020)	?	186, 21

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		6400	Kühne et al. (2005)	?	
	7.8		Yaws (1999)	?	21, 12
	1.1×10^{1}		Chiou et al. (1980)	?	80
2,3-dichlorophenol $C_6H_4Cl_2O$ [576-24-9] UMPSXRYVXUPCOS-UHFFFAOYSA-N	2.9		HSDB (2015)	V	
2,4-dichlorophenol	3.4		Sheikheldin et al. (2001)	M	12
$C_6H_4Cl_2O$	6.6	6800	Tabai et al. (1997)	M	11
[120-83-2]	2.3		Duchowicz et al. (2020)	V	187
HFZWRUODUSTPEG-UHFFFAOYSA-N	2.8		HSDB (2015)	V	
	2.3		Mackay et al. (2006c)	V	
	2.3		Mackay et al. (1995)	V	
	2.3		Shiu et al. (1994)	V	
	9.0		Leuenberger et al. (1985)	V	418
	1.5		Goldstein (1982)	X	448
	1.5	4900	Goldstein (1982)	X	299
	1.8		Ryan et al. (1988)	C	
	2.2×10^{1}		Duchowicz et al. (2020)	Q	
	3.2×10^{1}		Zhang et al. (2010)	Q	288, 289
	8.0		Zhang et al. (2010)	Q	288, 290
	1.1		Zhang et al. (2010)	Q	288, 291
	4.6		Zhang et al. (2010)	Q	288, 292
	8.2		Hilal et al. (2008)	Q	
	4.4		Modarresi et al. (2007)	Q	68
		6300	Kühne et al. (2005)	Q	
		7400	Kühne et al. (2005)	?	
2,5-dichlorophenol $C_6H_4Cl_2O$ [583-78-8] RANCECPPZPIPNO-UHFFFAOYSA-N	1.6		HSDB (2015)	V	
2,6-dichlorophenol	3.7		Duchowicz et al. (2020)	V	187
$C_6H_4Cl_2O$	3.7		HSDB (2015)	V	
[87-65-0]	1.3		Mackay et al. (2006c)	V	
HOLHYSJJBXSLMV-UHFFFAOYSA-N	3.3		Mackay et al. (1995)	V	
	1.2		Duchowicz et al. (2020)	Q	
	3.8		Yaffe et al. (2003)	Q	249, 250
	2.5×10^{1}		Katritzky et al. (1998)	Q	
3,4-dichlorophenol $C_6H_4Cl_2O$ [95-77-2] WDNBURPWRNALGP-UHFFFAOYSA-N	2.1×10^{1}		HSDB (2015)	Q	100

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,5-dichlorophenol	4.0×10^{1}		Duchowicz et al. (2020)	V	187
$C_6H_4Cl_2O$	4.1×10^{1}		HSDB (2015)	V	
[591-35-5]	1.8×10^{2}		Duchowicz et al. (2020)	Q	
VPOMSPZBQMDLTM-UHFFFAOYSA-N	4.6×10^{1}		Hilal et al. (2008)	Q	
	1.4×10^{1}		Modarresi et al. (2007)	Q	68
2,3,4-trichlorophenol	2.5		Mackay et al. (2006c)	V	
$C_6H_3Cl_3O$	2.5		Mackay et al. (1995)	V	
[15950-66-0]					
HSQFVBWFPBKHEB-UHFFFAOYSA-N					
2,3,5-trichlorophenol	2.5		Mackay et al. (2006c)	V	
$C_6H_3Cl_3O$	2.5		Mackay et al. (1995)	V	
[933-78-8]					
WWGQHTJIFOQAOC-UHFFFAOYSA-N					
2,4,5-trichlorophenol	6.1		Duchowicz et al. (2020)	V	187
$C_6H_3Cl_3O$	6.2		HSDB (2015)	V	
[95-95-4]	1.9		Mackay et al. (2006c)	V	
LHJGJYXLEPZJPM-UHFFFAOYSA-N	4.6×10^{-1}		Fogg and Sangster (2003)	V	
	1.9		Mackay et al. (1995)	V	
	7.6		Leuenberger et al. (1985)	V	418
	4.6×10^{1}		Duchowicz et al. (2020)	Q	
	2.0×10^{1}		Hilal et al. (2008)	Q	
	5.7		Modarresi et al. (2007)	Q	68
2,3,6-trichlorophenol	4.3×10^{1}		HSDB (2015)	Q	100
$C_6H_3Cl_3O$					
[933-75-5]					
XGCHAIDDPMFRLJ-UHFFFAOYSA-N					
2,4,6-trichlorophenol	1.9×10^{1}		Chao et al. (2017)	M	
$C_6H_3Cl_3O$	2.0		Yoshida et al. (1987)	M	732, 12
[88-06-2]	3.8		Duchowicz et al. (2020)	V	187
LINPIYWFGCPVIE-UHFFFAOYSA-N	3.8		HSDB (2015)	V	
	1.8		Mackay et al. (2006c)	V	
	1.6×10^{2}		Lide and Frederikse (1995)	V	
	1.8		Mackay et al. (1995)	V	
	7.6		Leuenberger et al. (1985)	V	418
	1.4	5000	Goldstein (1982)	X	299
	1.6×10^{1}		Howard (1989)	X	420
	2.4		Ryan et al. (1988)	C	
	2.5		Duchowicz et al. (2020)	Q	
	4.3×10^{1}		Zhang et al. (2010)	Q	288, 289
	2.8×10^{-2}		Zhang et al. (2010)	Q	288, 290
	8.8×10^{-1}		Zhang et al. (2010)	Q	288, 291
	9.7×10^{-1}		Zhang et al. (2010)	Q	288, 292
	2.2		Hilal et al. (2008)	Q	
	3.3		Modarresi et al. (2007)	Q	68

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		6400	Kühne et al. (2005)	Q	
	3.8		Yaffe et al. (2003)	Q	249, 250
	1.8×10^{1}		Katritzky et al. (1998)	Q	
		6500	Kühne et al. (2005)	?	
3,4,5-trichlorophenol $C_6H_3Cl_3O$ [609-19-8] GBNHEBQXJVDXSW-UHFFFAOYSA-N	4.3×10^{1}		HSDB (2015)	Q	100
2,3,4,5-tetrachlorophenol $C_6H_2Cl_4O$ [4901-51-3] RULKYXXCCZZKDZ-UHFFFAOYSA-N	7.2		Mackay et al. (2006c)	V	
	7.2		Mackay et al. (1995)	V	
	2.8×10^{1}		HSDB (2015)	Q	100
2,3,4,6-tetrachlorophenol $C_6H_2Cl_4O$ [58-90-2] VGVRPFIJEJYOFN-UHFFFAOYSA-N	1.1		Duchowicz et al. (2020)	V	187
	7.6		HSDB (2015)	V	
	2.8		Mackay et al. (2006c)	V	
	2.8		Mackay et al. (1995)	V	
	6.6		Duchowicz et al. (2020)	Q	
	5.8×10^{1}		Zhang et al. (2010)	Q	288, 289
	4.1×10^{-2}		Zhang et al. (2010)	Q	288, 290
	3.9		Zhang et al. (2010)	Q	288, 291
	3.1		Zhang et al. (2010)	Q	288, 292
2,3,5,6-tetrachlorophenol $C_6H_2Cl_4O$ [935-95-5] KEWNKZNZRIAIAK-UHFFFAOYSA-N	4.3		Mackay et al. (2006c)	V	
	4.3		Mackay et al. (1995)	V	
	2.8×10^{1}		HSDB (2015)	Q	100
hydroxypentachlorobenzene C_6HCl_5O (pentachlorophenol) [87-86-5] IZUPBVBPLAPZRR-UHFFFAOYSA-N	4.1×10^{2}		Hellmann (1987)	M	88
	1.3×10^{1}		Mackay et al. (2006c)	V	
			Mackay et al. (2006d)	V	560
	1.1×10^{-2}		Fogg and Sangster (2003)	V	
	1.3×10^{1}		Mackay et al. (1995)	V	
	2.3×10^{1}		Riederer (1990)	V	
	2.3×10^{1}		Suntio et al. (1988)	V	12
	2.2×10^{-1}		Barcelo and Hennion (1997)	X	569
	1.1×10^{-1}	1300	Goldstein (1982)	X	299
	4.7		McCarty (1980)	X	370
	3.4		Ryan et al. (1988)	C	
	7.9×10^{1}		Zhang et al. (2010)	Q	288, 289
	6.0×10^{-2}		Zhang et al. (2010)	Q	288, 290
	6.5		Zhang et al. (2010)	Q	288, 291
	4.0		Zhang et al. (2010)	Q	288, 292
	2.5×10^{-1}		Goodarzi et al. (2010)	Q	570, 571
	1.3×10^{1}		Modarresi et al. (2007)	Q	68
		7800	Kühne et al. (2005)	Q	
	7.9×10^{1}		Meylan and Howard (1991)	Q	

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.8		Fogg and Sangster (2003)	E	
		7400	Kühne et al. (2005)	?	
3,4,5-trichloro-1,2-benzenediol $C_6H_3Cl_3O_2$ (3,4,5-trichlorocatechol) [56961-20-7] FUTDYIMYZIMPBJ-UHFFFAOYSA-N	2.4×10^{2}		Lei et al. (1999)	V	
4,5-dichloro-1,2-benzenediol $C_6H_4Cl_2O_2$ (4,5-dichlorocatechol) [3428-24-8] ACCHWUWBKYGKNM-UHFFFAOYSA-N	1.3×10^{3}		Lei et al. (1999)	V	
3,4,5,6-tetrachloro-1,2-benzenediol $C_6H_2Cl_4O_2$ (tetrachlorocatechol) [1198-55-6] RRBMVWQICIXSEO-UHFFFAOYSA-N	2.9×10^{1}		Lei et al. (1999)	V	
2,3,5,6-tetrachloro-*p*-benzoquinone $C_6Cl_4O_2$ (chloranil) [118-75-2] UGNWTBMOAKPKBL-UHFFFAOYSA-N	1.5×10^{3}		HSDB (2015)	V	
2-chloro-5-methylphenol C_7H_7ClO [615-74-7] SMFHPCZZAAMJJO-UHFFFAOYSA-N	2.1×10^{1}		HSDB (2015)	Q	100
4-chloro-2-methylphenol	8.7		Duchowicz et al. (2020)	V	187
C_7H_7ClO	9.0		Woodrow et al. (1990)	V	
[1570-64-5]	8.5×10^{1}		Duchowicz et al. (2020)	Q	
RHPUJHQBPORFGV-UHFFFAOYSA-N	1.6×10^{1}		Hilal et al. (2008)	Q	
	1.5		Modarresi et al. (2007)	Q	68
4-chloro-3-methylphenol	4.0		Duchowicz et al. (2020)	V	187
C_7H_7ClO	4.1		HSDB (2015)	V	
[59-50-7]	3.9×10^{1}		Abraham et al. (1994a)	R	
CFKMVGJGLGKFKI-UHFFFAOYSA-N	4.0		Ryan et al. (1988)	C	
	8.5×10^{1}		Duchowicz et al. (2020)	Q	
	2.2×10^{1}		Zhang et al. (2010)	Q	288, 289
	1.3×10^{1}		Zhang et al. (2010)	Q	288, 290
	2.8×10^{1}		Zhang et al. (2010)	Q	288, 291
	9.2×10^{1}		Zhang et al. (2010)	Q	288, 292
	1.2×10^{1}		Hilal et al. (2008)	Q	
	8.8		Modarresi et al. (2007)	Q	68

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.9×10^{1}		Yaffe et al. (2003)	Q	249, 250
	1.7×10^{1}		English and Carroll (2001)	Q	231, 232
	1.3×10^{2}		Nirmalakhandan et al. (1997)	Q	
1-chloro-2-methoxybenzene C_7H_7ClO (2-chloroanisole) [766-51-8] QGRPVMLBTFGQDQ-UHFFFAOYSA-N	1.0×10^{-1}		Pfeifer et al. (2001)	M	733
	1.1×10^{-1}		Duchowicz et al. (2020)	V	187
	1.8×10^{-1}		Duchowicz et al. (2020)	Q	
1-chloro-3-methoxybenzene C_7H_7ClO (3-chloroanisole) [2845-89-8] YUKILTJWFRTXGB-UHFFFAOYSA-N	4.5×10^{-2}		Pfeifer et al. (2001)	M	733
1-chloro-4-methoxybenzene C_7H_7ClO (4-chloroanisole) [623-12-1] YRGAYAGBVIXNAQ-UHFFFAOYSA-N	5.8×10^{-2}		Pfeifer et al. (2001)	M	733
1,2-dichloro-3-methoxybenzene $C_7H_6Cl_2O$ (2,3-dichloroanisole) [1984-59-4] HFEASCCDHUVYKU-UHFFFAOYSA-N	2.2×10^{-2}		Pfeifer et al. (2001)	M	733
1,5-dichloro-2-methoxybenzene $C_7H_6Cl_2O$ (2,4-dichloroanisole) [553-82-2] CICQUFBZCADHHX-UHFFFAOYSA-N	1.2×10^{-2}		Pfeifer et al. (2001)	M	733
1,4-dichloro-2-methoxybenzene $C_7H_6Cl_2O$ (2,5-dichloroanisole) [1984-58-3] QKMNFFSBZRGHDJ-UHFFFAOYSA-N	2.1×10^{-2}		Pfeifer et al. (2001)	M	733
	5.7×10^{-2}		Zhang et al. (2010)	Q	288, 289
	1.4×10^{-2}		Zhang et al. (2010)	Q	288, 290
	1.4×10^{-1}		Zhang et al. (2010)	Q	288, 291
	4.8×10^{-2}		Zhang et al. (2010)	Q	288, 292
1,3-dichloro-2-methoxybenzene $C_7H_6Cl_2O$ (2,6-dichloroanisole) [1984-65-2] KZLMCDNAVVJKPX-UHFFFAOYSA-N	8.8×10^{-3}		Pfeifer et al. (2001)	M	733

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-dichloro-4-methoxybenzene $C_7H_6Cl_2O$ (3,4-dichloroanisole) [36404-30-5] VISJRVXHPNMYRH-UHFFFAOYSA-N	9.2×10^{-3}		Pfeifer et al. (2001)	M	733
1,3-dichloro-5-methoxybenzene $C_7H_6Cl_2O$ (3,5-dichloroanisole) [33719-74-3] SSNXYMVLSOMJLU-UHFFFAOYSA-N	2.3×10^{-3}		Pfeifer et al. (2001)	M	733
1,2,3-trichloro-4-methoxybenzene $C_7H_5Cl_3O$ (2,3,4-trichloroanisole) [54135-80-7] FRQUNVLMWIYOLV-UHFFFAOYSA-N	1.3×10^{-2}		Pfeifer et al. (2001)	M	733
1,2,5-trichloro-3-methoxybenzene $C_7H_5Cl_3O$ (2,3,5-trichloroanisole) [54135-81-8] MKERQGLKSFEKAE-UHFFFAOYSA-N	7.6×10^{-3}		Pfeifer et al. (2001)	M	733
1,2,4-trichloro-3-methoxybenzene $C_7H_5Cl_3O$ (2,3,6-trichloroanisole) [50375-10-5] OTFNCXLUCRUNCH-UHFFFAOYSA-N	1.1×10^{-2} 9.8×10^{-3} 1.8×10^{-2} 2.0×10^{-2} 7.6×10^{-2}	4500	Diaz et al. (2005) Pfeifer et al. (2001) Hilal et al. (2008) Modarresi et al. (2007) Meylan and Howard (1991)	M M Q Q Q	 733 68
1,2,4-trichloro-5-methoxybenzene $C_7H_5Cl_3O$ (2,4,5-trichloroanisole) [6130-75-2] SXKBHOQOOGRFJF-UHFFFAOYSA-N	1.1×10^{-2}		Pfeifer et al. (2001)	M	733
1,3,5-trichloro-2-methoxybenzene $C_7H_5Cl_3O$ (2,4,6-trichloroanisole) [87-40-1] WCVOGSZTONGSQY-UHFFFAOYSA-N	2.3×10^{-2} 4.4×10^{-3} 4.6×10^{-3}	5500 640	Wu et al. (2022a) Diaz et al. (2005) Pfeifer et al. (2001)	M M M	 733
1,2,3-trichloro-5-methoxybenzene $C_7H_5Cl_3O$ (3,4,5-trichloroanisole) [54135-82-9] GUCFBWGWRCILHN-UHFFFAOYSA-N	4.4×10^{-3}		Pfeifer et al. (2001)	M	733

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,4-tetrachloro-5-methoxybenzene $C_7H_4Cl_4O$ (2,3,4,5-tetrachloroanisole) [938-86-3] FUUHMSUPRUNWRQ-UHFFFAOYSA-N	6.5×10^{-3}		Pfeifer et al. (2001)	M	733
1,2,3,5-tetrachloro-4-methoxybenzene $C_7H_4Cl_4O$ (2,3,4,6-tetrachloroanisole) [938-22-7] ITXDBGLYYSJNPK-UHFFFAOYSA-N	3.1×10^{-3}		Pfeifer et al. (2001)	M	733
1,2,4,5-tetrachloro-3-methoxybenzene $C_7H_4Cl_4O$ (2,3,5,6-tetrachloroanisole) [6936-40-9] WMMFIDNWZNCBCT-UHFFFAOYSA-N	3.2×10^{-3}		Pfeifer et al. (2001)	M	733
pentachloromethoxybenzene $C_7H_3Cl_5O$ (pentachloroanisole) [1825-21-4] BBABSCYTNHOKOG-UHFFFAOYSA-N	2.1×10^{-3} 5.1×10^{-3}		Pfeifer et al. (2001) HSDB (2015)	M Q	733 100
4,5-dichloro-2-methoxyphenol $C_7H_6Cl_2O_2$ (4,5-dichloroguaiacol) [2460-49-3] HAAFFTHBNFBVKY-UHFFFAOYSA-N	5.2 2.3		Mackay et al. (2006c) Lei et al. (1999)	V V	
3,4,5-trichloro-2-methoxyphenol $C_7H_5Cl_3O_2$ (3,4,5-trichloroguaiacol) [57057-83-7] RKEHLKXRUVUBJN-UHFFFAOYSA-N	1.1×10^{1} 8.3 9.7×10^{1}		Duchowicz et al. (2020) Mackay et al. (2006c) Lei et al. (1999) Duchowicz et al. (2020)	V V V Q	187 422
4,5,6-trichloro-2-methoxyphenol $C_7H_5Cl_3O_2$ (4,5,6-trichloroguaiacol) [2668-24-8] NIAJPNQTKGWEOI-UHFFFAOYSA-N	7.4 7.1		Mackay et al. (2006c) Lei et al. (1999)	V V	

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4,5-tetrachloro-6-methoxyphenol $C_7H_4Cl_4O_2$ (tetrachloroguaiacol) [2539-17-5] YZZVKLJKDFFSFL-UHFFFAOYSA-N	1.4		Duchowicz et al. (2020)	V	187
	6.2		Mackay et al. (2006c)	V	
	6.7		Lei et al. (1999)	V	
	8.4		Duchowicz et al. (2020)	Q	
2-chlorobenzoic acid $C_7H_5ClO_2$ [118-91-2] IKCLCGXPQILATA-UHFFFAOYSA-N	1.5×10^{2}		Duchowicz et al. (2020)	V	187
	1.3×10^{2}		Yaws (2003)	X	238
	3.5×10^{2}		Duchowicz et al. (2020)	Q	
	1.4×10^{2}		Gharagheizi et al. (2010)	Q	247
3-chlorobenzoic acid $C_7H_5ClO_2$ [535-80-8] LULAYUGMBFYYEX-UHFFFAOYSA-N	5.7×10^{1}		Abraham et al. (2019)	Q	
	2.5×10^{2}		HSDB (2015)	Q	547
4-chlorobenzoic acid $C_7H_5ClO_2$ [74-11-3] XRHGYUZYPHTUJZ-UHFFFAOYSA-N	2.5×10^{1}		Abraham et al. (2019)	Q	
3,4-dichlorobenzoic acid $C_7H_4Cl_2O_2$ [51-44-5] VPHHJAOJUJHJKD-UHFFFAOYSA-N	2.1×10^{1}		Abraham et al. (2019)	Q	
2,3,6-trichlorobenzoic acid $C_7H_3Cl_3O_2$ [50-31-7] XZIDTOHMJBOSOX-UHFFFAOYSA-N	4.7×10^{2}		Duchowicz et al. (2020)	V	187
	6.5×10^{2}		Duchowicz et al. (2020)	Q	
1,2,3-trichloro-4,5-dimethoxybenzene $C_8H_7Cl_3O_2$ (3,4,5-trichloroveratrole) [16766-29-3] VKNITLPENCJQOP-UHFFFAOYSA-N	2.7×10^{-1}		Lei et al. (1999)	V	
1,2,3,4-tetrachloro-5,6-dimethoxybenzene $C_8H_6Cl_4O_2$ (tetrachloroveratrole) [944-61-6] NCYHCGGUQGDEQW-UHFFFAOYSA-N	9.1×10^{-2}		Lei et al. (1999)	V	
	1.7		Zhang et al. (2010)	Q	288, 289
	2.0		Zhang et al. (2010)	Q	288, 290
	2.6		Zhang et al. (2010)	Q	288, 291
	7.5×10^{-1}		Zhang et al. (2010)	Q	288, 292

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-chloro-2,6-dimethoxyphenol $C_8H_9ClO_3$ (3-chlorosyringol) [18113-22-9] WYEMCZZCZXKDNC-UHFFFAOYSA-N	4.2×10^{1}		Lei et al. (1999)	V	
3,5-dichloro-2,6-dimethoxyphenol $C_8H_8Cl_2O_3$ (3,5-dichlorosyringol) [78782-46-4] IDKMFABKPPHDBI-UHFFFAOYSA-N	1.4×10^{1}		Lei et al. (1999)	V	
3,5-dichloro-2-hydroxybenzoic acid	1.3×10^{3}		Zhang et al. (2010)	Q	288, 289
$C_7H_4Cl_2O_3$	4.3×10^{2}		Zhang et al. (2010)	Q	288, 290
[320-72-9]	7.5×10^{4}		Zhang et al. (2010)	Q	288, 291
CNJGWCQEGROXEE-UHFFFAOYSA-N	2.2×10^{2}		Zhang et al. (2010)	Q	288, 292
3,6-dichloro-2-hydroxybenzoic acid	1.3×10^{3}		Zhang et al. (2010)	Q	288, 289
$C_7H_4Cl_2O_3$	3.4×10^{3}		Zhang et al. (2010)	Q	288, 290
[3401-80-7]	1.1×10^{1}		Zhang et al. (2010)	Q	288, 291
FKIKPQHMWFZFEB-UHFFFAOYSA-N	2.2×10^{2}		Zhang et al. (2010)	Q	288, 292
5-chloro-2-methoxybenzoic acid	2.1×10^{3}		Zhang et al. (2010)	Q	288, 289
$C_8H_7ClO_3$	3.8×10^{1}		Zhang et al. (2010)	Q	288, 290
[3438-16-2]	9.5×10^{3}		Zhang et al. (2010)	Q	288, 291
HULDRQRKKXRXBI-UHFFFAOYSA-N	6.0×10^{3}		Zhang et al. (2010)	Q	288, 292
2-chloroacetophenone C_8H_7ClO [532-27-4] IMACFCSSMIZSPP-UHFFFAOYSA-N	2.8		HSDB (2015)	Q	100
2,2,2',4',5'-pentachloroacetophenone	2.0×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_8H_3Cl_5O$	5.7		Zhang et al. (2010)	Q	288, 290
[1203-86-7]	1.0		Zhang et al. (2010)	Q	288, 291
WKJXVVFAALGBOH-UHFFFAOYSA-N	6.0		Zhang et al. (2010)	Q	288, 292
tetrachloroterephthaloyl chloride	1.0×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_8Cl_6O_2$	1.9×10^{1}		Zhang et al. (2010)	Q	288, 290
[719-32-4]	3.4×10^{-2}		Zhang et al. (2010)	Q	288, 291
YJIRZJAZKDWEIJ-UHFFFAOYSA-N	1.3×10^{3}		Zhang et al. (2010)	Q	288, 292
chloroxylenol	1.9×10^{1}		HSDB (2015)	Q	100
C_8H_9ClO	1.9×10^{1}		Zhang et al. (2010)	Q	288, 289
[88-04-0]	1.5×10^{1}		Zhang et al. (2010)	Q	288, 290
OSDLLIBGSJNGJE-UHFFFAOYSA-N	2.0×10^{1}		Zhang et al. (2010)	Q	288, 291
	5.1×10^{1}		Zhang et al. (2010)	Q	288, 292

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,5,6,7-tetrachloro-1,3-isobenzofurandione	5.2		Zhang et al. (2010)	Q	288, 289
$C_8Cl_4O_3$	1.8×10^4		Zhang et al. (2010)	Q	288, 290
[117-08-8]	1.9×10^2		Zhang et al. (2010)	Q	288, 291
AUHHYELHRWCWEZ-UHFFFAOYSA-N	4.3×10^1		Zhang et al. (2010)	Q	288, 292
3,4,5-trichloro-2,6-dimethoxyphenol $C_8H_7Cl_3O_3$ (trichlorosyringol) [2539-26-6] ZZCSBXFJFLSDRR-UHFFFAOYSA-N	4.5×10^1		Lei et al. (1999)	V	
4,5,6,7-tetrachlorophthalide	1.8×10^1		Kawamoto and Urano (1989)	M	
$C_8H_2Cl_4O_2$	3.1×10^3		Duchowicz et al. (2020)	V	187
[27355-22-2]	8.6		Duchowicz et al. (2020)	Q	
NMWKWBPNKPGATC-UHFFFAOYSA-N					
dicamba	4.5×10^3		Duchowicz et al. (2020)	V	187
$C_8H_6Cl_2O_3$	2.3×10^4		HSDB (2015)	V	
(banvel)	4.5×10^3		Mackay et al. (2006d)	V	
[1918-00-9]	8.3×10^3		Suntio et al. (1988)	V	12
IWEDIXLBFLAXBO-UHFFFAOYSA-N	8.2×10^1		Barcelo and Hennion (1997)	X	569
	2.2×10^4		Armbrust (2000)	C	
	5.9×10^3		Duchowicz et al. (2020)	Q	
	1.2		Goodarzi et al. (2010)	Q	570, 571
	1.0×10^4		Maniere et al. (2011)	?	166
(2,4-dichlorophenoxy)-ethanoic acid	1.4×10^{-1}		Rice et al. (1997b)	M	734, 12
$C_8H_6Cl_2O_3$	1.2		Rice et al. (1997b)	M	734, 12
((2,4-dichlorophenoxy)-acetic acid; 2,4-D)	2.8×10^2		Duchowicz et al. (2020)	V	187
[94-75-7]	5.0×10^4		Mackay et al. (2006c)	V	
OVSKIKFHRZPJSS-UHFFFAOYSA-N	2.3×10^4		Mackay et al. (2006d)	V	
	4.0×10^3		Mackay et al. (2006d)	V	
	2.9×10^2		Mackay et al. (1995)	V	
	1.8		Riederer (1990)	V	
	1.8		Suntio et al. (1988)	V	12
	7.2×10^4		Howard (1991)	X	414
	9.7×10^2		Howard (1991)	X	414
	5.5×10^6		Armbrust (2000)	C	
	8.7×10^2		Duchowicz et al. (2020)	Q	
	2.5×10^5		Maniere et al. (2011)	?	12, 166

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4,5-trichlorophenoxyethanoic acid	1.7×10^{2}		Mackay et al. (2006d)	V	
$C_8H_5Cl_3O_3$	1.7×10^{2}		Riederer (1990)	V	
(2,4,5-T)	1.7×10^{2}		Suntio et al. (1988)	V	12
[93-76-5]	8.4×10^{5}		MacBean (2012a)	?	
SMYMJHWAQXWPDB-UHFFFAOYSA-N					
1,4-dichloro-2,5-dimethoxybenzene	9.7×10^{-2}		Duchowicz et al. (2020)	V	187
$C_8H_8Cl_2O_2$	9.9×10^{-2}		HSDB (2015)	V	
[2675-77-6]			Mackay et al. (2006d)	V	560
PFIADAMVCJPXSF-UHFFFAOYSA-N	9.4×10^{-1}		Duchowicz et al. (2020)	Q	
2,3,6-trichlorophenylacetic acid	8.3×10^{-1}		Mackay et al. (2006d)	V	
$C_8H_5Cl_3O_2$	5.5×10^{2}		HSDB (2015)	Q	100
[85-34-7]					
QZXCCPZJCKEPSA-UHFFFAOYSA-N					
4-methoxy-benzoyl chloride	1.3		HSDB (2015)	Q	100
$C_8H_7ClO_2$					
(*p*-anisoyl chloride)					
[100-07-2]					
MXMOTZIXVICDSD-UHFFFAOYSA-N					
(4-chlorophenoxy)acetic acid	1.0×10^{5}		Ebert et al. (2023)	?	317
$C_8H_7ClO_3$					
[122-88-3]					
SODPIMGUZLOIPE-UHFFFAOYSA-N					
isobenzan	1.7×10^{2}		HSDB (2015)	Q	100
$C_9H_4Cl_8O$					
[297-78-9]					
LRWHHSXTGZSMSN-UHFFFAOYSA-N					
2-chloro-4-hydroxy-3,5-dimethoxybenzaldehyde	9.1×10^{1}		Lei et al. (1999)	V	
$C_9H_9ClO_4$					
(2-chlorosyringaldehyde)					
[76341-69-0]					
GRIHRCLOUQZXPD-UHFFFAOYSA-N					
2,6-dichloro-4-hydroxy-3,5-dimethoxybenzaldehyde	2.7×10^{2}		Lei et al. (1999)	V	
$C_9H_8Cl_2O_4$					
(2,6-dichlorosyringaldehyde)					
[76330-06-8]					
CTFRWEPMHUGVMM-UHFFFAOYSA-N					

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl 2,4-dichlorophenoxyethanoate	3.6		Duchowicz et al. (2020)	V	187
$C_9H_8Cl_2O_3$	1.0×10^{1}		Duchowicz et al. (2020)	Q	
[1928-38-7]	1.8		Hilal et al. (2008)	Q	
HWIGZMADSFQMOI-UHFFFAOYSA-N	1.3		Modarresi et al. (2007)	Q	68
(2-methyl-4-chlorophenoxy)acetic acid	$>9.9\times10^{1}$		Mabury and Crosby (1996)	M	
$C_9H_9ClO_3$	7.4×10^{3}		Duchowicz et al. (2020)	V	187
(MCPA)	4.0×10^{4}		Mackay et al. (2006d)	V	
[94-74-6]	9.9×10^{3}		Woodrow et al. (1990)	V	
WHKUVVPPKQRRBV-UHFFFAOYSA-N	5.7×10^{2}		Duchowicz et al. (2020)	Q	
	1.8×10^{4}		Maniere et al. (2011)	?	166
α-(2,4-dichlorophenoxy)propionic acid	3.7×10^{3}		Mackay et al. (2006d)	V	
$C_9H_8Cl_2O_3$					
(dichloroprop)					
[120-36-5]					
MZHCENGPTKEIGP-UHFFFAOYSA-N					
(*R*)-2-(2,4-dichlorophenoxy)propanoic acid	4.0×10^{4}		Mackay et al. (2006d)	V	
$C_9H_8Cl_2O_3$	1.8×10^{4}		Maniere et al. (2011)	?	242, 166
(dichlorprop-p)					
[15165-67-0]					
MZHCENGPTKEIGP-RXMQYKEDSA-N					
2-(2,4,5-trichlorophenoxy)propanoic acid	3.9×10^{4}		Mackay et al. (2006d)	V	
$C_9H_7Cl_3O_3$					
[93-72-1]					
ZLSWBLPERHFHIS-UHFFFAOYSA-N					
cloxyfonac	1.0×10^{5}		Duchowicz et al. (2020)	V	187
$C_9H_9O_4Cl$	1.9×10^{6}		Duchowicz et al. (2020)	Q	
[6386-63-6]					
ZJRUTGDCLVIVRD-UHFFFAOYSA-N					
tridiphane	1.9×10^{-1}		MacBean (2012a)	?	
$C_{10}H_7Cl_5O$					
[58138-08-2]					
IBZHOAONZVJLOB-UHFFFAOYSA-N					
plifenat	1.1×10^{4}		MacBean (2012a)	?	
$C_{10}H_7O_2Cl_5$					
[21757-82-4]					
FSGNOVKGEXRRHD-UHFFFAOYSA-N					

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chlorfenprop-methyl $C_{10}H_{10}Cl_2O_2$ [14437-17-3] YJKIALIXRCSISK-UHFFFAOYSA-N	4.4		Ebert et al. (2023)	?	367
ethyl 2,4-dichlorophenoxyethanoate	3.0		Duchowicz et al. (2020)	V	187
$C_{10}H_{10}Cl_2O_3$	4.3		Duchowicz et al. (2020)	Q	
[533-23-3]	1.2		Hilal et al. (2008)	Q	
JSLBZIVMVVHMDJ-UHFFFAOYSA-N	1.1		Modarresi et al. (2007)	Q	68
mecoprop	1.1×10^4		Duchowicz et al. (2020)	V	187
$C_{10}H_{11}ClO_3$			Mackay et al. (2006d)	V	560
[93-65-2]	9.0×10^1		Barcelo and Hennion (1997)	X	569
WNTGYJSOUMFZEP-UHFFFAOYSA-N	9.0×10^3		Armbrust (2000)	C	
	2.6×10^2		Duchowicz et al. (2020)	Q	
	1.4×10^2		Goodarzi et al. (2010)	Q	570
(*R*)-2-(4-chloro-2-methylphenoxy)propanoic acid	1.0×10^4		Mackay et al. (2006d)	V	
$C_{10}H_{11}ClO_3$ (mecoprop-p) [16484-77-8]	1.8×10^4		Maniere et al. (2011)	?	12, 166
WNTGYJSOUMFZEP-SSDOTTSWSA-N					
dacthal	4.4		Muir et al. (2004)	L	369
$C_{10}H_6Cl_4O_4$	4.5		Duchowicz et al. (2020)	V	187
(DCPA)	4.5		HSDB (2015)	V	
[1861-32-1]	1.4×10^2		Duchowicz et al. (2020)	Q	
NPOJQCVWMSKXDN-UHFFFAOYSA-N					
4-(2,4-dichlorophenoxy)-butanoic acid	4.3×10^3		HSDB (2015)	Q	100
$C_{10}H_{10}Cl_2O_3$ (2,4-DB) [94-82-6]	2.2×10^5		Maniere et al. (2011)	?	242, 166
YIVXMZJTEQBPQO-UHFFFAOYSA-N					
dichlone	9.7×10^3		HSDB (2015)	Q	100
$C_{10}H_4Cl_2O_2$ [117-80-6]					
SVPKNMBRVBMTLB-UHFFFAOYSA-N					

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-[(2,3,6-trichlorophenyl)methoxy]propan-2-ol	2.0×10^{1}		Duchowicz et al. (2020)	V	187
$C_{10}H_{11}Cl_3O_2$	1.7×10^{1}		Duchowicz et al. (2020)	Q	
(tritac)					
[1861-44-5]					
LJWIIRATRWPHBA-UHFFFAOYSA-N					
(2,4-dichlorophenoxy)-acetic acid 1-methylethyl ester	4.6		Duchowicz et al. (2020)	V	187
$C_{11}H_{12}Cl_2O_3$	4.5		HSDB (2015)	V	
[94-11-1]	2.0		Duchowicz et al. (2020)	Q	
WHOKDONDRZNCBC-UHFFFAOYSA-N					
4-(4-chloro-2-methylphenoxy)butanoic acid	3.6×10^{3}		Duchowicz et al. (2020)	V	187
$C_{11}H_{13}ClO_3$	3.1×10^{3}		Mackay et al. (2006d)	V	
(MCPB)	1.7×10^{3}		Duchowicz et al. (2020)	Q	
[94-81-5]	3.3×10^{4}		Maniere et al. (2011)	?	242, 166
LLWADFLAOKUBDR-UHFFFAOYSA-N					
triclosan	4.7×10^{2}		HSDB (2015)	Q	100
$C_{12}H_7Cl_3O_2$	2.0×10^{3}		Zhang et al. (2010)	Q	288, 289
[3380-34-5]	5.7×10^{1}		Zhang et al. (2010)	Q	288, 290
XEFQLINVKFYRCS-UHFFFAOYSA-N	1.4×10^{3}		Zhang et al. (2010)	Q	288, 291
	8.2×10^{2}		Zhang et al. (2010)	Q	288, 292
monobutyl tetrachlorophthalate	2.0×10^{4}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_{10}Cl_4O_4$	7.5×10^{2}		Zhang et al. (2010)	Q	288, 290
[24261-19-6]	5.1×10^{4}		Zhang et al. (2010)	Q	288, 291
WKYMTJULVAGWJM-UHFFFAOYSA-N	5.1×10^{4}		Zhang et al. (2010)	Q	288, 292
(2,4-dichlorophenoxy)-acetic acid butyl ester	2.0×10^{1}		Duchowicz et al. (2020)	V	187
$C_{12}H_{14}Cl_2O_3$	2.0×10^{1}		HSDB (2015)	V	
[94-80-4]	5.7		Duchowicz et al. (2020)	Q	
UQMRAFJOBWOFNS-UHFFFAOYSA-N					
sucralose	2.5×10^{13}		HSDB (2015)	Q	100
$C_{12}H_{19}Cl_3O_8$					
[56038-13-2]					
BAQAVOSOZGMPRM-QBMZZYIRSA-N					
endrin aldehyde	2.4		Duchowicz et al. (2020)	V	187
$C_{12}H_8Cl_6O$	2.3		HSDB (2015)	V	
[7421-93-4]	4.8		Duchowicz et al. (2020)	Q	
HCTWZIFNBBCVGM-UHFFFAOYSA-N					

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
clorophene	3.7×10^{3}		Duchowicz et al. (2020)	V	187
$C_{13}H_{11}ClO$	3.7×10^{3}		HSDB (2015)	V	
(4-chloro-2-benzylphenol)	6.5×10^{2}		Duchowicz et al. (2020)	Q	
[120-32-1]					
NCKMMSIFQUPKCK-UHFFFAOYSA-N					
(4-chlorophenyl)phenylmethanone	7.0		HSDB (2015)	Q	100
$C_{13}H_9ClO$					
(4-chlorobenzophenone)					
[134-85-0]					
UGVRJVHOJNYEHR-UHFFFAOYSA-N					
1-(4-chlorophenyl)-4,4-dimethyl-3-pentanone	1.1		Zhang et al. (2010)	Q	288, 289
$C_{13}H_{17}ClO$	7.2×10^{-1}		Zhang et al. (2010)	Q	288, 290
[66346-01-8]	4.2		Zhang et al. (2010)	Q	288, 291
ILQGIJDYSLHIOX-UHFFFAOYSA-N	3.9×10^{-1}		Zhang et al. (2010)	Q	288, 292
hexachlorophene	1.8×10^{7}		HSDB (2015)	Q	100
$C_{13}H_6Cl_6O_2$	1.1×10^{7}		Zhang et al. (2010)	Q	288, 289
[70-30-4]	2.5×10^{5}		Zhang et al. (2010)	Q	288, 290
ACGUYXCXAPNIKK-UHFFFAOYSA-N	1.2×10^{4}		Zhang et al. (2010)	Q	288, 291
	6.5×10^{5}		Zhang et al. (2010)	Q	288, 292
2,4'-dichlorobenzophenone	9.2		Zhang et al. (2010)	Q	288, 289
$C_{13}H_8Cl_2O$	6.9		Zhang et al. (2010)	Q	288, 290
[85-29-0]	4.3×10^{1}		Zhang et al. (2010)	Q	288, 291
YXMYPHLWXBXNFF-UHFFFAOYSA-N	6.1×10^{1}		Zhang et al. (2010)	Q	288, 292
1-(4-chlorophenyl)-4,4-dimethylpent-1-en-3-one	4.8		Zhang et al. (2010)	Q	288, 289
$C_{13}H_{15}ClO$	2.2		Zhang et al. (2010)	Q	288, 290
[1577-03-3]	8.2		Zhang et al. (2010)	Q	288, 291
LXJZYHPGRKBVGF-UHFFFAOYSA-N	1.5		Zhang et al. (2010)	Q	288, 292
dichlorophen	8.2×10^{6}		HSDB (2015)	V	
$C_{13}H_{10}Cl_2O_2$	8.5×10^{6}		Mackay et al. (2006d)	V	
[97-23-4]					
MDNWOSOZYLHTCG-UHFFFAOYSA-N					
MCPB ethyl ester	2.0×10^{2}		Duchowicz et al. (2020)	V	187
$C_{13}H_{17}ClO_3$	2.9		Duchowicz et al. (2020)	Q	
[10443-70-6]					
XNKARWLGLZGMGX-UHFFFAOYSA-N					
2-chloro-9,10-anthracenedione	4.2×10^{3}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_7ClO_2$	6.7×10^{2}		Zhang et al. (2010)	Q	288, 290
[131-09-9]	1.4×10^{2}		Zhang et al. (2010)	Q	288, 291
FPKCTSIVDAWGFA-UHFFFAOYSA-N	3.3×10^{4}		Zhang et al. (2010)	Q	288, 292

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dicofol	4.1×10^{1}		Duchowicz et al. (2020)	V	187
$C_{14}H_9Cl_5O$	4.1×10^{1}		HSDB (2015)	V	
[115-32-2]	9.6×10^{2}		Duchowicz et al. (2020)	Q	
UOAMTSKGCBMZTC-UHFFFAOYSA-N	1.8×10^{4}		Zhang et al. (2010)	Q	288, 289
	3.1×10^{2}		Zhang et al. (2010)	Q	288, 290
	9.2×10^{1}		Zhang et al. (2010)	Q	288, 291
	3.2×10^{3}		Zhang et al. (2010)	Q	288, 292
bis(2,4-dichlorobenzoyl)peroxide	9.2		Zhang et al. (2010)	Q	288, 289
$C_{14}H_6Cl_4O_4$	1.4×10^{2}		Zhang et al. (2010)	Q	288, 290
[133-14-2]	1.6×10^{3}		Zhang et al. (2010)	Q	288, 291
WRXCBRHBHGNNQA-UHFFFAOYSA-N	3.5×10^{3}		Zhang et al. (2010)	Q	288, 292
dipropyl tetrachlorophthalate	4.7×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_{14}Cl_4O_4$	3.0×10^{1}		Zhang et al. (2010)	Q	288, 290
[6928-67-2]	1.0×10^{1}		Zhang et al. (2010)	Q	288, 291
QJRSPJSHRYYBJL-UHFFFAOYSA-N	2.8×10^{1}		Zhang et al. (2010)	Q	288, 292
2-(4-chlorobenzoyl)benzoic acid	3.4×10^{5}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_9ClO_3$	3.6×10^{4}		Zhang et al. (2010)	Q	288, 290
[85-56-3]	7.9×10^{7}		Zhang et al. (2010)	Q	288, 291
YWECCEXWKFHHQJ-UHFFFAOYSA-N	2.1×10^{6}		Zhang et al. (2010)	Q	288, 292
(2,4,5-trichlorophenoxy)acetic acid butoxyethanol ester $C_{14}H_{17}Cl_3O_4$ [2545-59-7] GLDWASBMYWLQGG-UHFFFAOYSA-N	1.2×10^{2}		HSDB (2015)	Q	100
(2,4-dichlorophenoxy)-acetic acid, 2-butoxyethyl ester	6.2×10^{1}		Duchowicz et al. (2020)	V	187
$C_{14}H_{18}Cl_2O_4$	6.2×10^{1}		HSDB (2015)	V	
[1929-73-3]	6.0×10^{1}		Duchowicz et al. (2020)	Q	
ZMWGIGHRZQTQRE-UHFFFAOYSA-N					
1-chloro-9,10-anthracenedione	4.3×10^{2}		Abraham et al. (2019)	Q	
$C_{14}H_7ClO_2$	4.2×10^{3}		HSDB (2015)	Q	100
(1-chloroanthraquinone) [82-44-0] BOCJQSFSGAZAPQ-UHFFFAOYSA-N					
chlorflurenol methyl $C_{15}H_{11}ClO_3$ [2536-31-4] LINPVWIEWJTEEJ-UHFFFAOYSA-N	1.3×10^{3}		Ebert et al. (2023)	?	367

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,4'-(1-methylethylidene)bis(2,6-dichlorophenol) $C_{15}H_{12}Cl_4O_2$ (2,2',6,6'-tetrachlorobisphenol A) [79-95-8] KYPYTERUKNKOLP-UHFFFAOYSA-N	3.5×10^{6}		HSDB (2015)	Q	449
diclofop $C_{15}H_{12}Cl_2O_4$ [40843-25-2] OOLBCHYXZDXLDS-UHFFFAOYSA-N	9.2×10^{5}		Ebert et al. (2023)	?	317
methoxychlor $C_{16}H_{15}Cl_3O_2$ [72-43-5] IAKOZHOLGAGEJT-UHFFFAOYSA-N	4.9×10^{1}		Altschuh et al. (1999)	M	
	1.0		Mackay et al. (2006d)	V	
	4.0		Keshavarz et al. (2022)	Q	
	5.5		Duchowicz et al. (2020)	Q	
	2.8		Hilal et al. (2008)	Q	
	6.4		Modarresi et al. (2007)	Q	68
	4.9×10^{1}		Duchowicz et al. (2020)	?	186, 21
diclofop-methyl $C_{16}H_{14}Cl_2O_4$ [51338-27-3] BACHBFVBHLGWSL-UHFFFAOYSA-N	5.0		Duchowicz et al. (2020)	V	187
	5.0		Mackay et al. (2006d)	V	
	1.3×10^{2}		Duchowicz et al. (2020)	Q	
	2.6×10^{2}		HSDB (2015)	Q	100
	9.5×10^{1}		Maniere et al. (2011)	?	12, 166
chlorobenzilate $C_{16}H_{14}Cl_2O_3$ [510-15-6] RAPBNVDSDCTNRC-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	V	
	2.6×10^{2}		MacBean (2012a)	?	
(2,4-dichlorophenoxy)-acetic acid 2-ethylhexyl ester	5.5×10^{-1}		MacBean (2012b)	X	352
$C_{16}H_{22}Cl_2O_3$ [1928-43-4] QZSFJRIWRPJUOH-UHFFFAOYSA-N	5.5×10^{-1}		Maniere et al. (2011)	?	242, 166
(2,4-dichlorophenoxy)-acetic acid, isooctyl ester	1.0×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{16}H_{22}Cl_2O_3$	3.3×10^{-1}		Duchowicz et al. (2020)	Q	
[25168-26-7]	1.7×10^{-1}		HSDB (2015)	Q	100
BBPLSOGERZQYQC-UHFFFAOYSA-N					
mecoprop-2-butoxyethyl ester $C_{16}H_{23}ClO_4$ [23359-62-8] GWFGUAFFJVHZKY-UHFFFAOYSA-N	5.0		Ebert et al. (2023)	?	319

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chloropropylate $C_{17}H_{16}Cl_2O_3$ [5836-10-2] AXGUBXVWZBFQGA-UHFFFAOYSA-N	1.2×10^{3} 1.0×10^{2}		HSDB (2015) MacBean (2012a)	V ?	
MCPA-2-ethylhexyl ester $C_{17}H_{25}ClO_3$ [29450-45-1] IDGRPSMONFWWEK-UHFFFAOYSA-N	2.3×10^{-1}		Ebert et al. (2023)	?	319
1-(2-(2-chloroethoxy)ethoxy)-4-(1,1,3,3-tetramethylbutyl)benzene $C_{18}H_{29}ClO_2$ [65925-28-2] FITQCDWGUKECBJ-UHFFFAOYSA-N	5.3×10^{-1} 1.6 3.8×10^{-1} 8.4×10^{-2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
fenofibrate $C_{20}H_{21}ClO_4$ [49562-28-9] YMTINGFKWWXKFG-UHFFFAOYSA-N	2.2×10^{3}		HSDB (2015)	Q	100
indanofan $C_{20}H_{17}O_3Cl$ [133220-30-1] PMAAYIYCDXGUAP-UHFFFAOYSA-N	1.5×10^{4} 5.4×10^{3}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
spirodiclofen $C_{21}H_{24}Cl_2O_4$ [148477-71-8] DTDSAWVUFPGDMX-UHFFFAOYSA-N	1.7×10^{2} $>5.0\times10^{2}$		HSDB (2015) Maniere et al. (2011)	V ?	 12, 166
permethrin $C_{21}H_{20}Cl_2O_3$ [52645-53-1] RLLPVAHGXHCWKJ-UHFFFAOYSA-N	5.3 4.1 9.0 1.2×10^{1}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Duchowicz et al. (2020)	V V V Q	187
chlorophacinone $C_{23}H_{15}ClO_3$ [3691-35-8] UDHXJZHVNHGCEC-UHFFFAOYSA-N	2.7×10^{6} 4.1×10^{4}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
chlormadinone acetate $C_{23}H_{29}ClO_4$ [302-22-7] QMBJSIBWORFWQT-UHFFFAOYSA-N	1.8×10^{4}		HSDB (2015)	Q	100
3,4,5,6-tetrachlorophthalic acid bis(2-ethylhexyl) ester $C_{24}H_{34}Cl_4O_4$ [34832-88-7] BELGUQVGZMFEAQ-UHFFFAOYSA-N	2.8 2.3×10^{1} 1.0×10^{4} 3.5		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
endosulfan alcohol	7.7×10^{3}		Zhang et al. (2010)	Q	288, 289
$C_9H_8Cl_6O_2$	3.0×10^{6}		Zhang et al. (2010)	Q	288, 290
[2157-19-9]	1.3×10^{5}		Zhang et al. (2010)	Q	288, 291
GTSJHTSVFKEASK-UHFFFAOYSA-N	1.8×10^{5}		Zhang et al. (2010)	Q	288, 292
chlorendic anhydride	1.1×10^{2}		Zhang et al. (2010)	Q	288, 289
$C_9H_2Cl_6O_3$	3.1×10^{4}		Zhang et al. (2010)	Q	288, 290
[115-27-5]	1.5×10^{4}		Zhang et al. (2010)	Q	288, 291
FLBJFXNAEMSXGL-UHFFFAOYSA-N	3.9×10^{7}		Zhang et al. (2010)	Q	288, 292
1,4,5,6,7,7-hexachloro-bicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid	3.3×10^{8}		HSDB (2015)	Q	100
$C_9H_4Cl_6O_4$	3.3×10^{8}		Zhang et al. (2010)	Q	288, 289
[115-28-6]	3.1×10^{9}		Zhang et al. (2010)	Q	288, 290
DJKGDNKYTKCJKD-UHFFFAOYSA-N	3.9×10^{9}		Zhang et al. (2010)	Q	288, 291
	7.3×10^{7}		Zhang et al. (2010)	Q	288, 292
heptachlorepoxide	4.8×10^{-1}		Shen and Wania (2005)	L	368
$C_{10}H_5Cl_7O$	5.9×10^{-1}		Shen and Wania (2005)	L	369
[1024-57-3]	9.6×10^{-1}		Chao et al. (2017)	M	
ZXFXBSWRVIQKOD-UHFFFAOYSA-N	5.0×10^{-1}	5200	Cetin et al. (2006)	M	
	4.7×10^{-1}		Altschuh et al. (1999)	M	
	3.1×10^{-1}		Warner et al. (1980)	M	
	5.4×10^{-1}		Hilal et al. (2008)	C	
	1.3×10^{1}		Ryan et al. (1988)	C	
	3.1×10^{-1}		Shen (1982)	C	
	6.6×10^{-1}		Keshavarz et al. (2022)	Q	
	7.7×10^{-1}		Duchowicz et al. (2020)	Q	
	7.3		Hilal et al. (2008)	Q	
	5.4		Modarresi et al. (2007)	Q	68
	4.7×10^{-1}		Duchowicz et al. (2020)	?	186, 21
dieldrin	1.0		Shen and Wania (2005)	L	368
$C_{12}H_8OCl_6$	9.1×10^{-1}		Shen and Wania (2005)	L	369
[60-57-1]	9.1×10^{-1}		Mackay and Shiu (1981)	L	
DFBKLUNHFCTMDC-NLUYNBKHSA-N	6.5×10^{-1}		Chao et al. (2017)	M	
	9.2×10^{-1}	5800	Cetin et al. (2006)	M	
	9.8×10^{-1}		Altschuh et al. (1999)	M	
	3.4×10^{-1}		Slater and Spedding (1981)	M	12
	1.7×10^{-1}		Warner et al. (1980)	M	
	8.9×10^{-1}		Mackay et al. (2006d)	V	
	8.9×10^{-1}		Suntio et al. (1988)	V	12
	4.9×10^{1}		Mackay and Leinonen (1975)	V	
	8.8×10^{-3}		Barcelo and Hennion (1997)	X	569
	1.7×10^{-1}		Hilal et al. (2008)	C	
	5.0×10^{1}		Suntio et al. (1988)	C	12

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{1}		Suntio et al. (1988)	C	683
	9.8×10^{-1}		Suntio et al. (1988)	C	683
	1.7×10^{-1}		Suntio et al. (1988)	C	
	4.7×10^{-2}		Suntio et al. (1988)	C	
	1.3		Ryan et al. (1988)	C	
	1.7×10^{-1}		Shen (1982)	C	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	7.2×10^{-1}		Duchowicz et al. (2020)	Q	
	7.4×10^{-4}		Goodarzi et al. (2010)	Q	570, 573
	1.1		Hilal et al. (2008)	Q	
	2.7		Modarresi et al. (2007)	Q	68
	9.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	1.2		MacBean (2012a)	?	
	5.7×10^{1}		Brimblecombe (1986)	?	81
endrin	1.6		Shen and Wania (2005)	L	368
$C_{12}H_8Cl_6O$	9.1×10^{-1}		Shen and Wania (2005)	L	369
[72-20-8]	1.5		Chao et al. (2017)	M	
DFBKLUNHFCTMDC-GKRDHZSOSA-N	1.8	4600	Cetin et al. (2006)	M	
	1.6		Altschuh et al. (1999)	M	
	3.0×10^{1}		Mackay et al. (2006d)	V	
	3.0×10^{1}		Suntio et al. (1988)	V	12
	5.6×10^{3}		Suntio et al. (1988)	C	
	2.4×10^{1}		Ryan et al. (1988)	C	
	1.2		Keshavarz et al. (2022)	Q	
	7.2×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.1		Hilal et al. (2008)	Q	
	2.7		Modarresi et al. (2007)	Q	68
	1.6		Duchowicz et al. (2020)	?	186, 21
1,4,5,6,7,7-hexachlorobicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid, dibutyl ester	5.8×10^{2}		Zhang et al. (2010)	Q	288, 289
$C_{17}H_{20}Cl_6O_4$	1.4×10^{2}		Zhang et al. (2010)	Q	288, 290
[1770-80-5]	4.6×10^{3}		Zhang et al. (2010)	Q	288, 291
UJAHPBDUQZFDLA-UHFFFAOYSA-N	8.0×10^{2}		Zhang et al. (2010)	Q	288, 292
di-2-ethylhexyl chlorendate	6.0×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_{25}H_{36}Cl_6O_4$	2.1×10^{2}		Zhang et al. (2010)	Q	288, 290
[4827-55-8]	5.2×10^{3}		Zhang et al. (2010)	Q	288, 291
ONIHOIFWLALAQH-UHFFFAOYSA-N	1.6×10^{2}		Zhang et al. (2010)	Q	288, 292

A6.5 Polychlorinated diphenyl ethers (PCDEs)

Table A6.5: Polychlorinated diphenyl ethers (PCDEs)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-chlorodiphenyl ether $C_{12}H_9ClO$ (PCDE-1) [2689-07-8] IPBRZLMGGXHHMS-UHFFFAOYSA-N	3.1×10^{-2}		Kurz and Ballschmiter (1999)	V	
3-chlorodiphenyl ether $C_{12}H_9ClO$ (PCDE-2) [6452-49-9] BMURONZFJJPAOK-UHFFFAOYSA-N	1.2×10^{-1} 2.7×10^{-2} 3.0×10^{-1}		Kurz and Ballschmiter (1999) Hilal et al. (2008) Modarresi et al. (2007)	V Q Q	 68
4-chlorodiphenyl ether $C_{12}H_9ClO$ (PCDE-3) [7005-72-3] PGPNJCAMHOJTEF-UHFFFAOYSA-N	1.1×10^{-1} 4.5×10^{-2} 9.0×10^{-2} 4.0×10^{-2} 3.1×10^{-2}		Kurz and Ballschmiter (1999) Mackay et al. (1993) Howard and Meylan (1997) Ryan et al. (1988) Hilal et al. (2008)	V V X C Q	 448
2,3-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-5) [68486-28-2] VSKSUBSGORDMQX-UHFFFAOYSA-N	2.4×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,4-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-7) [51892-26-3] KXIPYLZZJZMMPD-UHFFFAOYSA-N	1.9×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,4'-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-8) [6903-65-7] MWKULKMSBBSGTP-UHFFFAOYSA-N	3.2×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,5-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-9) [24910-69-8] VITXVDNQHXYQSK-UHFFFAOYSA-N	7.9×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,6-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-10) [28419-69-4] IRLZOQDGEAEIPX-UHFFFAOYSA-N	5.0×10^{-2}		Kurz and Ballschmiter (1999)	V	

Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-12) [55538-69-7] QFQLZVAAQOJUFS-UHFFFAOYSA-N	1.1×10^{-1}		Kurz and Ballschmiter (1999)	V	
3,4'-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-13) [6842-62-2] HPRGYUWRGCTBAV-UHFFFAOYSA-N	1.3×10^{-1}		Kurz and Ballschmiter (1999)	V	
3,5-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-14) [24910-68-7] LEKOWSSKXYFERR-UHFFFAOYSA-N	6.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
4,4'-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-15) [2444-89-5] URUJZHZLCCIILC-UHFFFAOYSA-N	2.1×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,2',4-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-17) [68914-97-6] YXMNUPKWUMIZAV-UHFFFAOYSA-N	4.5×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,3,4-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-21) [85918-32-7] ANKBTLMYMVMWBS-UHFFFAOYSA-N	2.8×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,3,4'-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-22) [157683-71-1] KOTNFWJIMRGVBR-UHFFFAOYSA-N	3.2×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,3,5-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-23) [162853-24-9] MDSPKCWGOVVFJD-UHFFFAOYSA-N	2.2×10^{-1}		Kurz and Ballschmiter (1999)	V	

Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,6-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-24) [162853-25-0] RQSRPDGSUDRYLH-UHFFFAOYSA-N	3.0×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3',4-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-25) [155999-93-2] BJFOCMRBCBZFJT-UHFFFAOYSA-N	1.5×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,4,4'-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-28) [59039-21-3] PIORTDHJOLELKR-UHFFFAOYSA-N	3.0×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,4,5-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-29) [52322-80-2] UWKZWXCTDPYXHU-UHFFFAOYSA-N	8.9×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,4,6-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-30) [63646-52-6] WXLQUFLKMICSSY-UHFFFAOYSA-N	1.4×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,4',5-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-31) [65075-00-5] FZBSTAVCYOMFMD-UHFFFAOYSA-N	1.6×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,4',6-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-32) [157683-72-2] ZMRFCSWFCKICQE-UHFFFAOYSA-N	4.2×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3',4'-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-33) [61328-44-7] VBNJGYOQZAENPO-UHFFFAOYSA-N	3.4×10^{-1}		Kurz and Ballschmiter (1999)	V	

Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3',4-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-35) [66794-60-3] BUKLLCIUMZELOH-UHFFFAOYSA-N	2.2×10^{-1}		Kurz and Ballschmiter (1999)	V	
3,4,4'-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-37) [63646-51-5] FTZDEZOARSJHGU-UHFFFAOYSA-N	1.6×10^{-1}		Kurz and Ballschmiter (1999)	V	
3,4,5-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-38) [63646-53-7] ZQCCHNBMSHOJAT-UHFFFAOYSA-N	9.1×10^{-3}		Kurz and Ballschmiter (1999)	V	
3,4',5-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-39) [24910-73-4] CCEZFZGXWFJQEF-UHFFFAOYSA-N	1.6×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,2',3,4-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-41) [220002-37-9] VTTDWGUAWMLHPR-UHFFFAOYSA-N	5.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-42) [147102-63-4] UYVBJPIPRAJEKW-UHFFFAOYSA-N	5.8×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',4,4'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-47) [28076-73-5] ZRWRPGGXCSSBAO-UHFFFAOYSA-N	2.9×10^{-2} 2.8×10^{-1}		Kurz and Ballschmiter (1999) HSDB (2015)	V Q	 100
2,2',4,5-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-48) [162853-26-1] DRVAMLZVBNYSQE-UHFFFAOYSA-N	1.6×10^{-2}		Kurz and Ballschmiter (1999)	V	

Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',4,5'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-49) [155999-92-1] XIXPEFLLHQAIOY-UHFFFAOYSA-N	2.6×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,3',4-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-55) [220002-39-1] IZISEKJPNSBPRX-UHFFFAOYSA-N	2.3×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,3',4'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-56) [162853-27-2] JVFGXWCLGNACOG-UHFFFAOYSA-N	4.4×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,4,4'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-60) [65075-01-6] ZPOBHUZRVVTGKB-UHFFFAOYSA-N	3.6×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,4,5-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-61) [220002-40-4] QAPPZLVGIXQUJW-UHFFFAOYSA-N	6.6×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,3,4,6-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-62) [85918-33-8] WJZPRRFFZWVZJL-UHFFFAOYSA-N	9.1×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,3,4',5-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-63) [220002-41-5] YHQRYZGDQCSHFO-UHFFFAOYSA-N	1.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,4',6-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-64) [220002-42-6] HJCNTJIMUWQMSA-UHFFFAOYSA-N	3.8×10^{-2}		Kurz and Ballschmiter (1999)	V	

Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,5,6-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-65) [63646-54-8] UFGXCDQXRUFDMA-UHFFFAOYSA-N	9.3×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,3',4,4'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-66) [61328-46-9] CAWSVYYOUZEMHA-UHFFFAOYSA-N	2.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3',4,5-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-67) [152833-52-8] QDQGECFQVPRMEO-UHFFFAOYSA-N	8.9×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,3',4,5'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-68) [147102-64-5] XORVNHCKWFPDLN-UHFFFAOYSA-N	1.0×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3',4',5-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-70) [159553-67-0] MFTPXFIGIJCNJM-UHFFFAOYSA-N	1.8×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3',4',6-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-71) [130892-66-9] IZZULMOBRTYHMH-UHFFFAOYSA-N	4.6×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,4,4',5-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-74) [61328-45-8] KXOJXWNARBQHNX-UHFFFAOYSA-N	1.9×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,4,4',6-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-75) [63553-30-0] YCWRSOTXXJYCKF-UHFFFAOYSA-N	1.7×10^{-2}		Kurz and Ballschmiter (1999)	V	

Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3',4,4'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-77) [56348-72-2] DHLVZXZRIZBPKG-UHFFFAOYSA-N	4.1×10^{-2}		Kurz and Ballschmiter (1999)	V	
3,3',4,5'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-79) [552884-22-7] BUPRSRBWDJVKGG-UHFFFAOYSA-N	1.0×10^{-2}		Kurz and Ballschmiter (1999)	V	
3,4,4',5-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-81) [62615-07-0] CAUBBRCOHHHCNG-UHFFFAOYSA-N	1.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,3',4-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-82) [160282-10-0] ABRDPORILGADAP-UHFFFAOYSA-N	8.3×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4,4'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-85) [71585-37-0] RSBUDFTVQYJNHK-UHFFFAOYSA-N	5.2×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4,5'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-87) [160282-09-7] SCLCXTQIVCULDR-UHFFFAOYSA-N	2.2×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4,6'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-89) [85918-35-0] JGXAONSRHOSPTJ-UHFFFAOYSA-N	6.5×10^{-2}		Kurz and Ballschmiter (1999)	V	

Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4',5-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-90) [157683-73-3] QPEBRZQSEUOWPA-UHFFFAOYSA-N	1.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4',6-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-91) [116995-20-1] BRNKJDZWZYZVNM-UHFFFAOYSA-N	3.9×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4',5'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-97) [160282-08-6] ABYZYVAIOYICJQ-UHFFFAOYSA-N	3.3×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',4,4',5-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-99) [60123-64-0] AVURWLKSFZBANQ-UHFFFAOYSA-N	1.8×10^{-2} 3.8×10^{-2}	 6100	Kurz and Ballschmiter (1999) Paasivirta et al. (1999)	V T	
2,2',4,4',6-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-100) [104294-16-8] FONWDRSQXQZNBN-UHFFFAOYSA-N	2.1×10^{-2} 1.3×10^{-2}	 5800	Kurz and Ballschmiter (1999) Paasivirta et al. (1999)	V T	
2,2',4,5,5'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-101) [131138-21-1] MKIAKZAWONVRFF-UHFFFAOYSA-N	1.6×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',4,5,6'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-102) [130892-67-0] BOJBTUWEQMUWHT-UHFFFAOYSA-N	3.7×10^{-2}		Kurz and Ballschmiter (1999)	V	

Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',4,4'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-105) [85918-31-6] PKEGIXYNAGGYPN-UHFFFAOYSA-N	4.2×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,3',4,5'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-108) [160282-07-5] HCTKORQPUZCIAO-UHFFFAOYSA-N	1.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,3',4,6-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-109) [727738-64-9] SEIXDCGLHKOBEO-UHFFFAOYSA-N	1.4×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,3',4',6-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-110) [159553-69-2] KASGFDPQAMDPAZ-UHFFFAOYSA-N	3.6×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,4,4',5-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-114) [113464-17-8] WSTVMACYLXUQIM-UHFFFAOYSA-N	1.2×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,4,4',6-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-115) [160282-05-3] LUNNFBBTEHRYMW-UHFFFAOYSA-N	1.1×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,4,5,6-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-116) [22274-42-6] JDWOFUWJURZFFF-UHFFFAOYSA-N	6.6×10^{-3}		Kurz and Ballschmiter (1999)	V	

Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4',5,6-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-117) [63646-55-9] UETIKWAWMZLQQZ-UHFFFAOYSA-N	1.1×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3',4,4',5-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-118) [60123-65-1] NRAVUGAGYOBXIG-UHFFFAOYSA-N	1.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3',4,4',6-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-119) [157683-74-4] POOXVKSDWCXIBU-UHFFFAOYSA-N	1.3×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3',4,5,5'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-120) [160282-04-2] XIFRTJZLSYOLIU-UHFFFAOYSA-N	4.8×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,3',4,4',5'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-123) [160282-06-4] BUAXMSGDEZZOJD-UHFFFAOYSA-N	1.3×10^{-2}		Kurz and Ballschmiter (1999)	V	
3,3',4,4',5-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-126) [94339-59-0] WDBLKMRZRGLISL-UHFFFAOYSA-N	1.0×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,3',4,4'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-128) [71585-39-2] GSWMXIIUDJOXNF-UHFFFAOYSA-N	8.3×10^{-2}		Kurz and Ballschmiter (1999)	V	

Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,5'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-130) [76621-14-2] JTEWACHFMNTRBB-UHFFFAOYSA-N	1.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,3',4,6'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-132) [124076-66-0] YDVYLSIVXYLBBX-UHFFFAOYSA-N	6.2×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4,4',5-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-137) [71585-38-1] LDPJEMNNPDFBCQ-UHFFFAOYSA-N	1.8×10^{-2} 1.9×10^{-2}	 6400	Kurz and Ballschmiter (1999) Paasivirta et al. (1999)	V T	
2,2',3,4,4',5'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-138) [71585-36-9] PHSJJYZIFPWCLZ-UHFFFAOYSA-N	2.9×10^{-2} 2.8×10^{-2}	 6500	Kurz and Ballschmiter (1999) Paasivirta et al. (1999)	V T	
2,2',3,4,4',6-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-139) [106220-83-1] BIWCEXHDIQZFHI-UHFFFAOYSA-N	9.8×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,2',3,4,4',6'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-140) [106220-82-0] XDAOZRZWYVKIAK-UHFFFAOYSA-N	3.0×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4',5,5'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-146) [162853-28-3] SFTBUGPDOJDENF-UHFFFAOYSA-N	1.0×10^{-2}		Kurz and Ballschmiter (1999)	V	

Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4',5,6-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-147) [116995-18-7] DIBYIHMYEPMGKC-UHFFFAOYSA-N	1.0×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4',5',6-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-149) [85918-37-2] RDKSFIZNZGWNLA-UHFFFAOYSA-N	3.1×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',4,4',5,5'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-153) [71859-30-8] PECXRRMHOQBOIE-UHFFFAOYSA-N	1.3×10^{-2} 1.1×10^{-2}	 6300	Kurz and Ballschmiter (1999) Paasivirta et al. (1999)	V T	
2,2',4,4',5,6'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-154) [106220-81-9] XKQUAQGQLZDDBV-UHFFFAOYSA-N	1.4×10^{-2} 4.4×10^{-3}	 5900	Kurz and Ballschmiter (1999) Paasivirta et al. (1999)	V T	
2,3,3',4,4',5-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-156) [109828-22-0] GHTWMHLFFDEYRE-UHFFFAOYSA-N	1.2×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,3',4,4',5'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-157) [94339-60-3] FEIDIWDEJQVIPO-UHFFFAOYSA-N	2.8×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,3',4',5,6-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-163) [155999-97-6] YLAYOOJLJKJGCF-UHFFFAOYSA-N	1.6×10^{-2}		Kurz and Ballschmiter (1999)	V	

Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4,4',5,6-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-166) [63646-56-0] MXDRLBNLTLOWGV-UHFFFAOYSA-N	5.0×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,3',4,4',5,5'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-167) [131138-20-0] DYSUSQZPGJXVAL-UHFFFAOYSA-N	8.3×10^{-3}		Kurz and Ballschmiter (1999)	V	
	9.0×10^{-3}	6200	Paasivirta et al. (1999)	T	
2,2',3,3',4,4',5-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-170) [71585-40-5] BLBURLWSCHSPIS-UHFFFAOYSA-N	2.0×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,3',4,5,6'-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-174) [159553-73-8] DQYYZAABYZAOOC-UHFFFAOYSA-N	1.8×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,3',4,5',6'-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-177) [83992-71-6] RXPQVFMDOJTCKE-UHFFFAOYSA-N	1.4×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4,4',5,5'-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-180) [83992-69-2] YBYYCWMPXZRBNJ-UHFFFAOYSA-N	5.0×10^{-3}		Kurz and Ballschmiter (1999)	V	
	1.9×10^{-2}	6800	Paasivirta et al. (1999)	T	

Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,4',5,6-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-181) [157683-75-5] RPNFRXWGMTYOPA-UHFFFAOYSA-N	3.4×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,2',3,4,4',5,6'-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-182) [88467-63-4] XWRZWPPSQDHTFU-UHFFFAOYSA-N	3.3×10^{-3}	6400	Paasivirta et al. (1999)	T	
2,2',3,4,4',6,6'-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-184) [106220-84-2] WTYSJAGEYAAIFW-UHFFFAOYSA-N	2.0×10^{-1}	7800	Paasivirta et al. (1999)	T	
2,2',3,4',5,5',6-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-187) [109828-23-1] BHJCMMGUFRZLKK-UHFFFAOYSA-N	7.4×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,3,3',4,4',5,5'-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-189) [83992-72-7] JUHPMUOWCYBMEY-UHFFFAOYSA-N	6.2×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,3,3',4,4',5,6-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-190) [83992-70-5] QLSBRXLSQINWHM-UHFFFAOYSA-N	5.8×10^{-3}		Kurz and Ballschmiter (1999)	V	

Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,4',5,5'- octachlorodiphenyl ether $C_{12}H_2Cl_8O$ (PCDE-194) [57379-40-5] IXZVOZCULZBCDY-UHFFFAOYSA-N	4.3×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,2',3,3',4,4',5,6- octachlorodiphenyl ether $C_{12}H_2Cl_8O$ (PCDE-195) [65075-02-7] YHUPMPHVHYBYJE-UHFFFAOYSA-N	1.8×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,2',3,3',4,4',5,6'- octachlorodiphenyl ether $C_{12}H_2Cl_8O$ (PCDE-196) [85918-38-3] HYNYIQBCBHJTOZ-UHFFFAOYSA-N	8.7×10^{-3}	7100	Paasivirta et al. (1999)	T	
2,2',3,3',4,4',6,6'- octachlorodiphenyl ether $C_{12}H_2Cl_8O$ (PCDE-197) [117948-62-6] GRWRDFGBFYSOKR-UHFFFAOYSA-N	7.7×10^{-3}	7000	Paasivirta et al. (1999)	T	
2,2',3,3',4,5,5',6'- octachlorodiphenyl ether $C_{12}H_2Cl_8O$ (PCDE-199) [83992-76-1] MRHQOXCYYPFGEE-UHFFFAOYSA-N	2.6×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,2',3,4,4',5,5',6- octachlorodiphenyl ether $C_{12}H_2Cl_8O$ (PCDE-203) [83992-75-0] PKOSPVZTRLMBSK-UHFFFAOYSA-N	2.3×10^{-3}		Kurz and Ballschmiter (1999)	V	

Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,4',5,5',6- nonachlorodiphenyl ether $C_{12}HCl_9O$ (PCDE-206) [83992-73-8] FPEYJPVHPGDXDD-UHFFFAOYSA-N	5.1×10^{-4}		Kurz and Ballschmiter (1999)	V	
decachlorodiphenyl ether $C_{12}Cl_{10}O$ (PCDE-209) [31710-30-2] CIPFDHFTBYJKQB-UHFFFAOYSA-N	7.1×10^{-5}		Kurz and Ballschmiter (1999)	V	

A6.6 Polychlorinated dibenzofuranes (PCDFs)

Table A6.6: Polychlorinated dibenzofuranes (PCDFs)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chlorodibenzofuran $C_{12}H_7ClO$ (PCDF-1) [84761-86-4] WRSMJZYBNIAAEE-UHFFFAOYSA-N	8.3×10^{-2}		Govers and Krop (1998)	Q	
2-chlorodibenzofuran $C_{12}H_7ClO$ (PCDF-2) [51230-49-0] PRKTYWJFCODJOA-UHFFFAOYSA-N	1.1×10^{-1}		Govers and Krop (1998)	Q	
3-chlorodibenzofuran $C_{12}H_7ClO$ (PCDF-3) [25074-67-3] BBOZMMAURMEVAR-UHFFFAOYSA-N	1.3×10^{-1}		Govers and Krop (1998)	Q	
4-chlorodibenzofuran $C_{12}H_7ClO$ (PCDF-4) [74992-96-4] RHRYBWFAHXCUCR-UHFFFAOYSA-N	8.9×10^{-2}		Govers and Krop (1998)	Q	
1,2-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-12) [64126-85-8] QVAPRJWSOUITIF-UHFFFAOYSA-N	1.5×10^{-1}		Govers and Krop (1998)	Q	
1,3-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-13) [94538-00-8] VKIBKEFGJSPRJC-UHFFFAOYSA-N	2.0×10^{-1}		Govers and Krop (1998)	Q	
1,4-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-14) [94538-01-9] VHQCMZLPHWGUDB-UHFFFAOYSA-N	1.5×10^{-1}		Govers and Krop (1998)	Q	
1,6-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-16) [74992-97-5] JRSRWACZUFLWKF-UHFFFAOYSA-N	1.4×10^{-1}		Govers and Krop (1998)	Q	

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,7-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-17) [94538-02-0] XRQNHPGZRFKBJW-UHFFFAOYSA-N	1.9×10^{-1}		Govers and Krop (1998)	Q	
1,8-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-18) [81638-37-1] UAFNQQBPUWFPGC-UHFFFAOYSA-N	2.5×10^{-1}		Govers and Krop (1998)	Q	
1,9-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-19) [70648-14-5] AEKSGHBVWJHELW-UHFFFAOYSA-N	2.0×10^{-1}		Govers and Krop (1998)	Q	
2,3-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-23) [64126-86-9] GETJJZZRPQFSFM-UHFFFAOYSA-N	2.3×10^{-1}		Govers and Krop (1998)	Q	
2,4-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-24) [24478-74-8] LHTCKMYRNOGUOA-UHFFFAOYSA-N	1.9×10^{-1}		Govers and Krop (1998)	Q	
2,6-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-26) [60390-27-4] XVLCNKFGFHUQNL-UHFFFAOYSA-N	1.8×10^{-1}		Govers and Krop (1998)	Q	
2,7-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-27) [74992-98-6] DOZUTNBCPVUMPY-UHFFFAOYSA-N	2.0×10^{-1}		Govers and Krop (1998)	Q	
2,8-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-28) [5409-83-6] IVVRJIDVYSPKFZ-UHFFFAOYSA-N	1.6×10^{-1} 1.6×10^{-1} 1.6×10^{-1} 4.2×10^{-1} 2.6×10^{-1} 2.2×10^{-1}		Duchowicz et al. (2020) Mackay et al. (2006b) Govers and Krop (1998) Duchowicz et al. (2020) Saçan et al. (2005) Govers and Krop (1998)	V V V Q Q Q	187

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-34) [94570-83-9] HYQGGNWDPQZLGX-UHFFFAOYSA-N	1.9×10^{-1}		Govers and Krop (1998)	Q	
3,6-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-36) [74918-40-4] DMOBGFAKTSXOHG-UHFFFAOYSA-N	2.2×10^{-1}		Govers and Krop (1998)	Q	
3,7-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-37) [58802-21-4] OLTYAGNRSNFHLK-UHFFFAOYSA-N	3.0×10^{-1}		Govers and Krop (1998)	Q	
4,6-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-46) [64560-13-0] BZFIZJNKNCJEAD-UHFFFAOYSA-N	2.2×10^{-1}		Govers and Krop (1998)	Q	
1,2,3-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-123) [83636-47-9] LADSWAAWPMGHBE-UHFFFAOYSA-N	2.9×10^{-1}		Govers and Krop (1998)	Q	
1,2,4-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-124) [24478-73-7] RQIWKWHVZLDXEJ-UHFFFAOYSA-N	2.5×10^{-1}		Govers and Krop (1998)	Q	
1,2,6-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-126) [64560-15-2] CYRZCBUWRUACKJ-UHFFFAOYSA-N	2.3×10^{-1}		Govers and Krop (1998)	Q	
1,2,7-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-127) [83704-37-4] AFOVQGPNOZDUEP-UHFFFAOYSA-N	2.3×10^{-1}		Govers and Krop (1998)	Q	

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,8-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-128) [83704-34-1] UYIGPSPCOXGBCS-UHFFFAOYSA-N	3.9×10^{-1}		Govers and Krop (1998)	Q	
1,2,9-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-129) [83704-38-5] ICTXINQOXPMQPM-UHFFFAOYSA-N	4.8×10^{-1}		Govers and Krop (1998)	Q	
1,3,4-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-134) [82911-61-3] FIPOITUDJFQRRN-UHFFFAOYSA-N	2.8×10^{-1}		Govers and Krop (1998)	Q	
1,3,6-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-136) [83704-39-6] AGPTXRLVBIRYLV-UHFFFAOYSA-N	3.3×10^{-1}		Govers and Krop (1998)	Q	
1,3,7-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-137) [64560-16-3] INRBXOGZPDFCLQ-UHFFFAOYSA-N	4.1×10^{-1}		Govers and Krop (1998)	Q	
1,3,8-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-138) [76621-12-0] PHFSTDOPTZHECA-UHFFFAOYSA-N	4.2×10^{-1}		Govers and Krop (1998)	Q	
1,3,9-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-139) [83704-40-9] SPPGDLROKBFNNO-UHFFFAOYSA-N	4.4×10^{-1}		Govers and Krop (1998)	Q	
1,4,6-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-146) [82911-60-2] XDQRWSUJOURTHK-UHFFFAOYSA-N	3.5×10^{-1}		Govers and Krop (1998)	Q	

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,4,7-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-147) [83704-41-0] XTLMVJUSIANHND-UHFFFAOYSA-N	3.2×10^{-1}		Govers and Krop (1998)	Q	
1,4,8-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-148) [64560-14-1] PCQCYDNFBUADOK-UHFFFAOYSA-N	3.9×10^{-1}		Govers and Krop (1998)	Q	
1,4,9-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-149) [70648-13-4] NVYUPBVXKLTYHV-UHFFFAOYSA-N	3.5×10^{-1}		Govers and Krop (1998)	Q	
1,6,7-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-167) [83704-46-5] HEWLCNCSWBMZHG-UHFFFAOYSA-N	2.7×10^{-1}		Govers and Krop (1998)	Q	
1,6,8-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-168) [82911-59-9] ZOBVYDQWZXUJNO-UHFFFAOYSA-N	4.1×10^{-1}		Govers and Krop (1998)	Q	
1,7,8-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-178) [58802-18-9] YNMCXGLWHTVMQO-UHFFFAOYSA-N	4.6×10^{-1}		Govers and Krop (1998)	Q	
2,3,4-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-234) [57117-34-7] YDLADWPBKZODCJ-UHFFFAOYSA-N	3.1×10^{-1}		Govers and Krop (1998)	Q	
2,3,6-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-236) [57117-33-6] CPMGJTLNRBIKQM-UHFFFAOYSA-N	3.4×10^{-1}		Govers and Krop (1998)	Q	

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,7-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-237) [58802-17-8] CKXMNTLGGAOERF-UHFFFAOYSA-N	3.5×10^{-1}		Govers and Krop (1998)	Q	
2,3,8-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-238) [57117-32-5] NUNSNNOYACKRIK-UHFFFAOYSA-N	3.1×10^{-1}		Govers and Krop (1998)	Q	
2,4,6-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-246) [58802-14-5] GTKURBTWZFQHHY-UHFFFAOYSA-N	4.2×10^{-1}		Govers and Krop (1998)	Q	
2,4,7-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-247) [83704-42-1] SZBZRVJHPZIGAY-UHFFFAOYSA-N	3.1×10^{-1}		Govers and Krop (1998)	Q	
2,4,8-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-248) [54589-71-8] WJURXKWTCOMRCE-UHFFFAOYSA-N	3.2×10^{-1}		Govers and Krop (1998)	Q	
3,4,6-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-346) [83704-43-2] XEUHBCMRIXEBTD-UHFFFAOYSA-N	4.3×10^{-1}		Govers and Krop (1998)	Q	
3,4,7-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-347) [83704-44-3] RPJJBTSXPNFUTA-UHFFFAOYSA-N	3.9×10^{-1}		Govers and Krop (1998)	Q	
3,4,8-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-348) [83704-45-4] YTZWNIQGGIJHJX-UHFFFAOYSA-N	2.5×10^{-1}		Govers and Krop (1998)	Q	

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,4-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1234) [24478-72-6] AETAPIFVELRIDN-UHFFFAOYSA-N	3.6×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,6-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1236) [83704-21-6] BBAXFLIBRPXRBP-UHFFFAOYSA-N	4.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1237) [83704-22-7] MDNZFYGATDCKRB-UHFFFAOYSA-N	3.9×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1238) [62615-08-1] KFQRHGKKSHJMCO-UHFFFAOYSA-N	5.0×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1239) [83704-23-8] GNQHLJHTOATTOJ-UHFFFAOYSA-N	7.9×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,6-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1246) [71998-73-7] NLVWEKPJFUPVMZ-UHFFFAOYSA-N	5.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1247) [83719-40-8] MFURKMJLDQBHRA-UHFFFAOYSA-N	3.5×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1248) [64126-87-0] BFTASCFRRBHFFK-UHFFFAOYSA-N	5.5×10^{-1}		Govers and Krop (1998)	Q	

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,4,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1249) [83704-24-9] ZUYYTCCHKQGGOV-UHFFFAOYSA-N	7.4×10^{-1}		Govers and Krop (1998)	Q	
1,2,6,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1267) [83704-25-0] AUEWYHHKDYUYMI-UHFFFAOYSA-N	2.8×10^{-1}		Govers and Krop (1998)	Q	
1,2,6,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1268) [83710-07-0] KCVGVSIBBGIJNZ-UHFFFAOYSA-N	5.5×10^{-1}		Govers and Krop (1998)	Q	
1,2,6,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1269) [70648-18-9] IEPGLLVEBKXASE-UHFFFAOYSA-N	7.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,7,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1278) [58802-20-3] JODWPAQNABOHDG-UHFFFAOYSA-N	1.1 4.8×10^{-1}		Saçan et al. (2005) Govers and Krop (1998)	Q Q	
1,2,7,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1279) [83704-26-1] PDMFRPIFZAKMLH-UHFFFAOYSA-N	6.9×10^{-1}		Govers and Krop (1998)	Q	
1,2,8,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1289) [70648-22-5] OHYCQUKMNPHFPT-UHFFFAOYSA-N	9.5×10^{-1}		Govers and Krop (1998)	Q	
1,3,4,6-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1346) [83704-27-2] CBBDONKZEJKFJP-UHFFFAOYSA-N	6.3×10^{-1}		Govers and Krop (1998)	Q	

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3,4,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1347) [70648-16-7] UMKCVDZTSZNWRH-UHFFFAOYSA-N	5.1×10^{-1}		Govers and Krop (1998)	Q	
1,3,4,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1348) [92341-04-3] XWKRJSMNDOXIHS-UHFFFAOYSA-N	5.0×10^{-1}		Govers and Krop (1998)	Q	
1,3,4,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1349) [83704-28-3] PNCYJHOTZSKZPA-UHFFFAOYSA-N	5.8×10^{-1}		Govers and Krop (1998)	Q	
1,3,6,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1367) [57117-36-9] PITDPGCTIMCYEZ-UHFFFAOYSA-N	5.1×10^{-1}		Govers and Krop (1998)	Q	
1,3,6,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1368) [71998-72-6] BDXKVABZWRZKOS-UHFFFAOYSA-N	6.2×10^{-1}		Govers and Krop (1998)	Q	
1,3,6,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1369) [83690-98-6] NJQQZRLWVLWNGD-UHFFFAOYSA-N	6.8×10^{-1}		Govers and Krop (1998)	Q	
1,3,7,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1378) [57117-35-8] CSXDVUGDFSYXTD-UHFFFAOYSA-N	6.5×10^{-1}		Govers and Krop (1998)	Q	
1,3,7,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1379) [64560-17-4] IEMJMCVYAORWJV-UHFFFAOYSA-N	7.9×10^{-1}		Govers and Krop (1998)	Q	

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,4,6,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1467) [66794-59-0] RBFNYMHNIOKXLA-UHFFFAOYSA-N	5.9×10^{-1}		Govers and Krop (1998)	Q	
1,4,6,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1468) [82911-58-8] VHOBVPNETFRJED-UHFFFAOYSA-N	8.5×10^{-1}		Govers and Krop (1998)	Q	
1,4,6,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1469) [70648-19-0] JAYSBJFHDJOMGZ-UHFFFAOYSA-N	7.9×10^{-1}		Govers and Krop (1998)	Q	
1,4,7,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1478) [83704-29-4] IVRDRRWQABCXLY-UHFFFAOYSA-N	6.5×10^{-1}		Govers and Krop (1998)	Q	
1,6,7,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1678) [83704-33-0] KOJMOXYETDLOPN-UHFFFAOYSA-N	5.8×10^{-1}		Govers and Krop (1998)	Q	
2,3,4,6-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-2346) [83704-30-7] JNVHSHPAAMRSKK-UHFFFAOYSA-N	6.2×10^{-1}		Govers and Krop (1998)	Q	
2,3,4,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-2347) [83704-31-8] BROFYOSLFHTGCQ-UHFFFAOYSA-N	4.4×10^{-1}		Govers and Krop (1998)	Q	
2,3,4,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-2348) [83704-32-9] IIKXRERKNIJJQY-UHFFFAOYSA-N	3.5×10^{-1}		Govers and Krop (1998)	Q	

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,6,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-2367) [57117-39-2] MJCNKMDTLRSHNK-UHFFFAOYSA-N	4.1×10^{-1}		Govers and Krop (1998)	Q	
2,3,6,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-2368) [57117-37-0] SPMZHWVRMWWTSY-UHFFFAOYSA-N	4.2×10^{-1}		Govers and Krop (1998)	Q	
2,3,7,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-2378) [51207-31-9] KSMVNVHUTQZITP-UHFFFAOYSA-N	5.9×10^{-1}		Friesen et al. (1993)	M	
	6.8×10^{-1}		Mackay et al. (2006b)	V	
	8.5×10^{-1}		Govers and Krop (1998)	V	
	2.2×10^{-3}	3700	Paasivirta et al. (1999)	T	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	
	6.4×10^{-1}		HSDB (2015)	Q	100
	7.2×10^{-1}		Saçan et al. (2005)	Q	
	3.7×10^{-1}		Govers and Krop (1998)	Q	
	5.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,4,6,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-2467) [57117-38-1] NSDXKMRVQOSASS-UHFFFAOYSA-N	5.4×10^{-1}		Govers and Krop (1998)	Q	
2,4,6,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-2468) [58802-19-0] ZSPJEACWUWSAGS-UHFFFAOYSA-N	6.6×10^{-1}		Govers and Krop (1998)	Q	
3,4,6,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-3467) [57117-40-5] LMJLCLBSUNZLNW-UHFFFAOYSA-N	7.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,4,6-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12346) [83704-47-6] LIQJBAPSLUZUTB-UHFFFAOYSA-N	7.1×10^{-1}		Govers and Krop (1998)	Q	

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,4,7-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12347) [83704-48-7] DOJZTBGOWIYFAC-UHFFFAOYSA-N	4.5×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,4,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12348) [67517-48-0] ZCTNDJSCLPJCRA-UHFFFAOYSA-N	5.5×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,4,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12349) [83704-49-8] IQSZNZVZXOFRJS-UHFFFAOYSA-N	9.8×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,6,7-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12367) [57117-42-7] NZUPQBVDIWCPBX-UHFFFAOYSA-N	4.2×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,6,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12368) [83704-51-2] VHQJZOFUPXEZQZ-UHFFFAOYSA-N	6.5×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,6,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12369) [83704-52-3] IPSFQAKXDJVQOX-UHFFFAOYSA-N	1.1		Govers and Krop (1998)	Q	
1,2,3,7,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12378) [57117-41-6] SBMIVUVRFPGOEB-UHFFFAOYSA-N	8.7×10^{-4} 5.2×10^{-1}	3000	Paasivirta et al. (1999) Govers and Krop (1998)	T Q	
1,2,3,7,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12379) [83704-53-4] JVUSEQPOWCBYNG-UHFFFAOYSA-N	1.0		Govers and Krop (1998)	Q	

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,8,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12389) [83704-54-5] NKGLWUJPCTUDEH-UHFFFAOYSA-N	2.0 1.1		Saçan et al. (2005) Govers and Krop (1998)	Q Q	
1,2,4,6,7-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12467) [83704-50-1] BQTCODOVGXJHRB-UHFFFAOYSA-N	5.8×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,6,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12468) [69698-57-3] JDTUAYPJSSXDNO-UHFFFAOYSA-N	1.0		Govers and Krop (1998)	Q	
1,2,4,6,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12469) [70648-24-7] QDQFGVXGPSYEJU-UHFFFAOYSA-N	1.5		Govers and Krop (1998)	Q	
1,2,4,7,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12478) [58802-15-6] GCFDWHIKRXCUPJ-UHFFFAOYSA-N	6.2×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,7,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12479) [71998-74-8] IYGVHNHWORPMFU-UHFFFAOYSA-N	9.8×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,8,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12489) [70648-23-6] ZSPAPWGNAGTCCA-UHFFFAOYSA-N	1.3		Govers and Krop (1998)	Q	
1,2,6,7,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12678) [69433-00-7] ZAAVDGLJEOXCMV-UHFFFAOYSA-N	5.2×10^{-1}		Govers and Krop (1998)	Q	

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,6,7,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12679) [70872-82-1] QQRRQEVOSMEVQB-UHFFFAOYSA-N	7.9×10^{-1}		Govers and Krop (1998)	Q	
1,3,4,6,7-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-13467) [83704-36-3] JVYYDUWJIJMOGW-UHFFFAOYSA-N	8.9×10^{-1}		Govers and Krop (1998)	Q	
1,3,4,6,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-13468) [83704-55-6] COKIAYPRHYHYCH-UHFFFAOYSA-N	1.0		Govers and Krop (1998)	Q	
1,3,4,6,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-13469) [70648-15-6] MYSAFUYQSBEEDR-UHFFFAOYSA-N	1.2		Govers and Krop (1998)	Q	
1,3,4,7,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-13478) [58802-16-7] ORSUQGVCWLXKLZ-UHFFFAOYSA-N	7.1×10^{-1}		Govers and Krop (1998)	Q	
1,3,4,7,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-13479) [70648-20-3] GFXPLABVZOBCCW-UHFFFAOYSA-N	9.5×10^{-1}		Govers and Krop (1998)	Q	
1,3,6,7,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-13678) [70648-21-4] FRLMQDUYUJIHCZ-UHFFFAOYSA-N	7.6×10^{-1}		Govers and Krop (1998)	Q	
1,4,6,7,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-14678) [83704-35-2] VANGHZRYKXDPRR-UHFFFAOYSA-N	1.1		Govers and Krop (1998)	Q	

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4,6,7-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-23467) [57117-43-8] SJFBZRQKGOGHEV-UHFFFAOYSA-N	6.9×10^{-1}		Govers and Krop (1998)	Q	
2,3,4,6,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-23468) [67481-22-5] MKRFORPSRBMAIP-UHFFFAOYSA-N	6.6×10^{-1}		Govers and Krop (1998)	Q	
2,3,4,7,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-23478) [57117-31-4] OGBQILNBLMPPDP-UHFFFAOYSA-N	2.0 2.0 2.0 1.7 2.3×10^{-3} 1.6 1.6 3.9×10^{-1}	 2900 	Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006b) Govers and Krop (1998) Paasivirta et al. (1999) Duchowicz et al. (2020) Saçan et al. (2005) Govers and Krop (1998)	V V V V T Q Q Q	187
1,2,3,4,6,7-hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123467) [79060-60-9] SNWFMKXFMVHBKD-UHFFFAOYSA-N	6.8×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,4,6,8-hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123468) [69698-60-8] UCFGNWHERVQWMZ-UHFFFAOYSA-N	2.4×10^{-4} 9.8×10^{-1}	2300 	Paasivirta et al. (1999) Govers and Krop (1998)	T Q	
1,2,3,4,6,9-hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123469) [91538-83-9] KFFUZIROJGXTQH-UHFFFAOYSA-N	1.8		Govers and Krop (1998)	Q	
1,2,3,4,7,8-hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123478) [70648-26-9] LVYBAQIVPKCOEE-UHFFFAOYSA-N	6.9×10^{-1} 3.8×10^{-1} 4.1×10^{-4} 2.0 5.2×10^{-1}	 2400 	Mackay et al. (2006b) Govers and Krop (1998) Paasivirta et al. (1999) Saçan et al. (2005) Govers and Krop (1998)	V V T Q Q	

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,4,7,9- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123479) [91538-84-0] BKIXWRBZCQEZAQ-UHFFFAOYSA-N	1.1		Govers and Krop (1998)	Q	
1,2,3,4,8,9- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123489) [92341-07-6] VSDUQUBUJRNREH-UHFFFAOYSA-N	2.7 1.1		Saçan et al. (2005) Govers and Krop (1998)	Q Q	
1,2,3,6,7,8- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123678) [57117-44-9] JEYJJJXOFWNEHN-UHFFFAOYSA-N	9.1×10^{-1} 1.1×10^{-3} 2.2 5.2×10^{-1}	 3300 	Govers and Krop (1998) Paasivirta et al. (1999) Saçan et al. (2005) Govers and Krop (1998)	V T Q Q	
1,2,3,6,7,9- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123679) [92341-06-5] JZVOLXQREJNTTL-UHFFFAOYSA-N	1.0		Govers and Krop (1998)	Q	
1,2,3,6,8,9- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123689) [75198-38-8] WLGQZUOHEXTWFH-UHFFFAOYSA-N	1.3		Govers and Krop (1998)	Q	
1,2,3,7,8,9- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123789) [72918-21-9] PYUSJFJVDVSXIU-UHFFFAOYSA-N	6.3×10^{-4} 2.6 1.0	2600 	Paasivirta et al. (1999) Saçan et al. (2005) Govers and Krop (1998)	T Q Q	
1,2,4,6,7,8- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-124678) [67562-40-7] CKDDYGBBKXIHRY-UHFFFAOYSA-N	3.2×10^{-4} 9.3×10^{-1}	2300 	Paasivirta et al. (1999) Govers and Krop (1998)	T Q	

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,4,6,7,9- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-124679) [75627-02-0] FAHIPPHRJJJQOG-UHFFFAOYSA-N	1.5		Govers and Krop (1998)	Q	
1,2,4,6,8,9- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-124689) [69698-59-5] FGZCXIPKUCJGHW-UHFFFAOYSA-N	2.2×10^{-4}	2600	Paasivirta et al. (1999)	T	
	2.4		Govers and Krop (1998)	Q	
1,3,4,6,7,8- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-134678) [71998-75-9] OGTZINCGZYXZCR-UHFFFAOYSA-N	1.1		Govers and Krop (1998)	Q	
1,3,4,6,7,9- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-134679) [92341-05-4] TURXXOIFVABBPW-UHFFFAOYSA-N	1.6		Govers and Krop (1998)	Q	
2,3,4,6,7,8- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-234678) [60851-34-5] XTAHLACQOVXINQ-UHFFFAOYSA-N	3.6×10^{-4}	2600	Paasivirta et al. (1999)	T	
	3.1		Saçan et al. (2005)	Q	
	5.6×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,4,6,7,8- heptachlorodibenzofuran $C_{12}HCl_7O$ (PCDF-1234678) [67562-39-4] WDMKCPIVJOGHBF-UHFFFAOYSA-N	7.0×10^{-1}		Duchowicz et al. (2020)	V	187
	7.0×10^{-1}		Mackay et al. (2006b)	V	
	2.9×10^{-1}		Govers and Krop (1998)	V	
	5.4×10^{-5}	1600	Paasivirta et al. (1999)	T	
	2.1		Duchowicz et al. (2020)	Q	
	3.9		Saçan et al. (2005)	Q	
	7.1×10^{-1}		Govers and Krop (1998)	Q	

Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,4,6,7,9- heptachlorodibenzofuran $C_{12}HCl_7O$ (PCDF-1234679) [70648-25-8] JWXWOEUKHXOUSK-UHFFFAOYSA-N	1.5		Govers and Krop (1998)	Q	
1,2,3,4,6,8,9- heptachlorodibenzofuran $C_{12}HCl_7O$ (PCDF-1234689) [69698-58-4] BADFHCOLISGRRW-UHFFFAOYSA-N	3.4×10^{-4}	1800	Paasivirta et al. (1999)	T	
	1.9		Govers and Krop (1998)	Q	
1,2,3,4,7,8,9- heptachlorodibenzofuran $C_{12}HCl_7O$ (PCDF-1234789) [55673-89-7] VEZCTZWLJYWARH-UHFFFAOYSA-N	5.5×10^{-4}	2100	Paasivirta et al. (1999)	T	
	3.2		Saçan et al. (2005)	Q	
	1.0		Govers and Krop (1998)	Q	
octachlorodibenzofuran $C_{12}Cl_8O$ (PCDF-12346789) [39001-02-0] RHIROFAGUQOFLU-UHFFFAOYSA-N	5.2		Duchowicz et al. (2020)	V	187
			Mackay et al. (2006b)	V	685
	7.6×10^{-1}		Govers and Krop (1998)	V	
	2.3×10^{-4}	2400	Paasivirta et al. (1999)	T	
	1.7		Duchowicz et al. (2020)	Q	
	4.9		Saçan et al. (2005)	Q	
	1.3		Govers and Krop (1998)	Q	

A6.7 Polychlorinated dibenzo-*p*-dioxins (PCDDs)

Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chlorodibenzo-*p*-dioxin	1.6×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{12}H_7ClO_2$	1.6×10^{-1}		Mackay et al. (2006b)	V	
(PCDD-1)	2.5×10^{-2}		Saçan et al. (2005)	V	
[39227-53-7]	1.6×10^{-1}		Govers and Krop (1998)	V	
VGGGRWRBGXENKI-UHFFFAOYSA-N	1.2×10^{-1}		Shiu et al. (1988)	V	
	2.1		Duchowicz et al. (2020)	Q	
		7100	Kühne et al. (2005)	Q	
	6.8×10^{-2}		Saçan et al. (2005)	Q	
	1.3×10^{-1}		Wang and Wong (2002)	Q	537
	1.7×10^{-1}		Govers and Krop (1998)	Q	
		6500	Kühne et al. (2005)	?	
2-chlorodibenzo-*p*-dioxin	8.6×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{12}H_7ClO_2$	7.9×10^{-2}		Mackay et al. (2006b)	V	
(PCDD-2)	7.9×10^{-2}		Govers and Krop (1998)	V	
[39227-54-8]	6.7×10^{-2}		Shiu et al. (1988)	V	
GIUGGRUEPHPVNR-UHFFFAOYSA-N	1.1		Duchowicz et al. (2020)	Q	
	9.8×10^{-2}		Saçan et al. (2005)	Q	
	1.3×10^{-1}		Wang and Wong (2002)	Q	537
	2.2×10^{-1}		Govers and Krop (1998)	Q	
1,2-dichlorodibenzo-*p*-dioxin	2.8×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_6Cl_2O_2$	3.2×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-12)					
[54536-18-4]					
DFGDMWHUCCHXIF-UHFFFAOYSA-N					
1,3-dichlorodibenzo-*p*-dioxin	2.2×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_6Cl_2O_2$	3.8×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-13)					
[50585-39-2]					
AZYJYMAKTBXNSX-UHFFFAOYSA-N					
1,4-dichlorodibenzo-*p*-dioxin	2.4×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_6Cl_2O_2$	3.2×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-14)					
[54536-19-5]					
MBMUPQZSDWVPQU-UHFFFAOYSA-N					
1,6-dichlorodibenzo-*p*-dioxin	2.5×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_6Cl_2O_2$	3.2×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-16)					
[38178-38-0]					
MAWMBEVNJGEDAD-UHFFFAOYSA-N					

Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,7-dichlorodibenzo-*p*-dioxin $C_{12}H_6Cl_2O_2$ (PCDD-17) [82291-26-7] IJUWLAFPPVRYGY-UHFFFAOYSA-N	2.6×10^{-1}		Wang and Wong (2002)	Q	537
	3.6×10^{-1}		Govers and Krop (1998)	Q	
1,8-dichlorodibenzo-*p*-dioxin $C_{12}H_6Cl_2O_2$ (PCDD-18) [82291-27-8] PLZYIHQBHROTFD-UHFFFAOYSA-N	2.6×10^{-1}		Wang and Wong (2002)	Q	537
	3.8×10^{-1}		Govers and Krop (1998)	Q	
1,9-dichlorodibenzo-*p*-dioxin $C_{12}H_6Cl_2O_2$ (PCDD-19) [82291-28-9] JZDVJXBKJDADAY-UHFFFAOYSA-N	2.6×10^{-1}		Wang and Wong (2002)	Q	537
	5.4×10^{-1}		Govers and Krop (1998)	Q	
2,3-dichlorodibenzo-*p*-dioxin $C_{12}H_6Cl_2O_2$ (PCDD-23) [29446-15-9] YCIYTXRUZSDMRZ-UHFFFAOYSA-N	1.5×10^{-1}		Duchowicz et al. (2020)	V	187
	1.5×10^{-1}		Mackay et al. (2006b)	V	
	1.5×10^{-1}		Saçan et al. (2005)	V	
	1.5×10^{-1}		Govers and Krop (1998)	V	
	1.5×10^{-1}		Shiu et al. (1988)	V	
	8.5×10^{-1}		Duchowicz et al. (2020)	Q	
	2.5×10^{-1}		Saçan et al. (2005)	Q	
	2.6×10^{-1}		Wang and Wong (2002)	Q	537
	4.0×10^{-1}		Govers and Krop (1998)	Q	
2,7-dichlorodibenzo-*p*-dioxin $C_{12}H_6Cl_2O_2$ (PCDD-27) [33857-26-0] NBFMTHWVRBOVPE-UHFFFAOYSA-N	1.7×10^{-1}		Santl et al. (1994)	M	735
			Mackay et al. (2006b)	V	685
	1.2×10^{-1}		Govers and Krop (1998)	V	
	1.2×10^{-1}		Shiu et al. (1988)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	6.6×10^{-1}		Duchowicz et al. (2020)	Q	300
	7.3×10^{-1}		Hilal et al. (2008)	Q	
	5.0		Modarresi et al. (2007)	Q	68
	1.0×10^{-1}		Saçan et al. (2005)	Q	
	2.6×10^{-1}		Wang and Wong (2002)	Q	537
	3.5×10^{-1}		Govers and Krop (1998)	Q	
	1.7×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,8-dichlorodibenzo-*p*-dioxin $C_{12}H_6Cl_2O_2$ (PCDD-28) [38964-22-6] WMWJCKBJUQDYLM-UHFFFAOYSA-N	4.7×10^{-1}		Duchowicz et al. (2020)	V	187
	4.7×10^{-1}		Mackay et al. (2006b)	V	
	4.7×10^{-1}		Govers and Krop (1998)	V	
	4.7×10^{-1}		Shiu et al. (1988)	V	
	1.2		Duchowicz et al. (2020)	Q	
	1.7×10^{-1}		Saçan et al. (2005)	Q	
	2.6×10^{-1}		Wang and Wong (2002)	Q	537
	4.4×10^{-1}		Govers and Krop (1998)	Q	

Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3-trichlorodibenzo-*p*-dioxin	5.0×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_5Cl_3O_2$	5.6×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-123)					
[54536-17-3]					
SKMFBGZVVNDVFR-UHFFFAOYSA-N					
1,2,4-trichlorodibenzo-*p*-dioxin	2.7×10^{-1}		Santl et al. (1994)	M	735
$C_{12}H_5Cl_3O_2$	2.9×10^{-1}		Mackay et al. (2006b)	V	
(PCDD-124)	2.6×10^{-1}		Govers and Krop (1998)	V	
[39227-58-2]	2.6×10^{-1}		Shiu et al. (1988)	V	
HRVUKLBFRPWXPJ-UHFFFAOYSA-N	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	9.1×10^{-1}		Duchowicz et al. (2020)	Q	
	1.3		Hilal et al. (2008)	Q	
	1.1×10^{1}		Modarresi et al. (2007)	Q	68
	3.0×10^{-1}		Saçan et al. (2005)	Q	
	4.4×10^{-1}		Wang and Wong (2002)	Q	537
	5.5×10^{-1}		Govers and Krop (1998)	Q	
	2.7×10^{-1}		Duchowicz et al. (2020)	?	186, 21
			Fogg and Sangster (2003)	W	736
1,2,6-trichlorodibenzo-*p*-dioxin	5.0×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_5Cl_3O_2$	5.1×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-126)					
[69760-96-9]					
XQBPVWBIUBCJJO-UHFFFAOYSA-N					
1,2,7-trichlorodibenzo-*p*-dioxin	5.1×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_5Cl_3O_2$	4.6×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-127)					
[82291-30-3]					
TXJMXDWFPQSYEQ-UHFFFAOYSA-N					
1,2,8-trichlorodibenzo-*p*-dioxin	5.1×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_5Cl_3O_2$	6.0×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-128)					
[82291-31-4]					
QBEOCKSANJLBAE-UHFFFAOYSA-N					
1,2,9-trichlorodibenzo-*p*-dioxin	5.2×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_5Cl_3O_2$	9.1×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-129)					
[82291-32-5]					
DQLRDBDQLSIOIX-UHFFFAOYSA-N					

Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3,6-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-136) [82291-33-6] LNPVMVSAUXUGHH-UHFFFAOYSA-N	4.2×10^{-1} 6.3×10^{-1}		Wang and Wong (2002) Govers and Krop (1998)	Q Q	537
1,3,7-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-137) [67028-17-5] RPKWIXFZKMDPMH-UHFFFAOYSA-N	4.3×10^{-1} 6.8×10^{-1}		Wang and Wong (2002) Govers and Krop (1998)	Q Q	537
1,3,8-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-138) [82306-61-4] FJAKCOBYQSEWMT-UHFFFAOYSA-N	4.3×10^{-1} 5.6×10^{-1}		Wang and Wong (2002) Govers and Krop (1998)	Q Q	537
1,3,9-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-139) [82306-62-5] DGDADRUTFAIIQQ-UHFFFAOYSA-N	4.4×10^{-1} 1.0		Wang and Wong (2002) Govers and Krop (1998)	Q Q	537
1,4,6-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-146) [82306-63-6] UTTYFTWIJLRXKB-UHFFFAOYSA-N	4.4×10^{-1} 9.3×10^{-1}		Wang and Wong (2002) Govers and Krop (1998)	Q Q	537
1,4,7-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-147) [82306-64-7] NBWAQBGJBSYXHV-UHFFFAOYSA-N	4.5×10^{-1} 6.0×10^{-1}		Wang and Wong (2002) Govers and Krop (1998)	Q Q	537
1,7,8-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-178) [82306-65-8] CAPCTZJHYADFNX-UHFFFAOYSA-N	4.9×10^{-1} 6.2×10^{-1}		Wang and Wong (2002) Govers and Krop (1998)	Q Q	537
2,3,7-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-237) [33857-28-2] ZSIZNEVHVVRPFF-UHFFFAOYSA-N	4.9×10^{-1} 5.6×10^{-1}		Wang and Wong (2002) Govers and Krop (1998)	Q Q	537

Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,4-tetrachlorodibenzo-*p*-dioxin	5.0×10^{-1}		Santl et al. (1994)	M	735
$C_{12}H_4Cl_4O_2$	2.7×10^{-1}		Mackay et al. (2006b)	V	
(PCDD-1234)	1.4		Mackay et al. (2006b)	V	
[30746-58-8]	3.3×10^{-1}		Govers and Krop (1998)	V	
DJHHDLMTUOLVHY-UHFFFAOYSA-N	2.7×10^{-1}		Shiu et al. (1988)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	7.0×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.4		Hilal et al. (2008)	Q	
	2.2×10^{1}		Modarresi et al. (2007)	Q	68
	6.3×10^{-1}		Saçan et al. (2005)	Q	
	8.7×10^{-1}		Wang and Wong (2002)	Q	537
	7.4×10^{-1}		Govers and Krop (1998)	Q	
	4.9×10^{-1}		Duchowicz et al. (2020)	?	186, 21
1,2,3,6-tetrachlorodibenzo-*p*-dioxin	8.7×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_4Cl_4O_2$	8.1×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-1236)					
[71669-25-5]					
XEZBZSVTUSXISZ-UHFFFAOYSA-N					
1,2,3,7-tetrachlorodibenzo-*p*-dioxin	1.3		Mackay et al. (2006b)	V	
$C_{12}H_4Cl_4O_2$	1.7		Govers and Krop (1998)	V	
(PCDD-1237)	1.3		Shiu et al. (1988)	V	
[67028-18-6]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
SKGXYFVQZVPEFP-UHFFFAOYSA-N	5.7×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.7		Hilal et al. (2008)	Q	
	2.1×10^{1}		Modarresi et al. (2007)	Q	68
	4.3×10^{-1}		Saçan et al. (2005)	Q	
	8.7×10^{-1}		Wang and Wong (2002)	Q	537
	6.8×10^{-1}		Govers and Krop (1998)	Q	
	1.3		Duchowicz et al. (2020)	?	186, 21
1,2,3,8-tetrachlorodibenzo-*p*-dioxin	8.7×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_4Cl_4O_2$	7.1×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-1238)					
[53555-02-5]					
BXKLTNKYLCZOHF-UHFFFAOYSA-N					
1,2,3,9-tetrachlorodibenzo-*p*-dioxin	9.1×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_4Cl_4O_2$	1.4		Govers and Krop (1998)	Q	
(PCDD-1239)					
[71669-26-6]					
CMVHZKSHSHQJHS-UHFFFAOYSA-N					

Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,4,6-tetrachlorodibenzo-*p*-dioxin $C_{12}H_4Cl_4O_2$ (PCDD-1246) [71669-27-7] KQNBZUDHTCXCNA-UHFFFAOYSA-N	8.1×10^{-1}		Wang and Wong (2002)	Q	537
	1.4		Govers and Krop (1998)	Q	
1,2,4,7-tetrachlorodibenzo-*p*-dioxin $C_{12}H_4Cl_4O_2$ (PCDD-1247) [71669-28-8] SMPHQCMJQUBTFZ-UHFFFAOYSA-N	7.8×10^{-1}		Wang and Wong (2002)	Q	537
	7.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,8-tetrachlorodibenzo-*p*-dioxin $C_{12}H_4Cl_4O_2$ (PCDD-1248) [71669-29-9] XGIKODBWQSAEFQ-UHFFFAOYSA-N	7.8×10^{-1}		Wang and Wong (2002)	Q	537
	8.9×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,9-tetrachlorodibenzo-*p*-dioxin $C_{12}H_4Cl_4O_2$ (PCDD-1249) [71665-99-1] WDAHVJCSSYOALR-UHFFFAOYSA-N	8.1×10^{-1}		Wang and Wong (2002)	Q	537
	1.5		Govers and Krop (1998)	Q	
1,2,6,7-tetrachlorodibenzo-*p*-dioxin $C_{12}H_4Cl_4O_2$ (PCDD-1267) [40581-90-6] SAMLAWFHXZIRMP-UHFFFAOYSA-N	9.5×10^{-1}		Wang and Wong (2002)	Q	537
	5.8×10^{-1}		Govers and Krop (1998)	Q	
1,2,6,8-tetrachlorodibenzo-*p*-dioxin $C_{12}H_4Cl_4O_2$ (PCDD-1268) [67323-56-2] YYUFYZDSYHKVDP-UHFFFAOYSA-N	8.1×10^{-1}		Wang and Wong (2002)	Q	537
	8.9×10^{-1}		Govers and Krop (1998)	Q	
1,2,6,9-tetrachlorodibenzo-*p*-dioxin $C_{12}H_4Cl_4O_2$ (PCDD-1269) [40581-91-7] ZKMXKYXNLFLUCD-UHFFFAOYSA-N	8.7×10^{-1}		Wang and Wong (2002)	Q	537
	1.4		Govers and Krop (1998)	Q	

Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,7,8-tetrachlorodibenzo-*p*-dioxin	7.8×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_4Cl_4O_2$	6.8×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-1278)					
[34816-53-0]					
YDZCLBKUTXYYKS-UHFFFAOYSA-N					
1,2,7,9-tetrachlorodibenzo-*p*-dioxin	8.3×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_4Cl_4O_2$	1.2		Govers and Krop (1998)	Q	
(PCDD-1279)					
[71669-23-3]					
QIKHBBZEUNSCAF-UHFFFAOYSA-N					
1,2,8,9-tetrachlorodibenzo-*p*-dioxin	9.8×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_4Cl_4O_2$	1.3		Govers and Krop (1998)	Q	
(PCDD-1289)					
[62470-54-6]					
WELWFAGPAZKSBG-UHFFFAOYSA-N					
1,3,6,8-tetrachlorodibenzo-*p*-dioxin	1.4×10^{-1}		Webster et al. (1985)	M	
$C_{12}H_4Cl_4O_2$	1.4		Govers and Krop (1998)	V	
(PCDD-1368)	1.4		Shiu et al. (1988)	V	
[33423-92-6]	1.2		Hilal et al. (2008)	Q	
OTQFXRBLGNEOGH-UHFFFAOYSA-N	2.9×10^{-1}		Saçan et al. (2005)	Q	
	6.8×10^{-1}		Wang and Wong (2002)	Q	537
	8.7×10^{-1}		Govers and Krop (1998)	Q	
1,3,6,9-tetrachlorodibenzo-*p*-dioxin	7.4×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_4Cl_4O_2$	1.7		Govers and Krop (1998)	Q	
(PCDD-1369)					
[71669-24-4]					
QAUIRDIJIUMMEP-UHFFFAOYSA-N					
1,3,7,8-tetrachlorodibenzo-*p*-dioxin	7.8×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_4Cl_4O_2$	7.9×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-1378)					
[50585-46-1]					
VPTDIAYLYJBYQG-UHFFFAOYSA-N					

Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3,7,9-tetrachlorodibenzo-*p*-dioxin	7.1×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_4Cl_4O_2$	1.7		Govers and Krop (1998)	Q	
(PCDD-1379)					
[62470-53-5]					
JMGYHLJVDHUACM-UHFFFAOYSA-N					
1,4,6,9-tetrachlorodibenzo-*p*-dioxin	7.9×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_4Cl_4O_2$	2.6		Govers and Krop (1998)	Q	
(PCDD-1469)					
[40581-93-9]					
QTIIAIRUSSSOHT-UHFFFAOYSA-N					
1,4,7,8-tetrachlorodibenzo-*p*-dioxin	8.1×10^{-1}		Wang and Wong (2002)	Q	537
$C_{12}H_4Cl_4O_2$	9.1×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-1478)					
[40581-94-0]					
FCRXUTCUWCJZJI-UHFFFAOYSA-N					
2,3,7,8-tetrachlorodibenzo-*p*-dioxin	2.0×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{12}H_4Cl_4O_2$	2.0×10^{-1}		HSDB (2015)	V	
(PCDD-2378; TCDD)	3.0×10^{-1}		Mackay et al. (2006b)	V	
[1746-01-6]	3.0×10^{-1}		Govers and Krop (1998)	V	
HGUFODBRKLSHSI-UHFFFAOYSA-N	5.8×10^{-1}		McLachlan et al. (1990)	V	375
	6.1×10^{-1}		Shiu et al. (1988)	V	
	3.0×10^{-1}		Shiu et al. (1988)	V	
	9.7×10^{-2}		Shiu et al. (1988)	V	
	6.3×10^{-1}		Podoll et al. (1986)	V	
	4.7		Schroy et al. (1985)	V	
	2.6×10^{-4}	3600	Paasivirta et al. (1999)	T	
	4.1×10^{-1}		Duchowicz et al. (2020)	Q	
	3.3×10^{-1}		Saçan et al. (2005)	Q	
	8.9×10^{-1}		Wang and Wong (2002)	Q	537
	6.2×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,4,6-pentachlorodibenzo-*p*-dioxin	1.5		Wang and Wong (2002)	Q	537
$C_{12}H_3Cl_5O_2$	1.8		Govers and Krop (1998)	Q	
(PCDD-12346)					
[67028-19-7]					
LNWDBNKKBLRAMH-UHFFFAOYSA-N					

Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,4,7-pentachlorodibenzo-*p*-dioxin	3.8		Duchowicz et al. (2020)	V	187
$C_{12}H_3Cl_5O_2$	3.8		Mackay et al. (2006b)	V	
(PCDD-12347)	4.5		Govers and Krop (1998)	V	
[39227-61-7]	3.8		Shiu et al. (1988)	V	
WRNGAZFESPEMCN-UHFFFAOYSA-N	4.5×10^{-1}		Duchowicz et al. (2020)	Q	
	7.0×10^{-1}		Saçan et al. (2005)	Q	
	1.4		Wang and Wong (2002)	Q	537
	8.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,6,7-pentachlorodibenzo-*p*-dioxin	1.5		Wang and Wong (2002)	Q	537
$C_{12}H_3Cl_5O_2$	7.8×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-12367)					
[71925-15-0]					
RLGWDUHOIIWPGN-UHFFFAOYSA-N					
1,2,3,6,8-pentachlorodibenzo-*p*-dioxin	1.3		Wang and Wong (2002)	Q	537
$C_{12}H_3Cl_5O_2$	9.5×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-12368)					
[71925-16-1]					
VKDGHBBUEIIEHL-UHFFFAOYSA-N					
1,2,3,6,9-pentachlorodibenzo-*p*-dioxin	1.4		Wang and Wong (2002)	Q	537
$C_{12}H_3Cl_5O_2$	1.9		Govers and Krop (1998)	Q	
(PCDD-12369)					
[82291-34-7]					
NWKWRHSKKNELND-UHFFFAOYSA-N					
1,2,3,7,8-pentachlorodibenzo-*p*-dioxin	5.2×10^{-5}	2500	Paasivirta et al. (1999)	T	
$C_{12}H_3Cl_5O_2$	6.4×10^{-1}		Saçan et al. (2005)	Q	
(PCDD-12378)	1.5		Wang and Wong (2002)	Q	537
[40321-76-4]	6.8×10^{-1}		Govers and Krop (1998)	Q	
FSPZPQQWDODWAU-UHFFFAOYSA-N					
1,2,3,7,9-pentachlorodibenzo-*p*-dioxin	1.3		Wang and Wong (2002)	Q	537
$C_{12}H_3Cl_5O_2$	1.5		Govers and Krop (1998)	Q	
(PCDD-12379)					
[71925-17-2]					
UAOYHTXYVWEPIB-UHFFFAOYSA-N					

Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,8,9-pentachlorodibenzo-*p*-dioxin $C_{12}H_3Cl_5O_2$ (PCDD-12389) [71925-18-3] VUMZAVNIADYKFC-UHFFFAOYSA-N	1.5		Wang and Wong (2002)	Q	537
	1.4		Govers and Krop (1998)	Q	
1,2,4,6,7-pentachlorodibenzo-*p*-dioxin $C_{12}H_3Cl_5O_2$ (PCDD-12467) [82291-35-8] SEKDDGLKEYEVQK-UHFFFAOYSA-N	1.4		Wang and Wong (2002)	Q	537
	1.4		Govers and Krop (1998)	Q	
1,2,4,6,8-pentachlorodibenzo-*p*-dioxin $C_{12}H_3Cl_5O_2$ (PCDD-12468) [71998-76-0] SJJWALZHAWITMS-UHFFFAOYSA-N	1.2		Wang and Wong (2002)	Q	537
	2.1		Govers and Krop (1998)	Q	
1,2,4,6,9-pentachlorodibenzo-*p*-dioxin $C_{12}H_3Cl_5O_2$ (PCDD-12469) [82291-36-9] GNQVSAMSAKZLKE-UHFFFAOYSA-N	1.3		Wang and Wong (2002)	Q	537
	3.6		Govers and Krop (1998)	Q	
1,2,4,7,8-pentachlorodibenzo-*p*-dioxin $C_{12}H_3Cl_5O_2$ (PCDD-12478) [58802-08-7] QUPLGUUISJOUPJ-UHFFFAOYSA-N	1.3		Wang and Wong (2002)	Q	537
	9.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,7,9-pentachlorodibenzo-*p*-dioxin $C_{12}H_3Cl_5O_2$ (PCDD-12479) [82291-37-0] QLBBXWPVEFJZEC-UHFFFAOYSA-N	1.2		Wang and Wong (2002)	Q	537
	1.8		Govers and Krop (1998)	Q	
1,2,4,8,9-pentachlorodibenzo-*p*-dioxin $C_{12}H_3Cl_5O_2$ (PCDD-12489) [82291-38-1] KLLFLRKEOJCTGC-UHFFFAOYSA-N	1.4		Wang and Wong (2002)	Q	537
	1.9		Govers and Krop (1998)	Q	

Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,4,6,7-hexachlorodibenzo-*p*-dioxin	2.5		Wang and Wong (2002)	Q	537
$C_{12}H_2Cl_6O_2$	1.5		Govers and Krop (1998)	Q	
(PCDD-123467)					
[58200-66-1]					
NLBQVWJHLWAFGJ-UHFFFAOYSA-N					
1,2,3,4,6,8-hexachlorodibenzo-*p*-dioxin	2.2		Wang and Wong (2002)	Q	537
$C_{12}H_2Cl_6O_2$	1.8		Govers and Krop (1998)	Q	
(PCDD-123468)					
[58200-67-2]					
IMALTUQZEIFHJW-UHFFFAOYSA-N					
1,2,3,4,6,9-hexachlorodibenzo-*p*-dioxin	2.3		Wang and Wong (2002)	Q	537
$C_{12}H_2Cl_6O_2$	4.0		Govers and Krop (1998)	Q	
(PCDD-123469)					
[58200-68-3]					
UDYXCMRDCOVQLG-UHFFFAOYSA-N					
1,2,3,4,7,8-hexachlorodibenzo-*p*-dioxin	2.5		Duchowicz et al. (2020)	V	187
$C_{12}H_2Cl_6O_2$	3.0		Mackay et al. (2006b)	V	
(PCDD-123478)	1.6		Govers and Krop (1998)	V	
[39227-28-6]	2.2×10^{-1}		Shiu et al. (1988)	V	
WCYYQNSQJHPVMG-UHFFFAOYSA-N	1.2×10^{-4}	2900	Paasivirta et al. (1999)	T	
	3.7×10^{-1}		Duchowicz et al. (2020)	Q	
		8800	Kühne et al. (2005)	Q	
	7.7×10^{-1}		Saçan et al. (2005)	Q	
	2.3		Wang and Wong (2002)	Q	537
	6.9×10^{-1}		Govers and Krop (1998)	Q	
		9400	Kühne et al. (2005)	?	
1,2,3,6,7,8-hexachlorodibenzo-*p*-dioxin	6.2×10^{-5}	2800	Paasivirta et al. (1999)	T	
$C_{12}H_2Cl_6O_2$	5.2		HSDB (2015)	Q	100
(PCDD-123678)	7.4×10^{-1}		Saçan et al. (2005)	Q	
[57653-85-7]	2.4		Wang and Wong (2002)	Q	537
YCLUIPQDHHPDJJ-UHFFFAOYSA-N	6.9×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,6,7,9-hexachlorodibenzo-*p*-dioxin	2.2		Wang and Wong (2002)	Q	537
$C_{12}H_2Cl_6O_2$	1.7		Govers and Krop (1998)	Q	
(PCDD-123679)					
[64461-98-9]					
BQOHWGKNRKCEFT-UHFFFAOYSA-N					

Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,6,8,9-hexachlorodibenzo-*p*-dioxin	2.2		Wang and Wong (2002)	Q	537
$C_{12}H_2Cl_6O_2$	1.8		Govers and Krop (1998)	Q	
(PCDD-123689)					
[58200-69-4]					
GZRQZUFXVFRKBI-UHFFFAOYSA-N					
1,2,3,7,8,9-hexachlorodibenzo-*p*-dioxin	2.5×10^{-4}	2700	Paasivirta et al. (1999)	T	
$C_{12}H_2Cl_6O_2$	5.2		HSDB (2015)	Q	100
(PCDD-123789)	1.1		Saçan et al. (2005)	Q	
[19408-74-3]	2.4		Wang and Wong (2002)	Q	537
LGIRBUBHIWTVCK-UHFFFAOYSA-N	1.2		Govers and Krop (1998)	Q	
1,2,4,6,7,9-hexachlorodibenzo-*p*-dioxin	2.1		Wang and Wong (2002)	Q	537
$C_{12}H_2Cl_6O_2$	3.5		Govers and Krop (1998)	Q	
(PCDD-124679)					
[39227-62-8]					
BSJDQMWAWFTDGD-UHFFFAOYSA-N					
1,2,4,6,8,9-hexachlorodibenzo-*p*-dioxin	2.0		Wang and Wong (2002)	Q	537
$C_{12}H_2Cl_6O_2$	4.4		Govers and Krop (1998)	Q	
(PCDD-124689)					
[58802-09-8]					
URELDHWUZUWPIU-UHFFFAOYSA-N					
1,2,3,4,6,7,8-heptachlorodibenzo-*p*-dioxin	5.6×10^{-2}		Duchowicz et al. (2020)	V	187
$C_{12}HCl_7O_2$	7.5		Mackay et al. (2006b)	V	
(PCDD-1234678)	2.3		Govers and Krop (1998)	V	
[35822-46-9]	7.5		Shiu et al. (1988)	V	
WCLNVRQZUKYVAI-UHFFFAOYSA-N	7.5×10^{-5}	2400	Paasivirta et al. (1999)	T	
	4.5×10^{-1}		Duchowicz et al. (2020)	Q	
	4.5×10^{-1}		HSDB (2015)	Q	547
	1.4		Saçan et al. (2005)	Q	
	3.6		Wang and Wong (2002)	Q	537
	1.2		Govers and Krop (1998)	Q	
1,2,3,4,6,7,9-heptachlorodibenzo-*p*-dioxin	3.4		Wang and Wong (2002)	Q	537
$C_{12}HCl_7O_2$	3.2		Govers and Krop (1998)	Q	
(PCDD-1234679)					
[58200-70-7]					
KTJJIBIRZGQFQZ-UHFFFAOYSA-N					

Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
octachlorodibenzo-*p*-dioxin	1.5		Duchowicz et al. (2020)	V	187
$C_{12}Cl_8O_2$	1.5		HSDB (2015)	V	
(PCDD-12346789)	1.5		Mackay et al. (2006b)	V	
[3268-87-9]	7.6×10^{-1}		Govers and Krop (1998)	V	
FOIBFBMSLDGNHL-UHFFFAOYSA-N	1.5		Shiu et al. (1988)	V	
	1.1×10^{-5}	2300	Paasivirta et al. (1999)	T	
	3.8×10^{-1}		Duchowicz et al. (2020)	Q	
		9600	Kühne et al. (2005)	Q	
	1.7		Saçan et al. (2005)	Q	
	5.2		Wang and Wong (2002)	Q	537
	1.9		Govers and Krop (1998)	Q	
		9500	Kühne et al. (2005)	?	

A6.8 Chlorocarbons with nitrogen (C, H, O, N, Cl)

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyanogen chloride NCCl [506-77-4] QPJDMGCKMHUXFD-UHFFFAOYSA-N	1.2×10^{-2} 5.1×10^{-3}		Hilal et al. (2008) Yaws (1999)	Q ?	 21
N,N-dichloromethylamine CH_3NCl_2 [7651-91-4] DWEYPOWXNBAIDU-UHFFFAOYSA-N	3.3×10^{-3} 3.3×10^{-3} 3.3×10^{-3}	4300 4300 4300	Burkholder et al. (2019) Burkholder et al. (2015) Cimetiere and de Laat (2009)	L L M	
chloroacetonitrile C_2H_2ClN [107-14-2] RENMDAKOXSCIGH-UHFFFAOYSA-N	9.1×10^{-1}	 4600 5400	HSDB (2015) Kühne et al. (2005) Kühne et al. (2005)	Q Q ?	449
dichloroacetonitrile C_2HCl_2N [3018-12-0] STZZWJCGRKXEFF-UHFFFAOYSA-N	2.6		HSDB (2015)	Q	100
trichloroacetonitrile C_2Cl_3N [545-06-2] DRUIESSIVFYOMK-UHFFFAOYSA-N	7.6 7.3 1.9×10^{-2} 3.9×10^{-3} 1.0×10^{-2}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	100 288, 289 288, 290 288, 291 288, 292
tetramethylammonium chloride $C_4H_{12}ClN$ [75-57-0] OKIZCWYLBDKLSU-UHFFFAOYSA-M	2.3×10^{6}		HSDB (2015)	Q	100
metformin hydrochloride $C_4H_{12}ClN_5$ [1115-70-4] OETHQSJEHLVLGH-UHFFFAOYSA-N	1.3×10^{10}		HSDB (2015)	Q	100
bis(2-chloroethyl)methylamine $C_5H_{11}Cl_2N$ [51-75-2] HAWPXGHAZFHHAD-UHFFFAOYSA-N	3.4 8.5×10^{-1}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
chlormequat chloride $C_5H_{13}Cl_2N$ [999-81-5] OLQFELZRGYJRAZ-UHFFFAOYSA-N	$>3.2\times10^{9}$		Maniere et al. (2011)	?	242, 166

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tris(2-chloroethyl)amine $C_6H_{12}Cl_3N$ [555-77-1] FDAYLTPAFBGXAB-UHFFFAOYSA-N	5.3×10^{-1} 5.3×10^{-1} 7.3×10^{-1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
bis(2-chloroethyl)ethylamine $C_6H_{13}Cl_2N$ (ethylbis(2-chloroethyl)amine) [538-07-8] UQZPGHOJMQTOHB-UHFFFAOYSA-N	2.8×10^{-2} 2.9×10^{-2} 3.0×10^{-1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
cetrimonium chloride $C_{19}H_{42}ClN$ (trimethylhexadecylammonium chloride) [112-02-7] WOWHHFRSBJGXCM-UHFFFAOYSA-M	3.4×10^{4}		HSDB (2015)	Q	100
dimethyldioctadecylammonium chloride $C_{38}H_{80}ClN$ [107-64-2] REZZEXDLIUJMMS-UHFFFAOYSA-M	1.5×10^{2}		HSDB (2015)	Q	100
1-amino-2-chlorobenzene C_6H_6ClN (*o*-chloroaniline) [95-51-2] AKCRQHGQIJBRMN-UHFFFAOYSA-N	1.9 7.8×10^{-1} 1.8 7.6×10^{-1} 1.8 1.3 1.3 1.3 2.4 1.6 7.4 2.3 9.6×10^{1} 2.8 1.1×10^{1} 5.4 7.0 1.1	7900	Brockbank (2013) Chao et al. (2017) Duchowicz et al. (2020) Chao et al. (2017) HSDB (2015) Mackay et al. (2006d) Lide and Frederikse (1995) Mackay et al. (1995) Meylan and Howard (1991) Abraham et al. (1994a) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) English and Carroll (2001) Katritzky et al. (1998) Nirmalakhandan et al. (1997) Meylan and Howard (1991) Yaws (1999)	L M V V V V V V V R Q Q Q Q Q Q Q ?	1, 737 187 68 231, 232 21, 12

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-amino-3-chlorobenzene	4.7		Chao et al. (2017)	M	
C_6H_6ClN	9.8		Altschuh et al. (1999)	M	
(*m*-chloroaniline)	2.7		Chao et al. (2017)	V	
[108-42-9]	4.5		Mackay et al. (2006d)	V	
PNPCRKVUWYDDST-UHFFFAOYSA-N	4.5		Mackay et al. (1995)	V	
	7.5		Abraham et al. (1994a)	R	
	7.5		Yaws (2003)	X	238, 12
	9.1		Keshavarz et al. (2022)	Q	
	8.8		Duchowicz et al. (2020)	Q	
	4.9		Gharagheizi et al. (2010)	Q	247
	7.7		Hilal et al. (2008)	Q	
	3.1×10^{1}		Modarresi et al. (2007)	Q	68
	4.6		Yao et al. (2002)	Q	230
	4.1		English and Carroll (2001)	Q	231, 275
	1.5×10^{1}		Katritzky et al. (1998)	Q	
	5.3		Nirmalakhandan et al. (1997)	Q	
	9.9		Duchowicz et al. (2020)	?	186, 21
	4.9		Yaws (1999)	?	21, 12
1-amino-4-chlorobenzene	8.5		Duchowicz et al. (2020)	V	187
C_6H_6ClN	3.2		HSDB (2015)	V	
(*p*-chloroaniline)	1.0×10^{1}		Mackay et al. (2006d)	V	
[106-47-8]	9.1×10^{-1}		Lide and Frederikse (1995)	V	
QSNSCYSYFYORTR-UHFFFAOYSA-N	1.0×10^{1}		Mackay et al. (1995)	V	
	2.5×10^{1}		Meylan and Howard (1991)	V	
	8.6		Abraham et al. (1994a)	R	
	3.4		Yaws (2003)	X	238, 12
	9.2×10^{-1}		Howard (1989)	X	414
	8.3		Duchowicz et al. (2020)	Q	
	4.9		Gharagheizi et al. (2010)	Q	247
	8.6		Hilal et al. (2008)	Q	
	1.6×10^{1}		Modarresi et al. (2007)	Q	68
	8.8		Yaffe et al. (2003)	Q	249, 250
	5.4		English and Carroll (2001)	Q	231, 261
	1.5×10^{1}		Katritzky et al. (1998)	Q	
	5.3		Nirmalakhandan et al. (1997)	Q	
	7.0		Meylan and Howard (1991)	Q	
2,3-dichlorobenzenamine	6.2		HSDB (2015)	Q	100
$C_6H_5Cl_2N$					
(2,3-dichloroaniline)					
[608-27-5]					
BRPSAOUFIJSKOT-UHFFFAOYSA-N					

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4-dichlorobenzenamine $C_6H_5Cl_2N$ (2,4-dichloroaniline) [554-00-7] KQCMTOWTPBNWDB-UHFFFAOYSA-N	6.2		HSDB (2015)	Q	100
3,4-dichlorobenzenamine	6.8×10^{-1}		Duchowicz et al. (2020)	V	187
$C_6H_5Cl_2N$	6.8×10^{-1}		HSDB (2015)	V	
(3,4-dichloroaniline)	4.4×10^{-1}		Mackay et al. (2006d)	V	
[95-76-1]	4.4×10^{-1}		Mackay et al. (1995)	V	
SDYWXFYBZPNOFX-UHFFFAOYSA-N	1.8×10^{1}		Duchowicz et al. (2020)	Q	
	2.0×10^{1}		Katritzky et al. (1998)	Q	
3,5-dichlorobenzenamine $C_6H_5Cl_2N$ (3,5-dichloroaniline) [626-43-7] UQRLKWGPEVNVHT-UHFFFAOYSA-N	6.2		HSDB (2015)	Q	100
2,5-dichlorobenzenamine	6.2		HSDB (2015)	Q	100
$C_6H_5Cl_2N$	9.5		Zhang et al. (2010)	Q	288, 289
(2,5-dichloroaniline)	2.6		Zhang et al. (2010)	Q	288, 290
[95-82-9]	2.7		Zhang et al. (2010)	Q	288, 291
AVYGCQXNNJPXSS-UHFFFAOYSA-N	1.9×10^{1}		Zhang et al. (2010)	Q	288, 292
2,4,5-trichlorobenzenamine	1.3×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_6H_4Cl_3N$	2.4		Zhang et al. (2010)	Q	288, 290
[636-30-6]	9.5		Zhang et al. (2010)	Q	288, 291
GUMCAKKKNKYFEB-UHFFFAOYSA-N	1.8×10^{1}		Zhang et al. (2010)	Q	288, 292
2,4,6-trichlorobenzenamine	7.4		HSDB (2015)	V	
$C_6H_4Cl_3N$	1.3×10^{1}		Zhang et al. (2010)	Q	288, 289
[634-93-5]	6.2×10^{-1}		Zhang et al. (2010)	Q	288, 290
NATVSFWWYVJTAZ-UHFFFAOYSA-N	4.1×10^{-1}		Zhang et al. (2010)	Q	288, 291
	1.5×10^{1}		Zhang et al. (2010)	Q	288, 292
2,3,4,5,6-pentachloroaniline $C_6H_2Cl_5N$ [527-20-8] KHCZSJXTDDHLGJ-UHFFFAOYSA-N	2.3×10^{1}		HSDB (2015)	Q	100
2,6-dichlorobenzenenitrile	4.8×10^{-1}	5400	Schoene and Steinhanses (1985)	M	
$C_6H_3Cl_2CN$	9.8×10^{-1}		Duchowicz et al. (2020)	V	187
(dichlobenil)	9.9×10^{-1}		HSDB (2015)	V	
[1194-65-6]	1.5		Mackay et al. (2006d)	V	
YOYAIZYFCNQIRF-UHFFFAOYSA-N	1.4		Schüürmann (2000)	V	
	1.5		Suntio et al. (1988)	V	12
	1.4		Burkhard and Guth (1981)	V	
	1.5×10^{-2}		Barcelo and Hennion (1997)	X	569
	3.5×10^{-1}		Duchowicz et al. (2020)	Q	

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.5×10^{-2}		Goodarzi et al. (2010)	Q	570, 571
	3.6×10^{-1}		Modarresi et al. (2007)	Q	68
		6000	Kühne et al. (2005)	Q	
		5500	Kühne et al. (2005)	?	
(2,4,6-trichlorophenyl)hydrazine	3.1×10^{3}		Zhang et al. (2010)	Q	288, 289
$C_6H_5Cl_3N_2$	3.7×10^{1}		Zhang et al. (2010)	Q	288, 290
[5329-12-4]	1.1×10^{1}		Zhang et al. (2010)	Q	288, 291
MULHANRBCQBHII-UHFFFAOYSA-N	5.4×10^{3}		Zhang et al. (2010)	Q	288, 292
4-chlorobenzonitrile	2.5×10^{-1}		Zhang et al. (2010)	Q	288, 289
C_7H_4ClN	3.8×10^{-1}		Zhang et al. (2010)	Q	288, 290
[623-03-0]	1.6		Zhang et al. (2010)	Q	288, 291
GJNGXPDXRVXSEH-UHFFFAOYSA-N	4.5×10^{-1}		Zhang et al. (2010)	Q	288, 292
3-chloro-2-methylbenzenamine C_7H_8ClN [87-60-5] ZUVPLKVDZNDZCM-UHFFFAOYSA-N	6.3		HSDB (2015)	Q	100
3-chloro-4-methylbenzenamine C_7H_8ClN [95-74-9] RQKFYFNZSHWXAW-UHFFFAOYSA-N	4.9		HSDB (2015)	Q	100
4-chloro-2-methylbenzenamine C_7H_8ClN [95-69-2] CXNVOWPRHWWCQR-UHFFFAOYSA-N	4.9		HSDB (2015)	Q	100
5-chloro-2-methylbenzenamine C_7H_8ClN [95-79-4] WRZOMWDJOLIVQP-UHFFFAOYSA-N	6.3		HSDB (2015)	Q	547
2,4,5,6-tetrachloro-1,3-dicyanobenzene	5.0×10^{1}		Kawamoto and Urano (1989)	M	
$C_8Cl_4N_2$	1.7×10^{-2}		Mackay et al. (2006d)	V	
(chlorothalonil)	3.9×10^{1}		MacBean (2012b)	X	352
[1897-45-6]	4.5×10^{1}		Armbrust (2000)	C	
CRQQGFGUEAVUIL-UHFFFAOYSA-N	4.1×10^{-1}		Keshavarz et al. (2022)	Q	
	1.8×10^{1}		Duchowicz et al. (2020)	Q	
	6.5×10^{1}		Zhang et al. (2010)	Q	288, 289
	1.5		Zhang et al. (2010)	Q	288, 290
	6.9×10^{1}		Zhang et al. (2010)	Q	288, 291
	2.7×10^{1}		Zhang et al. (2010)	Q	288, 292
	5.8		Hilal et al. (2008)	Q	
	2.4×10^{1}		Modarresi et al. (2007)	Q	68
	6.5×10^{1}		Meylan and Howard (1991)	Q	
	4.9		Duchowicz et al. (2020)	?	186, 21

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-chlorobenzalmalononitrile $C_{10}H_5ClN_2$ [2698-41-1] JJNZXLAFIPKXIG-UHFFFAOYSA-N	9.9×10^{2}		HSDB (2015)	Q	100
benzyltrimethylammonium chloride $C_{10}H_{16}ClN$ [56-93-9] KXHPPCXNWTUNSB-UHFFFAOYSA-M	2.9×10^{8}		HSDB (2015)	Q	100
chlordimeform $C_{10}H_{13}ClN_2$ [6164-98-3] STUSTWKEFDQFFZ-UHFFFAOYSA-N	2.9×10^{1} 2.6×10^{1}		HSDB (2015) MacBean (2012a)	V ?	 12
4,4'-dichloroazobenzene $C_{12}H_8Cl_2N_2$ [1602-00-2] XHQLXCFUPJSGOE-UHFFFAOYSA-N	1.2		HSDB (2015)	Q	100
bis(3,4-dichlorophenyl)diazene $C_{12}H_6Cl_4N_2$ (3,4,3',4'-tetrachloroazobenzene) [14047-09-7] SOBGIMQKWDUEPY-UHFFFAOYSA-N	2.2		HSDB (2015)	Q	449
2-(*p*-chlorophenyl)-3-methylbutyronitrile $C_{11}H_{12}ClN$ [2012-81-9] RBGSZIRWNWQDOK-UHFFFAOYSA-N	2.3 4.4 3.9 2.9×10^{-1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
3,3'-dichloro-(1,1'-biphenyl)-4,4'-diamine $C_{12}H_{10}Cl_2N_2$ (3,3'-dichlorobenzidine) [91-94-1] HUWXDEQWWKGHRV-UHFFFAOYSA-N	2.0×10^{2} 2.0×10^{2} 1.2×10^{1} 3.5×10^{5}		Mackay et al. (2006d) Mackay et al. (1995) Mackay et al. (1995) HSDB (2015)	V V C Q	 100
4-chloroazobenzene $C_{12}H_9ClN_2$ [4340-77-6] NJFDMENHTAYHMA-UHFFFAOYSA-N	7.4 2.2		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,4'-methylenebis(2-chlorobenzenamine) $C_{13}H_{12}Cl_2N_2$ [101-14-4] IBOFVQJTBBUKMU-UHFFFAOYSA-N	9.0×10^5		HSDB (2015)	Q	100
	3.0×10^5		Zhang et al. (2010)	Q	288, 289
	3.4×10^4		Zhang et al. (2010)	Q	288, 290
	2.9×10^4		Zhang et al. (2010)	Q	288, 291
	9.7×10^5		Zhang et al. (2010)	Q	288, 292
clofentezine $C_{14}H_8N_4Cl_2$ [74115-24-5] UXADOQPNKNTIHB-UHFFFAOYSA-N	2.5×10^4		Duchowicz et al. (2020)	V	187
	1.7×10^4		Duchowicz et al. (2020)	Q	
aniline, 4,4'-(imidocarbonyl)bis-(N,N-dimethyl)-, hydrochloride $C_{17}H_{22}ClN_3$ (auramine hydrochloride) [2465-27-2] KSCQDDRPFHTIRL-UHFFFAOYSA-N	3.5×10^{10}		HSDB (2015)	Q	100
amitriptyline hydrochloride $C_{20}H_{24}ClN$ [549-18-8] KFYRPLNVJVHZGT-UHFFFAOYSA-N	1.4×10^2		HSDB (2015)	Q	100
chlorhexidine $C_{22}H_{30}Cl_2N_{10}$ [55-56-1] GHXZTYHSJHQHIJ-UHFFFAOYSA-N	9.0×10^{24}		HSDB (2015)	Q	100
malachite green $C_{23}H_{25}ClN_2$ [569-64-2] FDZZZRQASAIRJF-UHFFFAOYSA-M	5.2×10^8		HSDB (2015)	Q	100
tetradecylbenzyldimethyl ammonium chloride $C_{23}H_{42}ClN$ [139-08-2] OCBHHZMJRVXXQK-UHFFFAOYSA-M	7.6×10^5		HSDB (2015)	Q	100
stearyldimethylbenzylammonium chloride $C_{27}H_{50}ClN$ (benzyldimethylstearylammonium chloride) [122-19-0] SFVFIFLLYFPGHH-UHFFFAOYSA-M	2.3×10^5		HSDB (2015)	Q	100

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4,6-trichloro-1,3,5-triazine	2.0×10^{1}		HSDB (2015)	Q	100
$C_3Cl_3N_3$	2.0×10^{1}		Zhang et al. (2010)	Q	288, 289
[108-77-0]	2.4×10^{1}		Zhang et al. (2010)	Q	288, 290
MGNCLNQXLYJVJD-UHFFFAOYSA-N	3.1×10^{-1}		Zhang et al. (2010)	Q	288, 291
	7.9		Zhang et al. (2010)	Q	288, 292
2-chloropyridine	7.4×10^{-1}	5900	Arnett and Chawla (1979)	M	561
C_5H_4ClN	6.1×10^{-1}		Duchowicz et al. (2020)	V	187
[109-09-1]	1.9×10^{-1}		Duchowicz et al. (2020)	Q	
OKDGRDCXVWSXDC-UHFFFAOYSA-N	5.8×10^{-1}		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	68
		6100	Kühne et al. (2005)	Q	
	6.7×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.9×10^{-1}		English and Carroll (2001)	Q	231, 275
	8.0×10^{-2}		Katritzky et al. (1998)	Q	
	1.5×10^{1}		Nirmalakhandan et al. (1997)	Q	
		6600	Kühne et al. (2005)	?	
3-chloropyridine	3.5×10^{-1}	5600	Arnett and Chawla (1979)	M	561
C_5H_4ClN	4.1×10^{-1}		Hilal et al. (2008)	Q	
[626-60-8]	8.3×10^{-1}		Modarresi et al. (2007)	Q	68
PWRBCZZQRRPXAB-UHFFFAOYSA-N	3.7×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.9×10^{-1}		English and Carroll (2001)	Q	231, 232
	1.5×10^{1}		Nirmalakhandan et al. (1997)	Q	
2,3,4,6-tetrachloropyridine	1.2×10^{-3}		Zhang et al. (2010)	Q	288, 289
C_5HCl_4N	1.1×10^{-1}		Zhang et al. (2010)	Q	288, 290
[14121-36-9]	7.9×10^{-2}		Zhang et al. (2010)	Q	288, 291
FZFNDUTVMQOPCT-UHFFFAOYSA-N	2.9×10^{-1}		Zhang et al. (2010)	Q	288, 292
2,3,5,6-tetrachloropyridine	1.2×10^{-3}		HSDB (2015)	Q	100
C_5HCl_4N	1.2×10^{-3}		Zhang et al. (2010)	Q	288, 289
[2402-79-1]	3.4×10^{-2}		Zhang et al. (2010)	Q	288, 290
FATBKZJZAHWCSL-UHFFFAOYSA-N	8.4×10^{-2}		Zhang et al. (2010)	Q	288, 291
	1.9×10^{-1}		Zhang et al. (2010)	Q	288, 292
pentachloropyridine	1.6×10^{-3}		HSDB (2015)	Q	100
C_5Cl_5N	1.6×10^{-3}		Zhang et al. (2010)	Q	288, 289
[2176-62-7]	1.3×10^{-2}		Zhang et al. (2010)	Q	288, 290
DNDPLEAVNVOOQZ-UHFFFAOYSA-N	2.5×10^{-2}		Zhang et al. (2010)	Q	288, 291
	1.8×10^{-1}		Zhang et al. (2010)	Q	288, 292
desethylatrazine	6.6×10^{3}		HSDB (2015)	Q	100
$C_6H_{10}ClN_5$					
[6190-65-4]					
DFWFIQKMSFGDCQ-UHFFFAOYSA-N					

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-chloro-6-(trichloromethyl)-pyridine	6.2×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_6H_3Cl_4N$	1.8		Zhang et al. (2010)	Q	288, 290
[1929-82-4]	2.7		Zhang et al. (2010)	Q	288, 291
DCUJJWWUNKIJPH-UHFFFAOYSA-N	4.2×10^{-1}		Zhang et al. (2010)	Q	288, 292
	1.8		Hilal et al. (2008)	Q	
	5.9×10^{-1}		Modarresi et al. (2007)	Q	68
2,3,4,5-tetrachloro-6-methylpyridine	6.7×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_6H_3Cl_4N$	3.6×10^{-2}		Zhang et al. (2010)	Q	288, 290
[10469-02-0]	3.6×10^{-2}		Zhang et al. (2010)	Q	288, 291
OZLPEWBQZDDFCQ-UHFFFAOYSA-N	1.1×10^{-1}		Zhang et al. (2010)	Q	288, 292
2-chloro-5-(trichloromethyl)pyridine	6.2×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_6H_3Cl_4N$	2.2		Zhang et al. (2010)	Q	288, 290
[69045-78-9]	7.7×10^{-1}		Zhang et al. (2010)	Q	288, 291
VLJIVLGVKMTBOD-UHFFFAOYSA-N	4.2×10^{-1}		Zhang et al. (2010)	Q	288, 292
2,3-dichloro-5-(trichloromethyl)pyridine	8.4×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_6H_2Cl_5N$	4.1×10^{-1}		Zhang et al. (2010)	Q	288, 290
[69045-83-6]	1.8×10^{-1}		Zhang et al. (2010)	Q	288, 291
XVBWGQSXLITICX-UHFFFAOYSA-N	6.1×10^{-1}		Zhang et al. (2010)	Q	288, 292
2,5-dichloro-6-(trichloromethyl)pyridine	8.4×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_6H_2Cl_5N$	1.2		Zhang et al. (2010)	Q	288, 290
[1817-13-6]	9.9×10^{-1}		Zhang et al. (2010)	Q	288, 291
MWFCRQNUHFSUNY-UHFFFAOYSA-N	5.7×10^{-1}		Zhang et al. (2010)	Q	288, 292
3,4,5-trichloro-2-(trichloromethyl)pyridine	7.2×10^{1}		Zhang et al. (2010)	Q	288, 289
C_6HCl_6N	9.0×10^{-2}		Zhang et al. (2010)	Q	288, 290
[1201-30-5]	1.0×10^{-1}		Zhang et al. (2010)	Q	288, 291
YWSFDYUMEBEQNZ-UHFFFAOYSA-N	4.1×10^{-1}		Zhang et al. (2010)	Q	288, 292
2,3,4,5-tetrachloro-6-(trichloromethyl)pyridine	1.5		Zhang et al. (2010)	Q	288, 289
C_6Cl_7N	6.7×10^{-2}		Zhang et al. (2010)	Q	288, 290
[1134-04-9]	7.0×10^{-2}		Zhang et al. (2010)	Q	288, 291
YMBFWRZKTZICHS-UHFFFAOYSA-N	2.3×10^{-1}		Zhang et al. (2010)	Q	288, 292
3,4,5,6-tetrachloropyridine-2-carbonitrile	7.5		Zhang et al. (2010)	Q	288, 289
$C_6Cl_4N_2$	1.7		Zhang et al. (2010)	Q	288, 290
[17824-83-8]	8.0×10^{-1}		Zhang et al. (2010)	Q	288, 291
KFPBGJYBKSQIAI-UHFFFAOYSA-N	1.5×10^{1}		Zhang et al. (2010)	Q	288, 292

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-amino-3,5,6-trichloropyridine-2-carbonitrile	1.6×10^{4}		Zhang et al. (2010)	Q	288, 289
$C_6H_2Cl_3N_3$	1.1×10^{3}		Zhang et al. (2010)	Q	288, 290
[14143-60-3]	9.0×10^{3}		Zhang et al. (2010)	Q	288, 291
AZYYQVGBVUCIEO-UHFFFAOYSA-N	1.0×10^{5}		Zhang et al. (2010)	Q	288, 292
crimidine	2.6×10^{2}		HSDB (2015)	Q	100
$C_7H_{10}ClN_3$					
[535-89-7]					
HJIUPFPIEBPYIE-UHFFFAOYSA-N					
simazine	1.0×10^{4}		HSDB (2015)	V	
$C_7H_{12}ClN_5$	2.9×10^{3}		Mackay et al. (2006d)	V	
[122-34-9]	2.9×10^{3}		Suntio et al. (1988)	V	12
ODCWYMIRDDJXKW-UHFFFAOYSA-N	1.6×10^{4}		Glotfelty et al. (1987)	V	
	2.9×10^{1}		Barcelo and Hennion (1997)	X	569
	6.2×10^{7}		Delgado and Alderete (2003)	C	
	1.1×10^{4}		Delgado and Alderete (2003)	C	
	9.1×10^{1}		Goodarzi et al. (2010)	Q	570
	1.7×10^{3}		Hilal et al. (2008)	Q	
	7.2×10^{3}		Abraham et al. (2007)	Q	
	5.5×10^{5}		Delgado and Alderete (2003)	Q	
	4.0×10^{6}		Delgado and Alderete (2003)	Q	
desethylterbuthylazine	2.2×10^{3}		Otto et al. (1997)	V	
$C_7H_{12}ClN_5$					
[30125-63-4]					
LMKQNTMFZLAJDV-UHFFFAOYSA-N					
mepiquat chloride	3.3×10^{11}		Maniere et al. (2011)	?	242, 166
$C_7H_{16}NCl$					
[24307-26-4]					
VHOVSQVSAAQANU-UHFFFAOYSA-M					
atrazine	1.9×10^{3}		Muir et al. (2004)	L	369
$C_8H_{14}ClN_5$	3.5×10^{3}		Mackay et al. (2006d)	V	
[1912-24-9]	1.0×10^{3}		Siebers et al. (1994)	V	
MXWJVTOOROXGIU-UHFFFAOYSA-N	3.3×10^{3}		Riederer (1990)	V	
	3.4×10^{3}		Suntio et al. (1988)	V	12
	2.0×10^{3}		Glotfelty et al. (1987)	V	
	3.4×10^{1}		Barcelo and Hennion (1997)	X	569
	8.3×10^{6}		Delgado and Alderete (2003)	C	
	4.3×10^{3}		Delgado and Alderete (2003)	C	
	7.2×10^{1}		Goodarzi et al. (2010)	Q	570
	7.2×10^{2}		Hilal et al. (2008)	Q	
	5.1×10^{3}		Abraham et al. (2007)	Q	
	2.8×10^{4}		Delgado and Alderete (2003)	Q	
	4.0×10^{5}		Delgado and Alderete (2003)	Q	

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
clonidine $C_9H_9Cl_2N_3$ [4205-90-7] GJSURZIOUXUGAL-UHFFFAOYSA-N	6.6×10^5		HSDB (2015)	Q	100
cyprazine $C_9H_{12}ClN_5$ [22936-86-3] OOHIAOSLOGDBCE-UHFFFAOYSA-N	7.6×10^3 7.7×10^4 3.8×10^3		Duchowicz et al. (2020) Duchowicz et al. (2020) HSDB (2015)	V Q Q	187 100
propazine $C_9H_{16}ClN_5$ [139-40-2] WJNRPILHGGKWCK-UHFFFAOYSA-N	2.1×10^3 1.0×10^4 9.9×10^1 1.7×10^2 3.6×10^2 4.0×10^3		HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Goodarzi et al. (2010) Hilal et al. (2008) Abraham et al. (2007)	V V V X Q Q Q	 560 12 569 570, 573
sebuthylazine $C_9H_{16}ClN_5$ [7286-69-3] BZRUVKZGXNSXMB-UHFFFAOYSA-N	8.4×10^2		Ebert et al. (2023)	?	319
terbuthylazine $C_9H_{16}ClN_5$ [5915-41-3] FZXISNSWEXTPMF-UHFFFAOYSA-N	4.3×10^2 2.5×10^2 2.5×10^2 2.4×10^2 2.9×10^2 9.0×10^2 4.3×10^2		HSDB (2015) Mackay et al. (2006d) Otto et al. (1997) Siebers et al. (1994) Hilal et al. (2008) Abraham et al. (2007) Maniere et al. (2011)	V V V V Q Q ?	 242, 166
cyanazine $C_9H_{13}ClN_6$ [21725-46-2] MZZBPDKVEFVLFF-UHFFFAOYSA-N	3.3×10^6 3.3×10^4 8.3×10^9 3.9×10^6 9.6×10^1 6.4×10^5 2.0×10^6 4.5×10^6 1.0×10^9		Mackay et al. (2006d) Barcelo and Hennion (1997) Delgado and Alderete (2003) Delgado and Alderete (2003) Goodarzi et al. (2010) Hilal et al. (2008) Abraham et al. (2007) Delgado and Alderete (2003) Delgado and Alderete (2003)	V X C C Q Q Q Q Q	 569 570
anilazine $C_9H_5Cl_3N_4$ [101-05-3] IMHBYKMAHXWHRP-UHFFFAOYSA-N	3.5×10^4 3.5×10^4 2.9×10^1 1.2×10^3 9.5 5.4×10^3 3.5×10^4		HSDB (2015) Mackay et al. (2006d) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) MacBean (2012a)	V V Q Q Q Q ?	 288, 289 288, 290 288, 291 288, 292

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,7-dichloroquinoline	2.6×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_9H_5Cl_2N$	6.9		Zhang et al. (2010)	Q	288, 290
[86-98-6]	1.5		Zhang et al. (2010)	Q	288, 291
HXEWMTXDBOQQKO-UHFFFAOYSA-N	7.0		Zhang et al. (2010)	Q	288, 292
fenclorim	5.6×10^{-1}		Ebert et al. (2023)	?	319
$C_{10}H_6Cl_2N_2$					
[3740-92-9]					
NRFQZTCQAYEXEE-UHFFFAOYSA-N					
acetamiprid	1.4×10^{2}		HSDB (2015)	Q	100
$C_{10}H_{11}ClN_4$	$>1.9\times10^{7}$		Maniere et al. (2011)	?	166
[135410-20-7]					
WCXDHFDTOYPNIE-UHFFFAOYSA-N					
pyrimethamine	9.1×10^{4}		HSDB (2015)	Q	449
$C_{12}H_{13}ClN_4$					
[58-14-0]					
WKSAUQYGYAYLPV-UHFFFAOYSA-N					
penconazole	6.9×10^{2}		Duchowicz et al. (2020)	V	187
$C_{13}H_{15}Cl_2N_3$	1.2×10^{3}		Mackay et al. (2006d)	V	
[66246-88-6]	2.1		Duchowicz et al. (2020)	Q	
WKBPZYKAUNRMKP-UHFFFAOYSA-N	1.5×10^{3}		Maniere et al. (2011)	?	12, 166
myclobutanil	2.3×10^{3}		Duchowicz et al. (2020)	V	187
$C_{15}H_{17}ClN_4$	2.3×10^{3}		HSDB (2015)	V	
[88671-89-0]	2.2×10^{2}		Duchowicz et al. (2020)	Q	
HZJKXKUJVSEEFU-UHFFFAOYSA-N	2.3×10^{3}		Maniere et al. (2011)	?	12, 166
2-chloro-4,6-bis(2,4-dimethylphenyl)-1,3,5-triazine	1.2×10^{3}		Zhang et al. (2010)	Q	288, 289
$C_{19}H_{18}N_3Cl$	1.3×10^{3}		Zhang et al. (2010)	Q	288, 290
[1237-53-2]	7.0		Zhang et al. (2010)	Q	288, 291
LVWOBZPDFCTAOU-UHFFFAOYSA-N	1.2×10^{3}		Zhang et al. (2010)	Q	288, 292
fenbuconazole	3.3×10^{4}		Maniere et al. (2011)	?	242, 166
$C_{19}H_{17}ClN_4$					
[114369-43-6]					
RQDJADAKIFFEKQ-UHFFFAOYSA-N					
trichloronitromethane	4.7×10^{-3}		Burkholder et al. (2019)	L	
CCl_3NO_2	4.7×10^{-3}		Burkholder et al. (2015)	L	
(chloropicrin)	4.7×10^{-3}		Sander et al. (2011)	L	
[76-06-2]	4.7×10^{-3}		Worthington and Wade (2007)	M	
LFHISGNCFUNFFM-UHFFFAOYSA-N	4.0×10^{-3}		Welke et al. (1998)	M	
	4.8×10^{-3}		Kawamoto and Urano (1989)	M	
			Mackay et al. (2006d)	V	560
	5.1×10^{-3}		Suntio et al. (1988)	V	12
	5.0×10^{-2}		Keshavarz et al. (2022)	Q	

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.6×10^{-2}		Duchowicz et al. (2020)	Q	185
	2.5×10^{-3}		Hilal et al. (2008)	Q	
	3.0×10^{-2}		Modarresi et al. (2007)	Q	68
	4.8×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.3×10^{-2}		Katritzky et al. (1998)	Q	
	4.8×10^{-3}		Duchowicz et al. (2020)	?	186, 21
phosgene oxime $CHCl_2NO$ [1794-86-1] JIRJHEXNDQBKRZ-UHFFFAOYSA-N	1.8×10^{1}		HSDB (2015)	Q	100
1,1-dichloro-1-nitroethane	7.7×10^{-3}		Duchowicz et al. (2020)	V	187
$C_2H_3Cl_2NO_2$	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
[594-72-9]	7.7×10^{-3}		HSDB (2015)	Q	100
OQOGEOLRYAOSKO-UHFFFAOYSA-N	2.0×10^{-2}		Hilal et al. (2008)	Q	
	1.1×10^{-1}		Modarresi et al. (2007)	Q	68
2-chloroacetamide C_2H_4ClNO [79-07-2] VXIVSQZSERGHQP-UHFFFAOYSA-N	2.5×10^{3}		HSDB (2015)	Q	100
MCM:CCL3PAN	1.0×10^{1}		Wang et al. (2017)	Q	81, 239
$C_2NO_5Cl_3$	7.3×10^{-1}		Wang et al. (2017)	Q	81, 240
LLOMRHYBAIQQGH-UHFFFAOYSA-N	3.6×10^{-5}		Wang et al. (2017)	Q	81, 241
MCM:CCLNO3COOH	2.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_2H_4NO_5Cl$	2.6×10^{3}		Wang et al. (2017)	Q	81, 240
GVGGZHVOOFUNFY-UHFFFAOYSA-N	4.2		Wang et al. (2017)	Q	81, 241
MCM:CHCL2PAN	2.2×10^{1}		Wang et al. (2017)	Q	81, 239
$C_2HNO_5Cl_2$	1.6×10^{1}		Wang et al. (2017)	Q	81, 240
BORKLXDOXKHVRO-UHFFFAOYSA-N	4.9×10^{-4}		Wang et al. (2017)	Q	81, 241
MCM:CLETPAN	9.8		Wang et al. (2017)	Q	81, 239
$C_2H_2NO_5Cl$	3.3×10^{1}		Wang et al. (2017)	Q	81, 240
IEQWXJNETVFAEB-UHFFFAOYSA-N	4.2×10^{-3}		Wang et al. (2017)	Q	81, 241
MCM:CNO3CLOOH	2.1×10^{3}		Wang et al. (2017)	Q	81, 239
$C_2H_4NO_5Cl$	3.0×10^{3}		Wang et al. (2017)	Q	81, 240
FBIXZLOOAAICML-UHFFFAOYSA-N	8.3		Wang et al. (2017)	Q	81, 241
MCM:CCLNO3COH	1.8×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_4NO_4Cl$	7.1×10^{2}		Wang et al. (2017)	Q	81, 240
PMLDKFZZOPGPNK-UHFFFAOYSA-N	7.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:CL2OHPAN	3.8×10^{3}		Wang et al. (2017)	Q	81, 239
$C_2HNO_6Cl_2$	1.5×10^{2}		Wang et al. (2017)	Q	81, 240
YJZUCQDIDXVPNP-UHFFFAOYSA-N	1.4×10^{-2}		Wang et al. (2017)	Q	81, 241

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CLOHPAN $C_2H_2NO_6Cl$ ZNYKQWDXHYNGTP-UHFFFAOYSA-N	4.2×10^{3} 1.0×10^{4} 8.9×10^{-2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
1-chloro-1-nitroethane $C_2H_4ClNO_2$ [598-92-5] LPIWIOBGUAPNQW-UHFFFAOYSA-N	2.0×10^{-2}		Ebert et al. (2023)	?	317
MCM:CNO3CLOH $C_2H_4NO_4Cl$ OUFVLIWCNZOATK-UHFFFAOYSA-N	2.8×10^{2} 1.4×10^{3} 1.4×10^{2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:CCLCONO3 $C_2H_2NO_4Cl$ XDEFPIDZLAIVCM-UHFFFAOYSA-N	2.6×10^{1} 1.6×10^{2} 2.5×10^{-3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:CNO3OCL $C_2H_2NO_4Cl$ ODQFUUDIEKKDDJ-UHFFFAOYSA-N	1.7×10^{1} 1.1×10^{1} 4.4×10^{-3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
symclosene $C_3Cl_3N_3O_3$ (trichloroisocyanuric acid) [87-90-1] YRIZYWQGELRKNT-UHFFFAOYSA-N	1.6×10^{5}		HSDB (2015)	Q	100
MCM:CL12PAN $C_3H_3NO_5Cl_2$ MSMFQRZPTBDNBF-UHFFFAOYSA-N	6.2×10^{1} 4.9×10^{1} 2.5×10^{-3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
1-chloro-1-nitropropane $C_3H_6ClNO_2$ [600-25-9] XEKUXTMJEFPWCG-UHFFFAOYSA-N	4.6×10^{-2}		Ebert et al. (2023)	?	317
1,3-dichloro-5,5-dimethylhydantoin $C_5H_6Cl_2N_2O_2$ [118-52-5] KEQGZUUPPQEDPF-UHFFFAOYSA-N	9.9		HSDB (2015)	Q	100
carmustine $C_5H_9Cl_2N_3O_2$ [154-93-8] DLGOEMSEDOSKAD-UHFFFAOYSA-N	2.1×10^{5}		HSDB (2015)	Q	100

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-chloro-N,N-di-2-propenylacetamide	9.2×10^{1}		Duchowicz et al. (2020)	V	187
$C_8H_{12}ClNO$	9.2×10^{1}		HSDB (2015)	V	
[93-71-0]	9.5		Duchowicz et al. (2020)	Q	
MDBGGTQNNUOQRC-UHFFFAOYSA-N	9.7×10^{1}		Hilal et al. (2008)	Q	
	1.9×10^{1}		Modarresi et al. (2007)	Q	68
2,2-dichloro-N,N-di-2-propenylacetamide	3.1×10^{1}		Hilal et al. (2008)	Q	
$C_8H_{11}Cl_2NO$ (dichlormid)	2.7×10^{1}		Modarresi et al. (2007)	Q	68
[37764-25-3]					
YRMLFORXOOIJDR-UHFFFAOYSA-N					
lomustine	5.5×10^{4}		HSDB (2015)	Q	100
$C_9H_{16}ClN_3O_2$					
[13010-47-4]					
GQYIWUVLTXOXAJ-UHFFFAOYSA-N					
semustine	3.9×10^{4}		HSDB (2015)	Q	100
$C_{10}H_{18}ClN_3O_2$					
[13909-09-6]					
FVLVBPDQNARYJU-UHFFFAOYSA-N					
furilazole	1.1×10^{5}		Duchowicz et al. (2020)	V	187
$C_{11}H_{13}Cl_2NO_3$	1.3×10^{3}		Duchowicz et al. (2020)	Q	
[121776-33-8]					
MCNOFYBITGAAGM-UHFFFAOYSA-N					
dimethazone	2.4×10^{2}		Duchowicz et al. (2020)	V	187
$C_{12}H_{14}ClNO_2$	2.4×10^{2}		MacBean (2012b)	X	352
(clomazone)	4.5		Duchowicz et al. (2020)	Q	
[81777-89-1]	2.4×10^{2}		Maniere et al. (2011)	?	242, 166
KIEDNEWSYUYDSN-UHFFFAOYSA-N					
2-chloronitrobenzene	1.1		Altschuh et al. (1999)	M	
$C_6H_4ClNO_2$	2.2×10^{-1}		Hellmann (1987)	M	88
(*o*-chloronitrobenzene)	2.8×10^{-1}		Lide and Frederikse (1995)	V	
[88-73-3]	1.1		Keshavarz et al. (2022)	Q	
BFCFYVKQTRLZHA-UHFFFAOYSA-N	3.1		Duchowicz et al. (2020)	Q	185
	6.2×10^{-1}		Zhang et al. (2010)	Q	288, 289
	1.5×10^{-1}		Zhang et al. (2010)	Q	288, 290
	1.2		Zhang et al. (2010)	Q	288, 291
	4.6×10^{-1}		Zhang et al. (2010)	Q	288, 292
	3.1×10^{-1}		Hilal et al. (2008)	Q	
	1.8×10^{-1}		Modarresi et al. (2007)	Q	68
		4700	Kühne et al. (2005)	Q	
	2.3×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	8.1×10^{-1}		Yao et al. (2002)	Q	230

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.5×10^{-1}		Katritzky et al. (1998)	Q	
	1.1		Duchowicz et al. (2020)	?	186, 21
		6000	Kühne et al. (2005)	?	
	9.7×10^{-1}		Yaws (1999)	?	21, 12
3-chloronitrobenzene	1.4		Chao et al. (2017)	M	
$C_6H_4ClNO_2$	7.3×10^{-1}		Altschuh et al. (1999)	M	
(*m*-chloronitrobenzene)	1.1×10^{-1}		Schüürmann (2000)	V	
[121-73-3]	1.1		Keshavarz et al. (2022)	Q	
KMAQZIILEGKYQZ-UHFFFAOYSA-N	1.8		Duchowicz et al. (2020)	Q	
	6.2×10^{-1}		Zhang et al. (2010)	Q	288, 289
	2.8×10^{-1}		Zhang et al. (2010)	Q	288, 290
	2.8×10^{-1}		Zhang et al. (2010)	Q	288, 291
	4.6×10^{-1}		Zhang et al. (2010)	Q	288, 292
	2.1×10^{-1}		Hilal et al. (2008)	Q	
	1.7×10^{-1}		Modarresi et al. (2007)	Q	68
	7.3×10^{-1}		Duchowicz et al. (2020)	?	186, 21
	3.4×10^{-1}		Yaws (1999)	?	21, 12
4-chloronitrobenzene	6.4×10^{-1}	5900	Brockbank (2013)	L	
$C_6H_4ClNO_2$	1.4		Chao et al. (2017)	M	
(*p*-chloronitrobenzene)	2.0		Altschuh et al. (1999)	M	
[100-00-5]	1.8×10^{-1}		Hellmann (1987)	M	88
CZGCEKJOLUNIFY-UHFFFAOYSA-N	2.8×10^{-1}		Lide and Frederikse (1995)	V	
	1.1		Keshavarz et al. (2022)	Q	
	1.7		Duchowicz et al. (2020)	Q	185
	6.2×10^{-1}		Zhang et al. (2010)	Q	288, 289
	3.0×10^{-1}		Zhang et al. (2010)	Q	288, 290
	6.1×10^{-1}		Zhang et al. (2010)	Q	288, 291
	4.6×10^{-1}		Zhang et al. (2010)	Q	288, 292
	2.3×10^{-1}		Hilal et al. (2008)	Q	
	2.3×10^{-1}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Modarresi et al. (2007)	Q	68
		4700	Kühne et al. (2005)	Q	
	1.9×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	1.6		Katritzky et al. (1998)	Q	
	2.0		Duchowicz et al. (2020)	?	186, 21
		4000	Kühne et al. (2005)	?	
1,2-dichloro-4-nitrobenzene	1.2		Altschuh et al. (1999)	M	
$C_6H_3Cl_2NO_2$	1.1		Keshavarz et al. (2022)	Q	
[99-54-7]	1.8		Duchowicz et al. (2020)	Q	
NTBYINQTYWZXLH-UHFFFAOYSA-N	2.1×10^{-1}		Abraham et al. (2019)	Q	
	8.4×10^{-1}		Zhang et al. (2010)	Q	288, 289
	3.1×10^{-1}		Zhang et al. (2010)	Q	288, 290
	4.6×10^{-1}		Zhang et al. (2010)	Q	288, 291
	6.7×10^{-1}		Zhang et al. (2010)	Q	288, 292
	2.7×10^{-1}		Hilal et al. (2008)	Q	

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.3×10^{-1}		Modarresi et al. (2007)	Q	68
	1.2		Duchowicz et al. (2020)	?	186, 21
1,4-dichloro-2-nitrobenzene	8.2×10^{-1}		Altschuh et al. (1999)	M	
$C_6H_3Cl_2NO_2$	1.1		Keshavarz et al. (2022)	Q	
[89-61-2]	1.8		Duchowicz et al. (2020)	Q	185
RZKKOBGFCAHLCZ-UHFFFAOYSA-N	3.2×10^{-1}		Abraham et al. (2019)	Q	
	8.4×10^{-1}		Zhang et al. (2010)	Q	288, 289
	1.5×10^{-1}		Zhang et al. (2010)	Q	288, 290
	7.3×10^{-1}		Zhang et al. (2010)	Q	288, 291
	6.1×10^{-1}		Zhang et al. (2010)	Q	288, 292
	3.1×10^{-1}		Hilal et al. (2008)	Q	
	2.2×10^{-1}		Modarresi et al. (2007)	Q	68
	8.2×10^{-1}		Duchowicz et al. (2020)	?	186, 21
2,3-dichloronitrobenzene	5.0×10^{-1}		Abraham et al. (2019)	Q	
$C_6H_3Cl_2NO_2$	8.2×10^{-1}		HSDB (2015)	Q	100
[3209-22-1]	8.4×10^{-1}		Zhang et al. (2010)	Q	288, 289
CMVQZRLQEOAYSW-UHFFFAOYSA-N	1.4×10^{-1}		Zhang et al. (2010)	Q	288, 290
	9.7×10^{-1}		Zhang et al. (2010)	Q	288, 291
	6.7×10^{-1}		Zhang et al. (2010)	Q	288, 292
2,4-dichloronitrobenzene	3.1×10^{-1}		HSDB (2015)	Q	100
$C_6H_3Cl_2NO_2$	8.4×10^{-1}		Zhang et al. (2010)	Q	288, 289
[611-06-3]	1.6×10^{-1}		Zhang et al. (2010)	Q	288, 290
QUIMTLZDMCNYGY-UHFFFAOYSA-N	8.4×10^{-1}		Zhang et al. (2010)	Q	288, 291
	2.9×10^{-1}		Zhang et al. (2010)	Q	288, 292
3,5-dichloronitrobenzene	8.4×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_6H_3Cl_2NO_2$	2.0×10^{-1}		Zhang et al. (2010)	Q	288, 290
[618-62-2]	1.1×10^{-1}		Zhang et al. (2010)	Q	288, 291
RNABGKOKSBUFHW-UHFFFAOYSA-N	2.9×10^{-1}		Zhang et al. (2010)	Q	288, 292
pentachloronitrobenzene	2.7		Kawamoto and Urano (1989)	M	
$C_6Cl_5NO_2$	2.2×10^{-1}		Duchowicz et al. (2020)	V	187
(quintozene)	2.2×10^{-1}		HSDB (2015)	V	
[82-68-8]	2.3×10^{-1}		Mackay et al. (2006d)	V	
LKPLKUMXSAEKID-UHFFFAOYSA-N	2.1×10^{-1}		Howard and Meylan (1997)	X	448
	1.1		Duchowicz et al. (2020)	Q	
	2.1		Zhang et al. (2010)	Q	288, 289
	2.3×10^{-2}		Zhang et al. (2010)	Q	288, 290
	2.2×10^{-2}		Zhang et al. (2010)	Q	288, 291
	2.2×10^{-1}		Zhang et al. (2010)	Q	288, 292
	6.9×10^{-2}		Hilal et al. (2008)	Q	
	2.1		Meylan and Howard (1991)	Q	

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-chloro-2-nitrophenol	7.8×10^{-1}		Duchowicz et al. (2020)	V	187
$C_6H_4ClNO_3$	7.8×10^{-1}		Schwarzenbach et al. (1988)	V	12
[89-64-5]	1.6×10^{1}		Duchowicz et al. (2020)	Q	
NWSIFTLPLKCTSX-UHFFFAOYSA-N	7.9×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	3.6×10^{1}		Katritzky et al. (1998)	Q	
2-chloro-4-nitrobenzenamine	1.0×10^{3}		Altschuh et al. (1999)	M	
$C_6H_5ClN_2O_2$	4.2×10^{3}		Keshavarz et al. (2022)	Q	
[121-87-9]	1.3×10^{3}		Duchowicz et al. (2020)	Q	185
LOCWBQIWHWIRGN-UHFFFAOYSA-N	1.8×10^{3}		Zhang et al. (2010)	Q	288, 289
	1.3×10^{3}		Zhang et al. (2010)	Q	288, 290
	6.7×10^{4}		Zhang et al. (2010)	Q	288, 291
	2.1×10^{3}		Zhang et al. (2010)	Q	288, 292
	4.6×10^{2}		Hilal et al. (2008)	Q	
	6.4×10^{2}		Modarresi et al. (2007)	Q	68
	1.0×10^{3}		Duchowicz et al. (2020)	?	186, 21
2-chloro-5-nitrobenzenamine	1.8×10^{3}		HSDB (2015)	Q	100
$C_6H_5ClN_2O_2$					
[6283-25-6]					
KWIXNFOTNVKIGM-UHFFFAOYSA-N					
4-chloro-2,6-dinitrobenzenamine	7.6×10^{1}		HSDB (2015)	Q	100
$C_6H_4ClN_3O_4$					
[5388-62-5]					
CLMQUEQFVUMDPC-UHFFFAOYSA-N					
1-chloro-2,4-dinitrobenzene	3.5		Duchowicz et al. (2020)	V	187
$C_6H_3ClN_2O_4$	4.0		HSDB (2015)	V	
[97-00-7]	1.1×10^{1}		Yaws (2003)	X	238, 81
VYZAHLCBVHPDDF-UHFFFAOYSA-N	1.8×10^{2}		Duchowicz et al. (2020)	Q	
	1.6×10^{2}		Zhang et al. (2010)	Q	288, 289
	6.0		Zhang et al. (2010)	Q	288, 290
	5.3		Zhang et al. (2010)	Q	288, 291
	3.9×10^{1}		Zhang et al. (2010)	Q	288, 292
	1.0×10^{1}		Gharagheizi et al. (2010)	Q	247
1-chloro-2,6-dinitrobenzene	1.6×10^{2}		Zhang et al. (2010)	Q	288, 289
$C_6H_3ClN_2O_4$	4.3		Zhang et al. (2010)	Q	288, 290
[606-21-3]	7.2		Zhang et al. (2010)	Q	288, 291
BPPMIQPXQVIZNJ-UHFFFAOYSA-N	3.9×10^{1}		Zhang et al. (2010)	Q	288, 292
2-chloro-1,3,5-trinitrobenzene	3.9×10^{4}		HSDB (2015)	Q	100
$C_6H_2ClN_3O_6$					
[88-88-0]					
HJRJRUMKQCMYDL-UHFFFAOYSA-N					

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4-trichloronitrobenzene	1.1		Zhang et al. (2010)	Q	288, 289
$C_6H_2Cl_3NO_2$	1.3×10^{-1}		Zhang et al. (2010)	Q	288, 290
[17700-09-3]	2.0×10^{-1}		Zhang et al. (2010)	Q	288, 291
BGKIECJVXXHLDP-UHFFFAOYSA-N	4.0×10^{-1}		Zhang et al. (2010)	Q	288, 292
2,3,4,5-tetrachloronitrobenzene	4.3×10^{-1}		HSDB (2015)	Q	100
$C_6HCl_4NO_2$					
[879-39-0]					
MTBYTWZDRVOMBR-UHFFFAOYSA-N					
1,2,4,5-tetrachloronitrobenzene	4.3×10^{-1}		HSDB (2015)	Q	100
$C_6HCl_4NO_2$					
(tecnazene)					
[117-18-0]					
XQTLDIFVVHJORV-UHFFFAOYSA-N					
4-chloro-2-nitrobenzenamine	8.2×10^{1}		HSDB (2015)	Q	100
$C_6H_5ClN_2O_2$	8.0×10^{1}		Zhang et al. (2010)	Q	288, 289
[89-63-4]	1.7×10^{2}		Zhang et al. (2010)	Q	288, 290
PBGKNXWGYQPUJK-UHFFFAOYSA-N	2.2×10^{3}		Zhang et al. (2010)	Q	288, 291
	2.9×10^{2}		Zhang et al. (2010)	Q	288, 292
4-chloro-3-nitrobenzenamine	1.8×10^{3}		HSDB (2015)	Q	100
$C_6H_5ClN_2O_2$	1.8×10^{3}		Zhang et al. (2010)	Q	288, 289
[635-22-3]	1.1×10^{3}		Zhang et al. (2010)	Q	288, 290
FOHHWGVAOVDVLP-UHFFFAOYSA-N	2.4×10^{3}		Zhang et al. (2010)	Q	288, 291
	3.5×10^{3}		Zhang et al. (2010)	Q	288, 292
botran	1.2×10^{2}		HSDB (2015)	V	
$C_6H_4Cl_2N_2O_2$	2.4×10^{3}		Zhang et al. (2010)	Q	288, 289
[99-30-9]	6.9×10^{1}		Zhang et al. (2010)	Q	288, 290
BIXZHMJUSMUDOQ-UHFFFAOYSA-N	1.7×10^{3}		Zhang et al. (2010)	Q	288, 291
	1.4×10^{3}		Zhang et al. (2010)	Q	288, 292
3,5-dichlorophenyl isocyanate	7.7×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_7H_3Cl_2NO$	2.8		Zhang et al. (2010)	Q	288, 290
[34893-92-0]	8.2×10^{-3}		Zhang et al. (2010)	Q	288, 291
XEFUJGURFLOFAN-UHFFFAOYSA-N	7.2×10^{-1}		Zhang et al. (2010)	Q	288, 292
2-chloro-5-nitrobenzoic acid	6.5×10^{3}		Abraham et al. (2019)	Q	
$C_7H_4ClNO_4$					
[2516-96-3]					
QUEKGYQTRJVEQC-UHFFFAOYSA-N					
4-chloro-3-nitrobenzoic acid	3.6×10^{3}		Abraham et al. (2019)	Q	
$C_7H_4ClNO_4$	3.1×10^{4}		Zhang et al. (2010)	Q	288, 289
[96-99-1]	2.1×10^{3}		Zhang et al. (2010)	Q	288, 290
DFXQXFGFOLXAPO-UHFFFAOYSA-N	1.6×10^{3}		Zhang et al. (2010)	Q	288, 291
	9.2×10^{4}		Zhang et al. (2010)	Q	288, 292

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloro-4-isocyanatobenzene	5.7×10^{-2}		Zhang et al. (2010)	Q	288, 289
C_7H_4ClNO	4.1		Zhang et al. (2010)	Q	288, 290
[104-12-1]	9.7×10^{-3}		Zhang et al. (2010)	Q	288, 291
ADAKRBAJFHTIEW-UHFFFAOYSA-N	3.4		Zhang et al. (2010)	Q	288, 292
1,2-dichloro-4-isocyanatobenzene	7.7×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_7H_3Cl_2NO$	4.5		Zhang et al. (2010)	Q	288, 290
[102-36-3]	1.6×10^{-2}		Zhang et al. (2010)	Q	288, 291
MFUVCHZWGSJKEQ-UHFFFAOYSA-N	2.2		Zhang et al. (2010)	Q	288, 292
2-chloro-1-methyl-4-nitrobenzene	2.4×10^{-1}		HSDB (2015)	Q	547
$C_7H_6ClNO_2$	5.7×10^{-1}		Zhang et al. (2010)	Q	288, 289
[121-86-8]	3.4×10^{-1}		Zhang et al. (2010)	Q	288, 290
LLYXJBROWQDVMI-UHFFFAOYSA-N	3.7×10^{-1}		Zhang et al. (2010)	Q	288, 291
	2.5×10^{-1}		Zhang et al. (2010)	Q	288, 292
2,4-dichloro-3-methyl-6-nitrophenol	2.3		Zhang et al. (2010)	Q	288, 289
$C_7H_5Cl_2NO_3$	2.9		Zhang et al. (2010)	Q	288, 290
[39549-27-4]	9.5×10^{1}		Zhang et al. (2010)	Q	288, 291
VMBRJHMTAZXHES-UHFFFAOYSA-N	3.3×10^{-1}		Zhang et al. (2010)	Q	288, 292
4-chloro-5-methyl-2-nitrophenol $C_7H_6ClNO_3$ (4-chloro-6-nitro-*m*-cresol) [7147-89-9] JBMGJOKJUYGIJH-UHFFFAOYSA-N	3.6×10^{-1}		Schwarzenbach et al. (1988)	V	12
3-amino-2,5-dichlorobenzoic acid	2.6×10^{5}		Duchowicz et al. (2020)	V	187
$C_7H_5Cl_2NO_2$	3.6		Mackay et al. (2006d)	V	
[133-90-4]	4.5×10^{5}		Duchowicz et al. (2020)	Q	
HSSBORCLYSCBJR-UHFFFAOYSA-N					
2,3,5,6-tetrachloro-4-nitroanisole $C_7H_3Cl_4NO_3$ (TCNA) [2438-88-2] BGPPUXMKKQMWLV-UHFFFAOYSA-N	5.2×10^{-1}		HSDB (2015)	Q	100
2,6-dichlorobenzamide $C_7H_5Cl_2NO$ [2008-58-4] JHSPCUHPSIUQRB-UHFFFAOYSA-N	8.2×10^{3}		HSDB (2015)	Q	100
swep $C_8H_7Cl_2NO$ [1918-18-9] WOZQBERUBLYCEG-UHFFFAOYSA-N	8.2×10^{2}		HSDB (2015)	Q	100

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-(4-chlorophenyl)acetamide C_8H_8ClNO (*p*-chloroacetanilide) [539-03-7] GGUOCFNAWIODMF-UHFFFAOYSA-N	2.1		HSDB (2015)	Q	100
methyl 5-chloro-2-nitrobenzoate	9.7×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_8H_6ClNO_4$	1.2×10^{2}		Zhang et al. (2010)	Q	288, 290
[51282-49-6]	3.7×10^{3}		Zhang et al. (2010)	Q	288, 291
JGBJHRKCUKTQOE-UHFFFAOYSA-N	6.7×10^{1}		Zhang et al. (2010)	Q	288, 292
4-chloro-2,5-dimethoxynitrobenzene	1.8×10^{2}		Zhang et al. (2010)	Q	288, 289
$C_8H_8ClNO_4$	1.6×10^{1}		Zhang et al. (2010)	Q	288, 290
[6940-53-0]	2.0×10^{2}		Zhang et al. (2010)	Q	288, 291
ORLPGMKKCAEWOW-UHFFFAOYSA-N	3.9×10^{1}		Zhang et al. (2010)	Q	288, 292
chloraniformethan	$>2.3\times10^{10}$		MacBean (2012a)	?	
$C_9H_7Cl_5N_2O$					
[20856-57-9]					
REEFSLKDEDEWAO-UHFFFAOYSA-N					
monuron	1.7×10^{4}		HSDB (2015)	V	
$C_9H_{11}ClN_2O$	1.5×10^{4}		Mackay et al. (2006d)	V	
[150-68-5]	3.3×10^{2}		Suntio et al. (1988)	V	12
BMLIZLVNXIYGCK-UHFFFAOYSA-N	1.7×10^{4}		Burkhard and Guth (1981)	V	
	1.7×10^{4}		Abraham et al. (2019)	Q	
	1.7×10^{4}		MacBean (2012a)	?	
monolinuron	2.1×10^{2}		HSDB (2015)	V	
$C_9H_{11}ClN_2O_2$	1.7×10^{2}		Mackay et al. (2006d)	V	
[1746-81-2]					
LKJPSUCKSLORMF-UHFFFAOYSA-N					
diuron	3.5×10^{1}		Chao et al. (2017)	M	
$C_9H_{10}Cl_2N_2O$	2.0×10^{4}		HSDB (2015)	V	
[330-54-1]			Mackay et al. (2006d)	V	560
XMTQQYYKAHVGBJ-UHFFFAOYSA-N	8.3×10^{2}		Suntio et al. (1988)	V	12
	8.2		Barcelo and Hennion (1997)	X	569
	4.0×10^{4}		Abraham et al. (2019)	Q	
	5.2×10^{1}		Goodarzi et al. (2010)	Q	570
linuron	1.6×10^{3}		Duchowicz et al. (2020)	V	187
$C_9H_{10}Cl_2N_2O_2$			Mackay et al. (2006d)	V	560
[330-55-2]	1.9×10^{2}		Suntio et al. (1988)	V	12
XKJMBINCVNINCA-UHFFFAOYSA-N	5.0×10^{3}		MacBean (2012b)	X	352
	1.8		Barcelo and Hennion (1997)	X	569
	6.5		Duchowicz et al. (2020)	Q	
	2.2×10^{1}		Goodarzi et al. (2010)	Q	570, 573

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
propanil	1.3×10^{1}		Chao et al. (2017)	M	
$C_9H_9Cl_2NO$	5.8×10^{3}		Duchowicz et al. (2020)	V	187
[709-98-8]	5.8×10^{3}		HSDB (2015)	V	
LFULEKSKNZEWOE-UHFFFAOYSA-N	1.8×10^{2}		Mackay et al. (2006d)	V	
	2.8×10^{2}		Suntio et al. (1988)	V	12
	2.7		Barcelo and Hennion (1997)	X	569
	2.8		Duchowicz et al. (2020)	Q	
	2.2×10^{3}		Zhang et al. (2010)	Q	288, 289
	8.0×10^{2}		Zhang et al. (2010)	Q	288, 290
	3.8×10^{3}		Zhang et al. (2010)	Q	288, 291
	8.4×10^{3}		Zhang et al. (2010)	Q	288, 292
	1.2×10^{-1}		Goodarzi et al. (2010)	Q	570, 573
methazole	4.3×10^{1}		HSDB (2015)	V	
$C_9H_6Cl_2N_2O_3$	4.8×10^{4}		Hilal et al. (2008)	Q	
[20354-26-1]	4.3×10^{1}		MacBean (2012a)	?	
LRUUNMYPIBZBQH-UHFFFAOYSA-N					
1,4-naphthalenedione, 2-amino-3-chloro- $C_{10}H_6ClNO_2$ (quinoclamine) [2797-51-5] OBLNWSCLAYSJJR-UHFFFAOYSA-N	3.3×10^{4}		Maniere et al. (2011)	?	242, 166
chlortoluron	7.0×10^{4}		HSDB (2015)	V	
$C_{10}H_{13}ClN_2O$	1.9×10^{4}		Mackay et al. (2006d)	V	
(chlorotoluron)	1.9×10^{2}		Barcelo and Hennion (1997)	X	569
[15545-48-9]	3.4×10^{1}		Goodarzi et al. (2010)	Q	570, 573
JXCGFZXSOMJFOA-UHFFFAOYSA-N					
metoxuron	6.9×10^{2}		Duchowicz et al. (2020)	V	187
$C_{10}H_{13}ClN_2O_2$	6.9×10^{2}		Mackay et al. (2006d)	V	
[19937-59-8]	6.6		Barcelo and Hennion (1997)	X	569
DSRNRYQBBJQVCW-UHFFFAOYSA-N	2.0×10^{2}		Duchowicz et al. (2020)	Q	
	1.2×10^{1}		Goodarzi et al. (2010)	Q	570
chlorpropham	2.3×10^{1}		Watanabe (1993)	M	
$C_{10}H_{12}ClNO_2$	1.7×10^{1}		Duchowicz et al. (2020)	V	187
[101-21-3]	1.7×10^{1}		HSDB (2015)	V	
CWJSHJJYOPWUGX-UHFFFAOYSA-N			Mackay et al. (2006d)	V	560
	4.8×10^{2}		Suntio et al. (1988)	V	12
	4.7×10^{1}		Barcelo and Hennion (1997)	X	569
	5.4×10^{-2}		Duchowicz et al. (2020)	Q	
	2.9		Goodarzi et al. (2010)	Q	570, 573

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pyrazon $C_{10}H_8ClN_3O$ [1698-60-8] WYKYKTKDBLFHCY-UHFFFAOYSA-N	3.0×10^{4} 3.0×10^{4} 2.3×10^{-1} 2.3×10^{-1} 8.3×10^{4} 1.9×10^{9}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Duchowicz et al. (2020) Maniere et al. (2011)	V V V V Q ?	187 12 12, 166
2,4-D dimethylamine $C_{10}H_{13}Cl_2NO_3$ ((2,4-dichlorophenoxy)acetic acid dimethylamine) [2008-39-1] IUQJDHJVPLLKFL-UHFFFAOYSA-N	2.1×10^{10} 4.9×10^{1} 7.0×10^{10}		Duchowicz et al. (2020) Duchowicz et al. (2020) HSDB (2015)	V Q Q	187 100
3',4'-dichlorocyclopropanecarboxanilide $C_{10}H_9Cl_2NO$ (cypromid) [2759-71-9] PLQDLOBGKJCDSZ-UHFFFAOYSA-N	3.8×10^{3}		HSDB (2015)	Q	100
triazoxide $C_{10}H_6N_5OCl$ [72459-58-6] IQGKIPDJXCAMSM-UHFFFAOYSA-N	4.6×10^{5} 7.9×10^{5}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
chlorbufam $C_{11}H_{10}ClNO_2$ [1967-16-4] ULBXWWGWDPVHAO-UHFFFAOYSA-N	1.1×10^{3} 1.1×10^{3}		HSDB (2015) MacBean (2012a)	V ?	
zarilamid $C_{11}H_{11}N_2O_2Cl$ [84527-51-5] VLBZAQJMGULJIU-UHFFFAOYSA-N	1.5×10^{5}		MacBean (2012a)	?	
chloramphenicol $C_{11}H_{12}Cl_2N_2O_5$ [56-75-7] WIIZWVCIJKGZOK-IUCAKERBSA-N	4.3×10^{12}		HSDB (2015)	Q	100
cloethocarb $C_{11}H_{14}ClNO_4$ [51487-69-5] PITWUHDDNUVBPT-UHFFFAOYSA-N	5.0×10^{5}		MacBean (2012a)	?	
formetanate hydrochloride $C_{11}H_{16}ClN_3O_2$ [23422-53-9] MYPKGPZHHQEODQ-UHFFFAOYSA-N	4.3×10^{13} 2.0×10^{9}		HSDB (2015) Maniere et al. (2011)	Q ?	100 242, 166

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyclanilide	1.4×10^{4}		MacBean (2012b)	X	352
$C_{11}H_9Cl_2NO_3$	1.2×10^{4}		Keshavarz et al. (2022)	Q	
[113136-77-9]	1.2×10^{5}		Duchowicz et al. (2020)	Q	
GLWWLNJJJCTFMZ-UHFFFAOYSA-N	1.4×10^{4}		Duchowicz et al. (2020)	?	186, 21
propachlor	2.7×10^{1}		HSDB (2015)	V	
$C_{11}H_{14}ClNO$	9.1×10^{1}		Mackay et al. (2006d)	V	
[1918-16-7]	9.1×10^{1}		Suntio et al. (1988)	V	12
MFOUDYKPLGXPGO-UHFFFAOYSA-N	9.0×10^{-1}		Barcelo and Hennion (1997)	X	569
	3.7×10^{-1}		Goodarzi et al. (2010)	Q	570
barban	8.4×10^{2}		Duchowicz et al. (2020)	V	187
$C_{11}H_9Cl_2NO_2$	8.2×10^{2}		HSDB (2015)	V	
[101-27-9]	8.5×10^{2}		Mackay et al. (2006d)	V	
MCOQHIWZJUDQIC-UHFFFAOYSA-N	3.3×10^{-1}		Duchowicz et al. (2020)	Q	
	8.5×10^{2}		MacBean (2012a)	?	
aclonifen	5.9×10^{2}		Duchowicz et al. (2020)	V	187
$C_{12}H_9ClN_2O_3$	7.1×10^{3}		Duchowicz et al. (2020)	Q	
[74070-46-5]	3.3×10^{2}		Maniere et al. (2011)	?	12, 166
DDBMQDADIHOWIC-UHFFFAOYSA-N					
propyzamide	1.0×10^{3}		Duchowicz et al. (2020)	V	187
$C_{12}H_{11}Cl_2NO$	5.2		HSDB (2015)	V	
(pronamide)	5.2×10^{-2}		Barcelo and Hennion (1997)	X	569
[23950-58-5]	1.5×10^{2}		Duchowicz et al. (2020)	Q	
PHNUZKMIPFFYSO-UHFFFAOYSA-N	6.6×10^{-2}		Goodarzi et al. (2010)	Q	570
	1.3×10^{8}		Maniere et al. (2011)	?	12, 166
			Mackay et al. (2006d)	W	738
2,4,6-trichlorophenyl 4-nitrophenyl ether $C_{12}H_6Cl_3NO_3$ (chlornitrofen) [1836-77-7] XQNAUQUKWRBODG-UHFFFAOYSA-N	>8.1		Kawamoto and Urano (1989)	M	
nitrofen	3.3		HSDB (2015)	V	
$C_{12}H_7Cl_2NO_3$	3.9×10^{1}		Zhang et al. (2010)	Q	288, 289
[1836-75-5]	2.8×10^{1}		Zhang et al. (2010)	Q	288, 290
XITQUSLLOSKDTB-UHFFFAOYSA-N	1.2×10^{2}		Zhang et al. (2010)	Q	288, 291
	1.1×10^{2}		Zhang et al. (2010)	Q	288, 292
buturon $C_{12}H_{13}ClN_2O$ [3766-60-7] BYYMILHAKOURNM-UHFFFAOYSA-N	1.3×10^{4}		MacBean (2012a)	?	

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
triclocarban	2.2×10^5		HSDB (2015)	Q	100
$C_{13}H_9Cl_3N_2O$	2.2×10^5		Zhang et al. (2010)	Q	288, 289
[101-20-2]	5.0×10^3		Zhang et al. (2010)	Q	288, 290
ICUTUKXCWQYESQ-UHFFFAOYSA-N	7.2×10^7		Zhang et al. (2010)	Q	288, 291
	1.8×10^7		Zhang et al. (2010)	Q	288, 292
dimethachlor	5.9×10^3		Maniere et al. (2011)	?	166
$C_{13}H_{18}ClNO_2$					
[50563-36-5]					
SCCDDNKJYDZXMM-UHFFFAOYSA-N					
3,5-dichloro-N-(3,4-dichlorophenyl)-2-hydroxybenzamide	2.1×10^5		HSDB (2015)	Q	100
$C_{13}H_7Cl_4NO_2$	2.1×10^5		Zhang et al. (2010)	Q	288, 289
[1154-59-2]	2.3×10^5		Zhang et al. (2010)	Q	288, 290
SJQBHPJLLIJASD-UHFFFAOYSA-N	3.9×10^6		Zhang et al. (2010)	Q	288, 291
	1.6×10^5		Zhang et al. (2010)	Q	288, 292
procymidone	8.5×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{13}H_{11}Cl_2NO_2$	8.5×10^{-1}		Mackay et al. (2006d)	V	
[32809-16-8]	9.0×10^{-3}		Barcelo and Hennion (1997)	X	569
QXJKBPAVAHBARF-UHFFFAOYSA-N	9.7×10^{-1}		Duchowicz et al. (2020)	Q	
	1.4×10^{-2}		Goodarzi et al. (2010)	Q	570
melphalan	2.3×10^7		HSDB (2015)	Q	100
$C_{13}H_{18}Cl_2N_2O_2$					
[148-82-3]					
SGDBTWWWUNNDEQ-LBPRGKRZSA-N					
niclosamide	1.5×10^4		HSDB (2015)	V	
$C_{13}H_8Cl_2N_2O_4$					
[50-65-7]					
RJMUSRYZPJIFPJ-UHFFFAOYSA-N					
iprodione	7.1×10^2		Barcelo and Hennion (1997)	X	569
$C_{13}H_{13}Cl_2N_3O_3$	4.0×10^4		Keshavarz et al. (2022)	Q	
[36734-19-7]	9.5×10^3		Duchowicz et al. (2020)	Q	
ONUFESLQCSAYKA-UHFFFAOYSA-N	2.0×10^1		Goodarzi et al. (2010)	Q	570, 571
	3.2×10^3		Duchowicz et al. (2020)	?	186, 21
zoxamide	4.9×10^3		HSDB (2015)	Q	100
$C_{14}H_{16}Cl_3NO_2$	$>1.5\times10^2$		Maniere et al. (2011)	?	242, 166
[156052-68-5]					
SOUGWDPPRBKJEX-UHFFFAOYSA-N					

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
fenhexamid	2.0×10^5		MacBean (2012b)	X	352
$C_{14}H_{17}Cl_2NO_2$	2.0×10^5		Maniere et al. (2011)	?	12, 495, 166
[126833-17-8]	3.3×10^6		Maniere et al. (2011)	?	12, 575, 166
VDLGAVXLJYLFDH-UHFFFAOYSA-N	1.1×10^5		Maniere et al. (2011)	?	12, 572, 166
chlorambucil	3.7×10^4		HSDB (2015)	Q	100
$C_{14}H_{19}Cl_2NO_2$					
[305-03-3]					
JCKYGMPEJWAADB-UHFFFAOYSA-N					
2-chloro-N-(ethoxymethyl)-N-(2-ethyl-6-methylphenyl)acetamide	3.7×10^4		HSDB (2015)	V	
$C_{14}H_{20}ClNO_2$					
(acetochlor)					
[34256-82-1]					
VTNQPKFIQCLBDU-UHFFFAOYSA-N					
alachlor	6.7×10^2		Muir et al. (2004)	L	369
$C_{14}H_{20}ClNO_2$	9.9×10^2		Muir et al. (2004)	L	368
[15972-60-8]	7.4		Chao et al. (2017)	M	
XCSGPAVHZFQHGE-UHFFFAOYSA-N	1.4×10^2	9200	Gautier et al. (2003)	M	
	9.0×10^2		Fendinger et al. (1989)	M	73
	1.2×10^3		Fendinger and Glotfelty (1988)	M	73
	4.5×10^2		Mackay et al. (2006d)	V	
	1.6×10^2		Suntio et al. (1988)	V	12
	3.1×10^2		Glotfelty et al. (1987)	V	
	1.6		Barcelo and Hennion (1997)	X	569
	3.6×10^{-2}		Goodarzi et al. (2010)	Q	570, 571
	3.1×10^3		Hilal et al. (2008)	Q	
	4.5×10^1		Modarresi et al. (2007)	Q	68
		11000	Kühne et al. (2005)	Q	
	8.2×10^4		Meylan and Howard (1991)	Q	
		9300	Kühne et al. (2005)	?	
	3.1×10^2		Chesters et al. (1989)	?	
bifenox	9.1×10^1		Duchowicz et al. (2020)	V	187
$C_{14}H_9Cl_2NO_3$	3.7		HSDB (2015)	V	
[42576-02-3]	3.2		Mackay et al. (2006d)	V	
SUSRORUBZHMPCO-UHFFFAOYSA-N	3.3×10^{-2}		Barcelo and Hennion (1997)	X	569
	6.2×10^3		Duchowicz et al. (2020)	Q	
	3.5×10^{-2}		Goodarzi et al. (2010)	Q	570, 573
	$<6.2\times10^3$		Maniere et al. (2011)	?	12, 166

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
S-metolachlor $C_{15}H_{22}ClNO_2$ [87392-12-9] WVQBLGZPHOPPFO-LBPRGKRZSA-N	4.5×10^{2}		Maniere et al. (2011)	?	166
metolachlor $C_{15}H_{22}ClNO_2$ [51218-45-2] WVQBLGZPHOPPFO-UHFFFAOYSA-N	7.5×10^{2}		Muir et al. (2004)	L	369
	7.2×10^{2}		Muir et al. (2004)	L	368
	6.2×10^{2}	15000	Fogg and Sangster (2003)	L	
	2.1×10^{2}	10000	Feigenbrugel et al. (2004a)	M	
	1.3×10^{2}		Rice et al. (1997b)	M	12
	5.7×10^{2}	15000	Lau et al. (1995)	M	739
	4.3×10^{2}		Mackay et al. (2006d)	V	
	4.1×10^{2}		Otto et al. (1997)	V	
	1.1×10^{3}		Glotfelty et al. (1987)	V	
	1.1×10^{3}		Burkhard and Guth (1981)	V	
	1.1×10^{1}		Barcelo and Hennion (1997)	X	569
	1.2×10^{3}		Rice et al. (1997b)	C	
	7.9×10^{-2}		Goodarzi et al. (2010)	Q	570
	6.2×10^{3}		Hilal et al. (2008)	Q	
	1.7×10^{2}		Modarresi et al. (2007)	Q	68
		12000	Kühne et al. (2005)	Q	
		10000	Kühne et al. (2005)	?	
	1.1×10^{3}		Chesters et al. (1989)	?	12
clonitralid $C_{15}H_{15}Cl_2N_3O_5$ [1420-04-8] XYCDHXSQODHSLG-UHFFFAOYSA-N	$>2.6\times10^{4}$		HSDB (2015)	V	
chloroxuron $C_{15}H_{15}ClN_2O_2$ [1982-47-4] IVUXTESCPZUGJC-UHFFFAOYSA-N	2.4×10^{4}		HSDB (2015)	V	
	5.3×10^{4}		MacBean (2012a)	?	
CGA 80000 $C_{15}H_{18}ClNO_4$ [67932-85-8] FHZMAAGOSXDIBJ-UHFFFAOYSA-N	4.4×10^{6}		MacBean (2012a)	?	
oxadiargyl $C_{15}H_{14}N_2O_3Cl_2$ [39807-15-3] DVOODWOZJVJKQR-UHFFFAOYSA-N	4.3×10^{2}		Duchowicz et al. (2020)	V	187
	8.2×10^{1}		Duchowicz et al. (2020)	Q	
diniconazole $C_{15}H_{17}Cl_2N_3O$ [83657-24-3] FBOUIAKEJMZPQG-UHFFFAOYSA-N	2.5×10^{1}		Duchowicz et al. (2020)	V	187
	2.8×10^{2}		Duchowicz et al. (2020)	Q	

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pethoxamid $C_{16}H_{22}ClNO_2$ [106700-29-2] CSWIKHNSBZVWNQ-UHFFFAOYSA-N	8.5×10^{2}		Maniere et al. (2011)	?	12, 166
pigment red 4 $C_{16}H_{10}ClN_3O_3$ [2814-77-9] XLTMWFMRJZDFFD-VHEBQXMUSA-N	1.1×10^{7}		HSDB (2015)	Q	100
darendoside b $C_{17}H_{15}Cl_2N_5O_2$ [13301-61-6] KHZRTXVUEZJYNE-UHFFFAOYSA-N	2.7×10^{7} 5.0×10^{6} 2.5×10^{7} 7.3×10^{4}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
butenachlor $C_{17}H_{24}NO_2Cl$ [87310-56-3] HZDIJTXDRLNTIS-DAXSKMNVSA-N	1.0×10^{2}		MacBean (2012a)	?	
butachlor $C_{17}H_{26}ClNO_2$ [23184-66-9] HKPHPIREJKHECO-UHFFFAOYSA-N	1.6×10^{2} 1.2×10^{2} 6.9×10^{2} 1.7×10^{2}		Watanabe (1993) Mackay et al. (2006d) Hilal et al. (2008) Modarresi et al. (2007)	M V Q Q	 68
pretilachlor $C_{17}H_{26}ClNO_2$ [51218-49-6] YLPGTOIOYRQOHV-UHFFFAOYSA-N	4.5×10^{3} 1.8×10^{2}		Hilal et al. (2008) Modarresi et al. (2007)	Q Q	 68
halofenozide $C_{18}H_{19}ClN_2O_2$ [112226-61-6] CNKHSLKYRMDDNQ-UHFFFAOYSA-N	2.7×10^{5}		HSDB (2015)	Q	100
benzoximate $C_{18}H_{18}ClNO_5$ [29104-30-1] BZMIHNKNQJJVRO-UHFFFAOYSA-N	1.8×10^{2} 1.5×10^{5}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
pencycuron $C_{19}H_{21}ClN_2O$ [66063-05-6] OGYFATSSENRIKG-UHFFFAOYSA-N	2.0×10^{6}		Maniere et al. (2011)	?	12, 166
valifenalate $C_{19}H_{27}ClN_2O_5$ [283159-90-0] DBXFMOWZRXXBRN-LWKPJOBUSA-N	6.2×10^{5}		Maniere et al. (2011)	?	12, 740, 166

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pyrazoxyfen $C_{20}H_{16}Cl_2N_2O_3$ [71561-11-0] FKERUJTUOYLBKB-UHFFFAOYSA-N	4.7×10^4 1.9×10^4		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
α-cypermethrin $C_{22}H_{19}Cl_2NO_3$ [67375-30-8] KAATUXNTWXVJKI-DXCJPMOASA-N	1.0 1.0×10^2 1.9×10^1		HSDB (2015) Mackay et al. (2006d) Maniere et al. (2011)	V V ?	 12, 166
cypermethrin-β $C_{22}H_{19}Cl_2NO_3$ [1224510-29-5] KAATUXNTWXVJKI-FLXSOZOKSA-N	5.6×10^1		Ebert et al. (2023)	?	319
β-cypermethrin $C_{22}H_{19}Cl_2NO_3$ [65731-84-2] KAATUXNTWXVJKI-NSHGMRRFSA-N			Mackay et al. (2006d)	V	560
δ-cypermethrin $C_{22}H_{19}Cl_2NO_3$ (cypermethrin; alphamethrin) [52315-07-8] KAATUXNTWXVJKI-UHFFFAOYSA-N	4.1×10^1 4.3×10^2 1.2×10^1 2.5×10^1 1.0×10^1 4.2×10^1 5.0×10^7		HSDB (2015) Mackay et al. (2006d) Siebers and Mattusch (1996) Barcelo and Hennion (1997) Goodarzi et al. (2010) Maniere et al. (2011) Maniere et al. (2011)	V V V X Q ? ?	 12 569 570, 571 12, 166 242, 166
θ-cypermethrin $C_{22}H_{19}Cl_2NO_3$ [71697-59-1] KAATUXNTWXVJKI-GGPKGHCWSA-N	6.1×10^2		Ebert et al. (2023)	?	319
ζ-cypermethrin $C_{22}H_{19}Cl_2NO_3$ [1315501-18-8] KAATUXNTWXVJKI-QPIRBTGLSA-N	4.3×10^2		Ebert et al. (2023)	?	367
ochratoxin C $C_{22}H_{22}ClNO_6$ [4865-85-4] BPZZWRPHVVDAPT-PXAZEXFGSA-N	7.6×10^8		HSDB (2015)	Q	100
quizalofop-p-tefuryl $C_{22}H_{21}N_2O_5Cl$ [119738-06-6] BBKDWPHJZANJGB-UHFFFAOYSA-N	1.8×10^4 3.4×10^6		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
mandipropamid	1.1×10^{4}		HSDB (2015)	V	
$C_{23}H_{22}ClNO_4$	$>1.1\times10^{4}$		Maniere et al. (2011)	?	166
[374726-62-2]					
KWLVWJPJKJMCSH-UHFFFAOYSA-N					
fenvalerate	2.9×10^{2}		Duchowicz et al. (2020)	V	187
$C_{25}H_{22}ClNO_3$	2.9×10^{2}		HSDB (2015)	V	
[51630-58-1]	4.7×10^{1}		Mackay et al. (2006d)	V	
NYPJDWWKZLNGGM-UHFFFAOYSA-N	7.0×10^{1}		Cotham and Bidleman (1989)	V	
	3.2×10^{3}		Duchowicz et al. (2020)	Q	
esfenvalerate	2.4×10^{1}		Duchowicz et al. (2020)	V	187
$C_{25}H_{22}ClNO_3$	2.4×10^{1}		HSDB (2015)	V	
[66230-04-4]	3.2×10^{3}		Duchowicz et al. (2020)	Q	
NYPJDWWKZLNGGM-ZEQRLZLVSA-N	2.0×10^{3}		Maniere et al. (2011)	?	242, 166
clopyralid	3.3×10^{3}		Duchowicz et al. (2020)	V	187
$C_6H_3Cl_2NO_2$	3.2×10^{2}		Barcelo and Hennion (1997)	X	569
[1702-17-6]	1.8×10^{3}		Duchowicz et al. (2020)	Q	
HUBANNPOLNYSAD-UHFFFAOYSA-N	3.6×10^{1}		Goodarzi et al. (2010)	Q	570
	3.0×10^{9}		Maniere et al. (2011)	?	12, 166
	4.5×10^{10}		Maniere et al. (2011)	?	12, 572, 166
	6.2×10^{10}		Maniere et al. (2011)	?	12, 575, 166
	5.6×10^{10}		Maniere et al. (2011)	?	12, 495, 166
picloram	3.0×10^{4}		Mackay et al. (2006d)	V	
$C_6H_3Cl_3N_2O_2$	2.9×10^{4}		Suntio et al. (1988)	V	12
[1918-02-1]	2.9×10^{2}		Barcelo and Hennion (1997)	X	569
NQQVFXUMIDALNH-UHFFFAOYSA-N	7.7×10^{6}		Zhang et al. (2010)	Q	288, 289
	2.5		Zhang et al. (2010)	Q	288, 290
	9.0×10^{4}		Zhang et al. (2010)	Q	288, 291
	1.6×10^{8}		Zhang et al. (2010)	Q	288, 292
	1.1×10^{3}		Goodarzi et al. (2010)	Q	570, 573
	2.1×10^{4}		Maniere et al. (2011)	?	242, 166
aminopyralid	5.8×10^{6}		HSDB (2015)	Q	100
$C_6H_4Cl_2N_2O_2$	1.0×10^{11}		Maniere et al. (2011)	?	242, 495, 166
[150114-71-9]					
NIXXQNOQHKNPEJ-UHFFFAOYSA-N					

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4,5,6-tetrachloropyridine-2-carboxylic acid	3.7×10^{3}		Zhang et al. (2010)	Q	288, 289
$C_6HCl_4NO_2$	2.4		Zhang et al. (2010)	Q	288, 290
[10469-09-7]	1.2×10^{2}		Zhang et al. (2010)	Q	288, 291
GXFRQLQUKBSYQL-UHFFFAOYSA-N	4.1×10^{4}		Zhang et al. (2010)	Q	288, 292
[(3,5,6-trichloro-2-pyridinyl)oxy]-acetic acid	1.0×10^{4}		Duchowicz et al. (2020)	V	187
$C_7H_4Cl_3NO_3$	1.0×10^{4}		HSDB (2015)	V	
(triclopyr)	1.2×10^{4}		Armbrust (2000)	C	
[55335-06-3]	3.2×10^{3}		Duchowicz et al. (2020)	Q	
REEQLXCGVXDJSQ-UHFFFAOYSA-N	1.1×10^{4}		Maniere et al. (2011)	?	12, 166
	2.1×10^{5}		Maniere et al. (2011)	?	12, 572, 166
	2.3×10^{5}		Maniere et al. (2011)	?	12, 495, 166
clopidol	9.9×10^{3}		HSDB (2015)	Q	100
$C_7H_7Cl_2NO$					
[2971-90-6]					
ZDPIZLCVJAAHHR-UHFFFAOYSA-N					
[(3,5,6-trichloro-2-pyridinyl)oxy]-acetic acid, methyl ester	6.0		Zhang et al. (2010)	Q	288, 289
$C_8H_6Cl_3NO_3$	3.1×10^{1}		Zhang et al. (2010)	Q	288, 290
[60825-26-5]	4.6×10^{3}		Zhang et al. (2010)	Q	288, 291
MNYBZEHWPRTNJY-UHFFFAOYSA-N	3.5×10^{2}		Zhang et al. (2010)	Q	288, 292
aminocyclopyrachlor	1.3×10^{7}		Ebert et al. (2023)	?	319
$C_8H_8ClN_3O_2$					
[858956-08-8]					
KWAIHLIXESXTJL-UHFFFAOYSA-N					
uracil mustard	2.5×10^{7}		HSDB (2015)	Q	100
$C_8H_{11}Cl_2N_3O_2$					
[66-75-1]					
IDPUKCWIGUEADI-UHFFFAOYSA-N					
imidacloprid	4.9×10^{9}		Armbrust (2000)	C	
$C_9H_{10}ClN_5O_2$	5.9×10^{9}		Maniere et al. (2011)	?	12, 166
[138261-41-3]					
YWTYJOPNNQFBPC-UHFFFAOYSA-N					

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethyl [(3,5,6-trichloro-2-pyridinyl)oxy]acetate	4.5		Zhang et al. (2010)	Q	288, 289
$C_9H_8Cl_3NO_3$	1.7×10^{1}		Zhang et al. (2010)	Q	288, 290
[60825-27-6]	2.3×10^{1}		Zhang et al. (2010)	Q	288, 291
KXAVVWXJUDQGDA-UHFFFAOYSA-N	3.1×10^{2}		Zhang et al. (2010)	Q	288, 292
N-methyl-3,4,5,6-tetrachlorophthalimide	1.5×10^{3}		Zhang et al. (2010)	Q	288, 289
$C_9H_3Cl_4NO_2$	1.2×10^{3}		Zhang et al. (2010)	Q	288, 290
[14737-80-5]	4.1×10^{1}		Zhang et al. (2010)	Q	288, 291
OHCSZUQRNNNMRG-UHFFFAOYSA-N	3.1×10^{3}		Zhang et al. (2010)	Q	288, 292
terbacil	5.2×10^{4}		HSDB (2015)	V	
$C_9H_{13}ClN_2O_2$	6.5×10^{4}		Mackay et al. (2006d)	V	
[5902-51-2]	7.9×10^{4}		Mackay et al. (2006d)	V	
NBQCNZYJJMBDKY-UHFFFAOYSA-N	5.6×10^{4}		Suntio et al. (1988)	V	12
	5.5×10^{2}		Barcelo and Hennion (1997)	X	569
	4.4×10^{2}		Goodarzi et al. (2010)	Q	570
eglinazine-ethyl $C_9H_{14}ClN_5O_2$ [6616-80-4] YESXTECNXIKUMM-UHFFFAOYSA-N	4.1×10^{4}		Ebert et al. (2023)	?	319
proglinazine ethyl ester $C_{10}H_{16}ClN_5O_2$ [68228-18-2] QQADVTSTCZBBOE-UHFFFAOYSA-N	1.0×10^{4}		Ebert et al. (2023)	?	319
triforine	2.6×10^{3}		HSDB (2015)	V	
$C_{10}H_{14}Cl_6N_4O_2$	2.6×10^{3}		Mackay et al. (2006d)	V	
[26644-46-2]					
RROQIUMZODEXOR-UHFFFAOYSA-N					
drazoxolon $C_{10}H_8ClN_3O_2$ [5707-69-7] OOTHTARUZHONSW-UHFFFAOYSA-N	1.4×10^{2}		Ebert et al. (2023)	?	319
anagrelide $C_{10}H_7Cl_2N_3O$ [68475-42-3] OTBXOEAOVRKTNQ-UHFFFAOYSA-N	3.7×10^{7}		HSDB (2015)	Q	100
fenpiclonil	1.8×10^{3}		Duchowicz et al. (2020)	V	187
$C_{11}H_6Cl_2N_2$	5.4×10^{2}		Duchowicz et al. (2020)	Q	
[74738-17-3]	1.9×10^{3}		MacBean (2012a)	?	
FKLFBQCQQYDUAM-UHFFFAOYSA-N					

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benoxacor	1.3×10^2		Duchowicz et al. (2020)	V	187
$C_{11}H_{11}Cl_2NO_2$	2.9×10^2		Duchowicz et al. (2020)	Q	
[98730-04-2]	1.3×10^2		Maniere et al. (2011)	?	12, 166
PFJJMJDEVDLPNE-UHFFFAOYSA-N					
ethychlozate	1.6×10^4		Ebert et al. (2023)	?	319
$C_{11}H_{11}ClN_2O_2$					
[27512-72-7]					
GLPZEHFBLBYFHN-UHFFFAOYSA-N					
quinmerac	1.0×10^{10}		Maniere et al. (2011)	?	242, 166
$C_{11}H_8ClNO_2$					
[90717-03-6]					
ALZOLUNSQWINIR-UHFFFAOYSA-N					
quinonamid	8.0×10^2		Ebert et al. (2023)	?	367
$C_{12}H_6Cl_3NO_3$					
[27541-88-4]					
ZIEWAMOXCOLNSJ-UHFFFAOYSA-N					
fenchlorazole-ethyl	2.7×10^3		MacBean (2012a)	?	12
$C_{12}H_8N_3O_2Cl_5$					
[103112-35-2]					
GMBRUAIJEFRHFQ-UHFFFAOYSA-N					
vinclozoline	5.8×10^2		HSDB (2015)	V	
$C_{12}H_9Cl_2NO_3$	2.6×10^5		Mackay et al. (2006d)	V	
(vinclozolin)	9.1×10^1		Siebers et al. (1994)	V	
[50471-44-8]	7.6		Barcelo and Hennion (1997)	X	569
FSCWZHGZWWDELK-UHFFFAOYSA-N	1.7		Goodarzi et al. (2010)	Q	570
forchlorfenuron	3.4×10^6		Duchowicz et al. (2020)	V	187
$C_{12}H_{10}ClN_3O$	3.5×10^6		MacBean (2012b)	X	352
[68157-60-8]	1.7×10^1		Duchowicz et al. (2020)	Q	
GPXLRLUVLMHHIK-UHFFFAOYSA-N	3.4×10^6		Maniere et al. (2011)	?	242, 166
azaconazole	5.1×10^4		Ebert et al. (2023)	?	319
$C_{12}H_{11}Cl_2N_3O_2$					
[60207-31-0]					
AKNQMEBLVAMSNZ-UHFFFAOYSA-N					
myclozolin	3.7×10^2		MacBean (2012a)	?	
$C_{12}H_{11}NO_4Cl_2$					
[54864-61-8]					
FTCOKXNKPOUEFH-UHFFFAOYSA-N					
triclopyr-butotyl	3.4×10^2		Maniere et al. (2011)	?	12, 166
$C_{13}H_{16}Cl_3NO_4$					
[64700-56-7]					
IVDRCZNHVGQBHZ-UHFFFAOYSA-N					

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
clofencet $C_{13}H_{11}ClN_2O_3$ [129025-54-3] PIZCXVUFSNPNON-UHFFFAOYSA-N	$>1.9\times10^{8}$ $>2.3\times10^{10}$		HSDB (2015) MacBean (2012a)	V ?	
chlozolinate $C_{13}H_{11}NO_5Cl_2$ [84332-86-5] IGUYEXXAGBDLLX-UHFFFAOYSA-N	7.6×10^{3} 4.7×10^{2} 2.8×10^{1} 2.8×10^{1} 4.4×10^{2}		Duchowicz et al. (2020) Duchowicz et al. (2020) Duchowicz et al. (2020) Duchowicz et al. (2020) MacBean (2012a)	V V Q Q ?	187 187
monalide $C_{13}H_{18}ClNO$ [7287-36-7] KXGYBSNVFXBPNO-UHFFFAOYSA-N	4.0×10^{2}		MacBean (2012a)	?	
chlomethoxyfen $C_{13}H_9Cl_2NO_4$ [32861-85-1] DXXVCXKMSWHGTF-UHFFFAOYSA-N	5.1×10^{-1}		Ebert et al. (2023)	?	319
metazachlor $C_{14}H_{16}ClN_3O$ [67129-08-2] STEPQTYSZVCJPV-UHFFFAOYSA-N	1.3×10^{1} 3.5×10^{2} 7.1×10^{3} 1.7×10^{4}		Barcelo and Hennion (1997) Goodarzi et al. (2010) Modarresi et al. (2007) Maniere et al. (2011)	X Q Q ?	569 570 68 12, 166
etaconazole $C_{14}H_{15}Cl_2N_3O_2$ [60207-93-4] DWRKFAJEBUWTQM-UHFFFAOYSA-N	7.9×10^{3}		MacBean (2012a)	?	
triadimenol $C_{14}H_{18}ClN_3O_2$ [55219-65-3] BAZVSMNPJJMILC-UHFFFAOYSA-N	7.6×10^{6} 3.8×10^{6} 4.5×10^{5}		HSDB (2015) Mackay et al. (2006d) Maniere et al. (2011)	V V ?	 242, 166
hexaconazole $C_{14}H_{17}Cl_2N_3O$ [79983-71-4] STMIIPIFODONDC-UHFFFAOYSA-N	2.8×10^{1} 6.0×10^{1}		Barcelo and Hennion (1997) Goodarzi et al. (2010)	X Q	569 570
triadimefon $C_{14}H_{16}ClN_3O_2$ [43121-43-3] WURBVZBTWMNKQT-UHFFFAOYSA-N	1.2×10^{5} 1.2×10^{5} 1.2×10^{5} 1.5×10^{2}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Duchowicz et al. (2020)	V V V Q	187
imazalil $C_{14}H_{14}Cl_2N_2O$ [35554-44-0] PZBPKYOVPCNPJY-UHFFFAOYSA-N	3.8×10^{3} 5.1×10^{5} 9.3×10^{3}		HSDB (2015) Mackay et al. (2006d) Maniere et al. (2011)	V V ?	 242, 166

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pyrifenox $C_{14}H_{12}Cl_2N_2O$ [88283-41-4] CKPCAYZTYMHQEX-UHFFFAOYSA-N	2.3×10^{2}		Ebert et al. (2023)	?	319
chlorphthalim $C_{14}H_{12}ClNO_2$ [39985-63-2] MJQBFSWPMMHVSM-UHFFFAOYSA-N	5.1×10^{2}		Ebert et al. (2023)	?	319
cyprofuram $C_{14}H_{14}ClNO_3$ [69581-33-5] KRZUZYJEQBXUIN-UHFFFAOYSA-N	3.1×10^{5}		Ebert et al. (2023)	?	317
ofurace $C_{14}H_{16}ClNO_3$ [58810-48-3] OWDLFBLNMPCXSD-UHFFFAOYSA-N	1.1×10^{4}		Ebert et al. (2023)	?	319
triadimenol B $C_{14}H_{18}ClN_3O_2$ [82200-72-4]	1.1×10^{5}		Ebert et al. (2023)	?	367
triadimenol A $C_{14}H_{18}ClN_3O_2$ [89482-17-7]	1.3×10^{5}		Ebert et al. (2023)	?	319
propiconazole $C_{15}H_{17}Cl_2N_3O_2$ [60207-90-1] STJLVHWMYQXCPB-UHFFFAOYSA-N	1.1×10^{4} 5.7×10^{3} 2.5×10^{3} 2.4×10^{1} 3.1×10^{1}		HSDB (2015) Mackay et al. (2006d) Siebers et al. (1994) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V V X Q	 569 570, 573
clonazepam $C_{15}H_{10}ClN_3O_3$ [1622-61-3] DGBIGWXXNGSACT-UHFFFAOYSA-N	1.4×10^{7}		HSDB (2015)	Q	100
oxazepam $C_{15}H_{12}ClN_2O_2$ [604-75-1] ADIMAYPTOBDMTL-UHFFFAOYSA-N	1.8×10^{4}		HSDB (2015)	Q	100
oxadiazon $C_{15}H_{18}Cl_2N_2O_3$ [19666-30-9] CHNUNORXWHYHNE-UHFFFAOYSA-N	1.4×10^{2} 1.4×10^{2}		HSDB (2015) Armbrust (2000)	V C	

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyproconazole	1.4×10^{4}		HSDB (2015)	V	
$C_{15}H_{18}ClN_3O$	1.3×10^{2}		Barcelo and Hennion (1997)	X	569
[94361-06-5]	3.4×10^{2}		Goodarzi et al. (2010)	Q	570
UFNOUKDBUJZYDE-UHFFFAOYSA-N	2.0×10^{4}		Maniere et al. (2011)	?	242, 166
diclobutrazol	8.0×10^{3}		MacBean (2012a)	?	
$C_{15}H_{19}Cl_2N_3O$					
[75736-33-3]					
URDNHJIVMYZFRT-UHFFFAOYSA-N					
paclobutrazol	4.2×10^{4}		Maniere et al. (2011)	?	242, 166
$C_{15}H_{20}ClN_3O$					
[76738-62-0]					
RMOGWMIKYWRTKW-UHFFFAOYSA-N					
prochloraz	6.0×10^{2}		Duchowicz et al. (2020)	V	187
$C_{15}H_{16}Cl_3N_3O_2$	5.8		Barcelo and Hennion (1997)	X	569
[67747-09-5]	6.4×10^{3}		Duchowicz et al. (2020)	Q	
TVLSRXXIMLFWEO-UHFFFAOYSA-N	5.9×10^{-1}		Goodarzi et al. (2010)	Q	570
	6.1×10^{2}		Maniere et al. (2011)	?	242, 166
cis-propiconazole	1.2×10^{4}		Ebert et al. (2023)	?	319
$C_{15}H_{17}Cl_2N_3O_2$					
[112721-87-6]					
trans-propiconazole	7.8×10^{3}		Ebert et al. (2023)	?	319
$C_{15}H_{17}Cl_2N_3O_2$					
[120523-07-1]					
fenoxanil	5.0×10^{6}		Ebert et al. (2023)	?	319
$C_{15}H_{18}Cl_2N_2O_2$					
[115852-48-7]					
IUOKJNROJISWRO-UHFFFAOYSA-N					
carpropamid	8.4×10^{2}		Ebert et al. (2023)	?	319
$C_{15}H_{18}Cl_3NO$					
[104030-54-8]					
RXDMAYSSBPYBFW-UHFFFAOYSA-N					
propisochlor	5.6×10^{1}		Ebert et al. (2023)	?	319
$C_{15}H_{22}ClNO_2$					
[86763-47-5]					
KZNDFYDURHAESM-UHFFFAOYSA-N					
mefenpyr-diethyl	3.8×10^{3}		Maniere et al. (2011)	?	166
$C_{16}H_{18}Cl_2N_2O_4$	8.5×10^{3}		Maniere et al. (2011)	?	12, 166
[135590-91-9]					
OPGCOAPTHCZZIW-UHFFFAOYSA-N					

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
diazepam $C_{16}H_{13}ClN_2O$ [439-14-5] AAOVKJBEBIDNHE-UHFFFAOYSA-N	2.7×10^{3}		HSDB (2015)	Q	100
bendamustine $C_{16}H_{21}Cl_2N_3O_2$ [16506-27-7] YTKUWDBFDASYHO-UHFFFAOYSA-N	2.5×10^{7}		HSDB (2015)	Q	100
fentrazamide $C_{16}H_{20}ClN_5O_2$ [158237-07-1] LLQPHQFNMLZJMP-UHFFFAOYSA-N	5.1×10^{4}		Ebert et al. (2023)	?	319
piperalin $C_{16}H_{21}Cl_2NO_2$ [3478-94-2] BZGLBXYQOMFXAU-UHFFFAOYSA-N	4.3×10^{2}		HSDB (2015)	Q	100
tebuconazole $C_{16}H_{22}ClN_3O$ [107534-96-3] PXMNMQRDXWABCY-UHFFFAOYSA-N	7.0×10^{4} 1.1×10^{3} 2.2×10^{2} 1.0×10^{5}		HSDB (2015) Barcelo and Hennion (1997) Goodarzi et al. (2010) Maniere et al. (2011)	V X Q ?	 569 570, 573 12, 166
diethatyl-ethyl $C_{16}H_{22}ClNO_3$ [38727-55-8] WFKSADNZWSKCRZ-UHFFFAOYSA-N	7.9×10^{2}		Ebert et al. (2023)	?	319
fenarimol $C_{17}H_{12}Cl_2N_2O$ [60168-88-9] NHOWDZOIZKMVAI-UHFFFAOYSA-N	1.4×10^{3} 1.4×10^{3} 7.8×10^{5}		Duchowicz et al. (2020) Mackay et al. (2006d) Duchowicz et al. (2020)	V V Q	187
cumyluron $C_{17}H_{19}ClN_2O$ [99485-76-4] VYNOULHXXDFBLU-UHFFFAOYSA-N	2.5×10^{6}		Ebert et al. (2023)	?	319
triticonazole $C_{17}H_{20}N_3OCl$ [131983-72-7] PPDBOQMNKNNODG-ZROIWOOFSA-N	6.6×10^{4} 3.3×10^{4}		HSDB (2015) Maniere et al. (2011)	Q ?	100 242, 166
furametpyr $C_{17}H_{20}ClN_3O_2$ [123572-88-3] NRTLIYOWLVMQBO-UHFFFAOYSA-N	6.0×10^{6}		Ebert et al. (2023)	?	319

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
metconazole	3.8×10^3		Duchowicz et al. (2020)	V	187
$C_{17}H_{22}ClN_3O$	1.3×10^3		Duchowicz et al. (2020)	Q	
[125116-23-6]	4.5×10^6		Maniere et al. (2011)	?	12, 166
XWPZUHJBOLQNMN-UHFFFAOYSA-N					
tepraloxydim	5.2×10^4		Ebert et al. (2023)	?	319
$C_{17}H_{24}ClNO_4$					
[149979-41-9]					
IOYNQIMAUDJVEI-BMVIKAAMSA-N					
cloquintocet-mexyl	1.2×10^4		Duchowicz et al. (2020)	V	187
$C_{18}H_{22}ClNO_3$	3.4×10^2		Duchowicz et al. (2020)	Q	
[99607-70-2]	3.3×10^2		Maniere et al. (2011)	?	166
COYBRKAVBMYYSF-UHFFFAOYSA-N					
fenoxaprop-p-ethyl	6.2×10^2		Duchowicz et al. (2020)	V	187
$C_{18}H_{16}ClNO_5$	2.3×10^3		Duchowicz et al. (2020)	Q	
[71283-80-2]	3.7×10^3		Maniere et al. (2011)	?	12, 166
PQKBPHSEKWERTG-LLVKDONJSA-N					
ipconazole	3.9×10^3		Duchowicz et al. (2020)	V	187
$C_{18}H_{24}ClN_3O$	1.3×10^3		Duchowicz et al. (2020)	Q	
[125225-28-7]	3.3×10^4		Maniere et al. (2011)	?	242, 166
QTYCMDBMOLSEAM-UHFFFAOYSA-N					
pyriofenone	5.3×10^3		Maniere et al. (2011)	?	242, 166
$C_{18}H_{20}ClNO_5$					
[688046-61-9]					
NMVCBWZLCXANER-UHFFFAOYSA-N					
cintofen	1.4×10^7		Maniere et al. (2011)	?	12, 579, 166
$C_{18}H_{15}ClN_2O_5$	5.4×10^9		Maniere et al. (2011)	?	12, 575, 166
(sintofen)	6.1×10^9		Maniere et al. (2011)	?	12, 495, 166
[130561-48-7]					
QLMNCUHSDAGQGT-UHFFFAOYSA-N					
boscalid	1.9×10^4		MacBean (2012b)	X	352
$C_{18}H_{12}Cl_2N_2O$	1.9×10^4		Maniere et al. (2011)	?	242, 166
[188425-85-6]					
WYEMLYFITZORAB-UHFFFAOYSA-N					
tebufenpyrad	$>8.2\times10^2$		HSDB (2015)	V	
$C_{18}H_{24}ClN_3O$	$>9.1\times10^2$		Maniere et al. (2011)	?	242, 166
[119168-77-3]					
ZZYSLNWGKKDOML-UHFFFAOYSA-N					

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
8,9,10,11-tetrachloro-12-phthaloperinone	4.8×10^{5}		Zhang et al. (2010)	Q	288, 289
$C_{18}H_6Cl_4N_2O$	7.5×10^{9}		Zhang et al. (2010)	Q	288, 290
[20749-68-2]	5.7×10^{3}		Zhang et al. (2010)	Q	288, 291
UBZVRROHBDDCQY-UHFFFAOYSA-N	1.9×10^{5}		Zhang et al. (2010)	Q	288, 292
pigment red 254	3.4×10^{9}		Zhang et al. (2010)	Q	288, 289
$C_{18}H_{10}Cl_2N_2O_2$	3.9×10^{6}		Zhang et al. (2010)	Q	288, 290
[84632-65-5]	1.9×10^{13}		Zhang et al. (2010)	Q	288, 291
JNNHVXMCVRYTTN-UHFFFAOYSA-N	2.2×10^{12}		Zhang et al. (2010)	Q	288, 292
fenoxaprop-ethyl $C_{18}H_{16}ClNO_5$ [66441-23-4] PQKBPHSEKWERTG-UHFFFAOYSA-N	6.2×10^{2}		Ebert et al. (2023)	?	317
benzoylprop-ethyl $C_{18}H_{17}Cl_2NO_3$ [22212-55-1] SLCGUGMPSUYJAY-UHFFFAOYSA-N	1.2×10^{4}		Ebert et al. (2023)	?	741
difenoconazole	1.1×10^{6}		Duchowicz et al. (2020)	V	187
$C_{19}H_{17}Cl_2N_3O_3$	6.6×10^{3}		Barcelo and Hennion (1997)	X	569
[119446-68-3]	3.1×10^{4}		Duchowicz et al. (2020)	Q	
BQYJATMQXGBDHF-UHFFFAOYSA-N	7.7×10^{1}		Goodarzi et al. (2010)	Q	570
	1.1×10^{6}		Maniere et al. (2011)	?	166
quizalofop ethyl	9.3×10^{2}		Duchowicz et al. (2020)	V	187
$C_{19}H_{17}ClN_2O_4$	9.0×10^{2}		HSDB (2015)	V	
[76578-14-8]	4.0×10^{4}		Duchowicz et al. (2020)	Q	
OSUHJPCHFDQAIT-UHFFFAOYSA-N	1.5×10^{4}		Maniere et al. (2011)	?	12, 166
quizalofop-p-ethyl $C_{19}H_{17}ClN_2O_4$ [100646-51-3] OSUHJPCHFDQAIT-GFCCVEGCSA-N	4.8×10^{3}		Ebert et al. (2023)	?	319
pyraclostrobine	1.9×10^{5}		MacBean (2012b)	X	352
$C_{19}H_{18}ClN_3O_4$	1.9×10^{5}		Maniere et al. (2011)	?	12, 166
[175013-18-0] HZRSNVGNWUDEFX-UHFFFAOYSA-N					
pyrimidifen $C_{20}H_{28}ClN_3O_2$ [105779-78-0] ITKAIUGKVKDENI-UHFFFAOYSA-N	3.6×10^{4}		Ebert et al. (2023)	?	319

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ponsol red violet 2rnx	2.4×10^{10}		Zhang et al. (2010)	Q	288, 289
$C_{21}H_8Cl_3NO_3$	4.1×10^{7}		Zhang et al. (2010)	Q	288, 290
[6373-31-5]	9.9×10^{8}		Zhang et al. (2010)	Q	288, 291
SQAQTWYUQXFOMH-UHFFFAOYSA-N	4.6×10^{9}		Zhang et al. (2010)	Q	288, 292
dimethomorph	4.9×10^{4}		Duchowicz et al. (2020)	V	187
$C_{21}H_{22}NO_4Cl$	9.3×10^{5}		Duchowicz et al. (2020)	Q	
[110488-70-5]	9.9×10^{9}		HSDB (2015)	Q	100
QNBTYORWCCMPQP-JXAWBTAJSA-N	1.9×10^{5}		Maniere et al. (2011)	?	242, 166
	4.0×10^{4}		Maniere et al. (2011)	?	242, 166
propaquizafop	3.2×10^{6}		Duchowicz et al. (2020)	V	187
$C_{22}H_{22}ClN_3O_5$	1.1×10^{7}		Duchowicz et al. (2020)	Q	
[111479-05-1]	1.1×10^{7}		Maniere et al. (2011)	?	12, 166
FROBCXTULYFHEJ-UHFFFAOYSA-N					
aripiprazole	9.9×10^{11}		HSDB (2015)	Q	100
$C_{23}H_{27}Cl_2N_3O_2$					
[129722-12-9]					
CEUORZQYGODEFX-UHFFFAOYSA-N					
ag-g-86814	1.8×10^{14}		Zhang et al. (2010)	Q	288, 289
$C_{26}H_6Cl_8N_2O_4$	9.7×10^{12}		Zhang et al. (2010)	Q	288, 290
[30125-47-4]	1.1×10^{11}		Zhang et al. (2010)	Q	288, 291
ZEHOVWPIGREOPO-UHFFFAOYSA-N	4.1×10^{14}		Zhang et al. (2010)	Q	288, 292
8,18-dichloro-5,15-diethyl-5,15-dihydrodiindolo(3,2-b:3',2'-m)triphenodioxazine	8.0×10^{6}		Zhang et al. (2010)	Q	288, 289
$C_{34}H_{22}Cl_2N_4O_2$	1.8×10^{12}		Zhang et al. (2010)	Q	288, 290
[6358-30-1]	6.2×10^{6}		Zhang et al. (2010)	Q	288, 291
CGLVZFOCZLHKOH-UHFFFAOYSA-N	1.0×10^{10}		Zhang et al. (2010)	Q	288, 292

A6.9 Chlorofluorocarbons (C, H, O, N, F, Cl)

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chlorofluoromethane	1.5×10^{-3}	2600	Wilhelm et al. (1977)	L	
CH_2FCl	1.5×10^{-3}	2300	Boggs and Buck (1958)	M	
(R31)	1.5×10^{-3}		Duchowicz et al. (2020)	V	187
[593-70-4]	1.5×10^{-3}		Hine and Mookerjee (1975)	V	
XWCDCDSDNJVCLO-UHFFFAOYSA-N	1.6×10^{-3}		Yaws (2003)	X	238
	1.5×10^{-3}		Duchowicz et al. (2020)	Q	
	3.9×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.6×10^{-3}		Gharagheizi et al. (2010)	Q	247
	3.4×10^{-3}		Hilal et al. (2008)	Q	
	5.9×10^{-4}		Modarresi et al. (2007)	Q	68
		2600	Kühne et al. (2005)	Q	
	6.6×10^{-4}		Yao et al. (2002)	Q	230
	1.8×10^{-3}		English and Carroll (2001)	Q	231, 232
	6.1×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	1.8×10^{-3}		Irmann (1965)	Q	
		2500	Kühne et al. (2005)	?	
	1.6×10^{-3}		Yaws (1999)	?	21
	1.5×10^{-3}		Yaws and Yang (1992)	?	21
chlorodifluoromethane	3.5×10^{-4}	2600	Burkholder et al. (2019)	L	
CHF_2Cl	3.2×10^{-4}	2700	Burkholder et al. (2019)	L	71
(R22)	3.5×10^{-4}	2600	Burkholder et al. (2015)	L	
[75-45-6]	3.2×10^{-4}	2700	Burkholder et al. (2015)	L	71
VOPWNXZWBYDODV-UHFFFAOYSA-N	3.4×10^{-4}	3400	Sander et al. (2011)	L	1
	3.4×10^{-4}	3400	Wilhelm et al. (1977)	L	
	2.9×10^{-4}	3100	Ooki and Yokouchi (2011)	M	71
	3.4×10^{-4}	3000	Zheng et al. (1997)	M	742
	3.5×10^{-4}	3100	Maaßen (1995)	M	743
	3.5×10^{-4}	3000	Reichl (1995)	M	744
	1.7×10^{-4}	3500	Chang and Criddle (1995)	M	745
	3.5×10^{-4}	2600	Boggs and Buck (1958)	M	
	3.3×10^{-4}		Mackay et al. (2006b)	V	
	3.3×10^{-4}		Mackay et al. (1993)	V	
	3.3×10^{-4}	3600	McLinden (1989)	V	746, 747
	3.4×10^{-4}		Hine and Mookerjee (1975)	V	
	3.2×10^{-4}		Irmann (1965)	V	
	3.3×10^{-4}		Yaws (2003)	X	238
			Kanakidou et al. (1995)	C	748
	3.1×10^{-4}		Hayer et al. (2022)	Q	20
	3.4×10^{-4}	3100	Li et al. (2019)	Q	1
	1.4×10^{-4}		Gharagheizi et al. (2012)	Q	

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-5}		Raventos-Duran et al. (2010)	Q	246
	3.7×10^{-4}		Gharagheizi et al. (2010)	Q	247
	6.0×10^{-4}		Hilal et al. (2008)	Q	
	1.9×10^{-4}		Modarresi et al. (2007)	Q	68
		2600	Kühne et al. (2005)	Q	
	3.4×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	8.4×10^{-4}		English and Carroll (2001)	Q	231, 232
	1.0×10^{-4}		Katritzky et al. (1998)	Q	
	4.0×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	3.5×10^{-4}		Irmann (1965)	Q	
		3000	Kühne et al. (2005)	?	
	3.3×10^{-4}		Yaws (1999)	?	21
	2.4×10^{-4}		Abraham and Weathersby (1994)	?	21
	3.3×10^{-4}		Yaws and Yang (1992)	?	21
dichlorofluoromethane	9.1×10^{-4}		HSDB (2015)	V	
$CHFCl_2$	1.8×10^{-3}		Mackay et al. (1993)	V	
(R21)	6.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[75-43-4]	1.6×10^{-3}		Hilal et al. (2008)	Q	
UMNKXPULIDJLSU-UHFFFAOYSA-N	5.9×10^{-4}		Modarresi et al. (2007)	Q	68
	9.2×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	1.5×10^{-3}		Yao et al. (2002)	Q	230
	7.2×10^{-4}		Katritzky et al. (1998)	Q	
	1.9×10^{-3}		Yaws (1999)	?	21
	3.8×10^{-5}		Mackay et al. (1993)	?	
	1.9×10^{-3}		Yaws and Yang (1992)	?	21
chlorotrifluoromethane	9.9×10^{-6}	1700	Burkholder et al. (2019)	L	749
CF_3Cl	8.0×10^{-6}	1500	Burkholder et al. (2019)	L	71
(R13)	9.9×10^{-6}	1700	Burkholder et al. (2015)	L	750
[75-72-9]	8.0×10^{-6}	1500	Burkholder et al. (2015)	L	71
AFYPFACVUDMOHA-UHFFFAOYSA-N	9.9×10^{-6}	1700	Sander et al. (2011)	L	751
	9.3×10^{-6}	1600	Wilhelm et al. (1977)	L	
	8.9×10^{-6}	1900	Reichl (1995)	M	752
	9.0×10^{-6}	2100	Scharlin and Battino (1995)	M	753
	9.0×10^{-6}	2100	Scharlin and Battino (1994)	M	754
	7.8×10^{-6}		Park et al. (1982)	M	
	1.5×10^{-4}		Mackay et al. (1993)	V	
	5.7×10^{-6}		Hine and Mookerjee (1975)	V	
	8.8×10^{-6}		Yaws (2003)	X	238
	7.2×10^{-6}		Hilal et al. (2008)	C	
	5.7×10^{-6}		Irmann (1965)	C	
	8.3×10^{-6}		Hayer et al. (2022)	Q	20
	6.4×10^{-6}		Keshavarz et al. (2022)	Q	
	4.0×10^{-5}		Duchowicz et al. (2020)	Q	

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.3×10^{-5}		Gharagheizi et al. (2012)	Q	
	6.9×10^{-6}		Gharagheizi et al. (2010)	Q	247
	2.6×10^{-5}		Hilal et al. (2008)	Q	
	2.1×10^{-5}		Modarresi et al. (2007)	Q	68
		2600	Kühne et al. (2005)	Q	
	7.7×10^{-6}		Yaffe et al. (2003)	Q	249, 250
	6.7×10^{-7}		Katritzky et al. (1998)	Q	
	1.4×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	5.1×10^{-6}		Irmann (1965)	Q	
	7.2×10^{-6}		Duchowicz et al. (2020)	?	186, 21
		2000	Kühne et al. (2005)	?	
	8.8×10^{-6}		Yaws (1999)	?	21
	8.7×10^{-6}		Yaws and Yang (1992)	?	21
dichlorodifluoromethane	3.0×10^{-5}	3500	Burkholder et al. (2019)	L	
CF_2Cl_2	2.6×10^{-5}	2100	Burkholder et al. (2019)	L	71
(R12)	3.0×10^{-5}	3500	Burkholder et al. (2015)	L	
[75-71-8]	2.6×10^{-5}	2100	Burkholder et al. (2015)	L	71
PXBRQCKWGAHEHS-UHFFFAOYSA-N	3.1×10^{-5}	3200	Brockbank (2013)	L	1
	3.0×10^{-5}	3400	Warneck and Williams (2012)	L	
	3.0×10^{-5}	3500	Sander et al. (2011)	L	
	3.0×10^{-5}	3500	Sander et al. (2006)	L	
	3.1×10^{-5}	3500	Staudinger and Roberts (2001)	L	
	2.1×10^{-5}	1800	Wilhelm et al. (1977)	L	
	1.3×10^{-4}	5500	Hiatt (2013)	M	
	3.0×10^{-5}	3000	Reichl (1995)	M	755
	2.9×10^{-5}	2900	Scharlin and Battino (1995)	M	756
	2.9×10^{-5}	2900	Scharlin and Battino (1994)	M	757
	3.1×10^{-5}	3500	Munz and Roberts (1987)	M	
	2.9×10^{-5}	3200	Warner and Weiss (1985)	M	
	2.3×10^{-5}	3400	Wisegarver and Cline (1985)	M	71
	2.9×10^{-5}		Park et al. (1982)	M	
	2.5×10^{-5}		Pearson and McConnell (1975)	M	651, 12
	2.4×10^{-5}		Mackay et al. (2006b)	V	
	2.4×10^{-5}		Mackay et al. (1993)	V	
	2.3×10^{-5}		Mackay and Shiu (1981)	V	
	2.3×10^{-5}		Hine and Mookerjee (1975)	V	
	2.5×10^{-5}		Yaws (2003)	X	238
	3.5×10^{-6}	-210	Goldstein (1982)	X	299
	3.6×10^{-5}		Hilal et al. (2008)	C	
	6.4×10^{-6}		Ryan et al. (1988)	C	
	2.3×10^{-5}		Irmann (1965)	C	
	2.4×10^{-5}		Hayer et al. (2022)	Q	20
	1.9×10^{-5}		Keshavarz et al. (2022)	Q	
	1.1×10^{-4}		Duchowicz et al. (2020)	Q	185
	2.8×10^{-5}	3300	Li et al. (2019)	Q	1

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	2.4×10^{-5}		Gharagheizi et al. (2010)	Q	247
	5.4×10^{-5}		Hilal et al. (2008)	Q	
	7.7×10^{-5}		Modarresi et al. (2007)	Q	68
		3000	Kühne et al. (2005)	Q	
	2.5×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	1.1×10^{-5}		Katritzky et al. (1998)	Q	
	4.7×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	2.0×10^{-5}		Irmann (1965)	Q	
	2.9×10^{-5}		Duchowicz et al. (2020)	?	186, 21
		3400	Kühne et al. (2005)	?	
	2.5×10^{-5}		Yaws (1999)	?	21
	2.3×10^{-5}		Abraham and Weathersby (1994)	?	21
	2.5×10^{-5}		Yaws and Yang (1992)	?	21
trichlorofluoromethane	1.1×10^{-4}	3300	Burkholder et al. (2019)	L	
$CFCl_3$	7.3×10^{-5}	3900	Burkholder et al. (2019)	L	71
(R11)	1.1×10^{-4}	3300	Burkholder et al. (2015)	L	
[75-69-4]	7.3×10^{-5}	3900	Burkholder et al. (2015)	L	71
CYRMSUTZVYGINF-UHFFFAOYSA-N	1.0×10^{-4}	3400	Brockbank (2013)	L	
	1.1×10^{-4}	3400	Warneck and Williams (2012)	L	
	1.1×10^{-4}	3300	Sander et al. (2011)	L	
	1.1×10^{-4}	3300	Sander et al. (2006)	L	
	1.1×10^{-4}	3300	Staudinger and Roberts (2001)	L	
	1.0×10^{-4}	3100	Staudinger and Roberts (1996)	L	
	2.8×10^{-4}	5100	Hiatt (2013)	M	
	6.0×10^{-5}	4900	Ooki and Yokouchi (2011)	M	71
	1.0×10^{-4}	3700	Maaßen (1995)	M	758
	1.5×10^{-4}	3700	Reichl (1995)	M	759
	9.8×10^{-5}	3500	Ashworth et al. (1988)	M	279
	1.0×10^{-4}	3600	Warner and Weiss (1985)	M	
	7.8×10^{-5}	3900	Wisegarver and Cline (1985)	M	71
	1.1×10^{-4}	2700	Hunter-Smith et al. (1983)	M	660
	1.1×10^{-4}		Park et al. (1982)	M	
	1.7×10^{-4}		Warner et al. (1980)	M	
	1.1×10^{-4}	2100	Balls (1980)	M	
	1.2×10^{-5}		Pearson and McConnell (1975)	M	651, 12
	7.8×10^{-5}		Mackay et al. (2006b)	V	
	9.9×10^{-5}	6100	Fogg and Sangster (2003)	V	
	7.8×10^{-5}		Mackay et al. (1993)	V	
	9.0×10^{-5}		Yoshida et al. (1983)	V	
	9.0×10^{-5}		Mackay and Shiu (1981)	V	
	9.5×10^{-5}		Warner et al. (1980)	V	
	9.8×10^{-5}		Irmann (1965)	V	
	8.0×10^{-5}		Yaws (2003)	X	238, 38
	1.7×10^{-4}	730	Goldstein (1982)	X	299

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.0×10^{-4}		Hilal et al. (2008)	C	
	1.7×10^{-4}		Ryan et al. (1988)	C	
	1.7×10^{-4}		Shen (1982)	C	
	8.1×10^{-5}		Liss and Slater (1974)	C	
	9.4×10^{-5}		Hayer et al. (2022)	Q	20
	5.9×10^{-5}		Keshavarz et al. (2022)	Q	
	2.7×10^{-4}		Duchowicz et al. (2020)	Q	300
	6.5×10^{-4}		Gharagheizi et al. (2012)	Q	
	8.4×10^{-5}		Gharagheizi et al. (2010)	Q	247
	1.7×10^{-4}		Hilal et al. (2008)	Q	
	2.5×10^{-4}		Modarresi et al. (2007)	Q	68
		3300	Kühne et al. (2005)	Q	
	1.1×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	8.6×10^{-5}		Katritzky et al. (1998)	Q	
	8.6×10^{-5}		Irmann (1965)	Q	
	1.0×10^{-4}		Duchowicz et al. (2020)	?	186, 21
	9.8×10^{-5}		Mackay et al. (2006b)	?	
		3800	Kühne et al. (2005)	?	
	8.1×10^{-5}		Yaws (1999)	?	21, 38
	8.2×10^{-5}		Abraham and Weathersby (1994)	?	21
	9.8×10^{-5}		Mackay et al. (1993)	?	
	8.1×10^{-5}		Yaws and Yang (1992)	?	21
1,1,1,2-tetrachlorodifluoroethane	6.1×10^{-5}		Duchowicz et al. (2020)	V	187
$C_2Cl_4F_2$	6.2×10^{-5}		HSDB (2015)	V	
[76-11-9]	7.3×10^{-4}		Duchowicz et al. (2020)	Q	
SLGOCMATMKJJCE-UHFFFAOYSA-N	5.1×10^{-4}		Hilal et al. (2008)	Q	
	2.8×10^{-4}		Modarresi et al. (2007)	Q	68
	2.4×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	3.2×10^{-5}		Katritzky et al. (1998)	Q	
1,1,2,2-tetrachlorodifluoroethane	9.0×10^{-5}		HSDB (2015)	V	
$C_2F_2Cl_4$	1.0×10^{-4}		Hine and Mookerjee (1975)	V	
(R112)	7.9×10^{-5}		Yaws (2003)	X	238
[76-12-0]	2.4×10^{-3}		Gharagheizi et al. (2012)	Q	
UGCSPKPEHQEOSR-UHFFFAOYSA-N	7.1×10^{-5}		Gharagheizi et al. (2010)	Q	247
	5.1×10^{-4}		Hilal et al. (2008)	Q	
	3.2×10^{-4}		Modarresi et al. (2007)	Q	68
	1.1×10^{-4}		Yao et al. (2002)	Q	230
	7.9×10^{-5}		Yaws (1999)	?	21
1,1,1-trichloro-2,2,2-trifluoroethane	3.7×10^{-5}		HSDB (2015)	Q	100
$C_2F_3Cl_3$	3.7×10^{-5}		Zhang et al. (2010)	Q	288, 289
(R113a)	2.1×10^{-4}		Zhang et al. (2010)	Q	288, 290
[354-58-5]	5.8×10^{-5}		Zhang et al. (2010)	Q	288, 291
BOSAWIQFTJIYIS-UHFFFAOYSA-N	3.0×10^{-5}		Zhang et al. (2010)	Q	288, 292

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1,2-trichloro-1,2,2-trifluoroethane	3.4×10^{-5}	3200	Burkholder et al. (2019)	L	
$C_2F_3Cl_3$	3.4×10^{-5}	3200	Burkholder et al. (2015)	L	
(R113)	2.9×10^{-5}	4100	Brockbank (2013)	L	
[76-13-1]	2.0×10^{-4}	5700	Hiatt (2013)	M	
AJDIZQLSFPQPEY-UHFFFAOYSA-N	2.9×10^{-5}	4300	Dewulf et al. (1999)	M	
	2.9×10^{-5}	4000	Bu and Warner (1995)	M	760
	2.8×10^{-5}	6500	Reichl (1995)	M	761
	3.4×10^{-5}	3200	Ashworth et al. (1988)	M	279
	1.9×10^{-5}		HSDB (2015)	V	
			Mackay et al. (2006b)	V	685
	8.8×10^{-6}		Mackay et al. (1993)	V	
	2.0×10^{-5}		Hine and Mookerjee (1975)	V	
	2.0×10^{-5}		Yaws (2003)	X	238
	7.0×10^{-4}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-5}		Gharagheizi et al. (2010)	Q	247
	1.8×10^{-4}		Hilal et al. (2008)	Q	
	1.1×10^{-4}		Modarresi et al. (2007)	Q	68
		3700	Kühne et al. (2005)	Q	
	3.1×10^{-5}		Mackay et al. (2006b)	?	
		3800	Kühne et al. (2005)	?	
	2.1×10^{-5}		Yaws (1999)	?	21
	3.1×10^{-5}		Mackay et al. (1993)	?	
	2.0×10^{-5}		Yaws and Yang (1992)	?	21
	2.0×10^{-5}		Abraham et al. (1990)	?	
1,1-dichlorotetrafluoroethane	8.2×10^{-6}		HSDB (2015)	V	
$C_2F_4Cl_2$	5.8×10^{-6}		Hine and Mookerjee (1975)	V	
(R114a)	7.5×10^{-6}		Hilal et al. (2008)	C	
[374-07-2]	5.8×10^{-6}		Irmann (1965)	C	295
BAMUEXIPKSRTBS-UHFFFAOYSA-N	8.8×10^{-5}		Hilal et al. (2008)	Q	
	6.6×10^{-6}		Irmann (1965)	Q	
1,2-dichlorotetrafluoroethane	9.0×10^{-6}	2800	Reichl (1995)	M	762
$C_2F_4Cl_2$	7.9×10^{-6}		Mackay et al. (1993)	V	
(R114)	8.0×10^{-6}		Hine and Mookerjee (1975)	V	
[76-14-2]	8.1×10^{-6}		Yaws (2003)	X	238
DDMOUSALMHHKOS-UHFFFAOYSA-N	8.1×10^{-6}		Irmann (1965)	C	12
	7.1×10^{-4}		Hayer et al. (2022)	Q	20
	1.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	8.1×10^{-6}		Gharagheizi et al. (2010)	Q	247
	8.4×10^{-5}		Hilal et al. (2008)	Q	
	2.8×10^{-5}		Modarresi et al. (2007)	Q	68
		3300	Kühne et al. (2005)	Q	
	1.1×10^{-4}		Yao et al. (2002)	Q	230
	6.6×10^{-6}		Irmann (1965)	Q	
		2700	Kühne et al. (2005)	?	

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.2×10^{-6}		Yaws (1999)	?	21
	7.9×10^{-6}		Abraham and Weathersby (1994)	?	21
	8.1×10^{-6}		Yaws and Yang (1992)	?	21
chloropentafluoroethane	3.4×10^{-6}	2800	Wilhelm et al. (1977)	L	
C_2F_5Cl	3.1×10^{-6}	2100	Reichl (1995)	M	763
(R115)	1.8×10^{-6}		Duchowicz et al. (2020)	V	187
[76-15-3]	1.8×10^{-6}		HSDB (2015)	V	
RFCAUADVODFSLZ-UHFFFAOYSA-N	3.8×10^{-6}		Mackay et al. (1993)	V	
	3.7×10^{-6}		Meylan and Howard (1991)	V	
	3.2×10^{-6}		Hine and Mookerjee (1975)	V	
	3.8×10^{-6}		Yaws (2003)	X	238
	3.2×10^{-6}		Irmann (1965)	C	
	3.1×10^{-6}		Hayer et al. (2022)	Q	20
	6.5×10^{-5}		Duchowicz et al. (2020)	Q	
	4.9×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-6}		Gharagheizi et al. (2010)	Q	247
	3.4×10^{-5}		Hilal et al. (2008)	Q	
	7.6×10^{-6}		Modarresi et al. (2007)	Q	68
		2900	Kühne et al. (2005)	Q	
	2.4×10^{-5}		Yao et al. (2002)	Q	230
	1.2×10^{-6}		Meylan and Howard (1991)	Q	
	2.1×10^{-6}		Irmann (1965)	Q	
		2000	Kühne et al. (2005)	?	
	3.8×10^{-6}		Yaws (1999)	?	21
	3.8×10^{-6}		Yaws and Yang (1992)	?	21
1,1,2,2-tetrachloro-1-fluoroethane C_2HCl_4F [354-14-3] LUBCGHUOCJOIJA-UHFFFAOYSA-N	3.3×10^{-3}		HSDB (2015)	Q	100
1,1-dichloro-1,2,2-trifluoroethane $C_2HCl_2F_3$ [812-04-4] AFTSHZRGGNMLHC-UHFFFAOYSA-N	1.0×10^{-4}		HSDB (2015)	Q	100
1,2-dichloro-1,1,2-trifluoroethane $C_2HCl_2F_3$ [354-23-4] YMRMDGSNYHCUCL-UHFFFAOYSA-N	1.0×10^{-4}		HSDB (2015)	Q	100
2,2-dichloro-1,1,1-trifluoroethane	2.3×10^{-4}	2400	Kutsuna (2013)	M	
$C_2HF_3Cl_2$	3.2×10^{-4}	3100	Chang and Criddle (1995)	M	764
(R123)	2.8×10^{-4}	2600	McLinden (1989)	V	
[306-83-2]	5.0×10^{-4}		Hilal et al. (2008)	Q	
OHMHBGPWCHTMQE-UHFFFAOYSA-N	1.8×10^{-4}		Modarresi et al. (2007)	Q	68

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloro-1,1,2,2-tetrafluoroethane C_2HClF_4 [354-25-6] JQZFYIGAYWLRCC-UHFFFAOYSA-N	1.8×10^{-5}		HSDB (2015)	Q	100
1-chloro-1,2,2,2-tetrafluoroethane	1.1×10^{-4}	2800	Kutsuna (2013)	M	
C_2HF_4Cl	1.0×10^{-4}	3500	Maaßen (1995)	M	765
(R124)	1.1×10^{-4}	3400	Reichl (1995)	M	766
[2837-89-0]	1.1×10^{-4}		Duchowicz et al. (2020)	V	187
BOUGCJDAQLKBQH-UHFFFAOYSA-N	1.0×10^{-4}	3200	McLinden (1989)	V	
	1.2×10^{-4}		Hayer et al. (2022)	Q	20
	1.3×10^{-3}		Duchowicz et al. (2020)	Q	
		2900	Kühne et al. (2005)	Q	
		3400	Kühne et al. (2005)	?	
1,2-dichloro-1,1-difluoroethane	1.4×10^{-4}		Duchowicz et al. (2020)	V	187
$C_2H_2Cl_2F_2$	1.4×10^{-4}		HSDB (2015)	V	
[1649-08-7]	1.1×10^{-3}		Duchowicz et al. (2020)	Q	
SKDFWEPBABSFMG-UHFFFAOYSA-N					
2-chloro-1,1,1-trifluoroethane	3.7×10^{-4}	3600	Maaßen (1995)	M	767
$C_2H_2F_3Cl$	4.1×10^{-4}	3500	Reichl (1995)	M	768
(R133a)	3.7×10^{-4}		Hine and Mookerjee (1975)	V	
[75-88-7]	3.7×10^{-4}		Irmann (1965)	C	
CYXIKYKBLDZZNW-UHFFFAOYSA-N	4.8×10^{-4}		Hayer et al. (2022)	Q	20
	3.7×10^{-5}		HSDB (2015)	Q	100
	3.0×10^{-4}		Hilal et al. (2008)	Q	
	4.6×10^{-4}		English and Carroll (2001)	Q	231, 232
	3.9×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	2.9×10^{-4}		Irmann (1965)	Q	
	2.7×10^{-4}		Abraham and Weathersby (1994)	?	21
1,1-dichloro-1-fluoroethane	2.9×10^{-4}	2800	Kutsuna (2013)	M	
CH_3CFCl_2	2.8×10^{-4}	3700	Maaßen (1995)	M	769
(R141b)	4.5×10^{-4}		Duchowicz et al. (2020)	V	187
[1717-00-6]	4.5×10^{-4}		HSDB (2015)	V	
FRCHKSNAZZFGCA-UHFFFAOYSA-N	7.7×10^{-5}	5200	McLinden (1989)	V	
	2.9×10^{-4}		Hayer et al. (2022)	Q	20
	6.8×10^{-4}		Duchowicz et al. (2020)	Q	
	2.9×10^{-4}	3500	Li et al. (2019)	Q	1
		3300	Kühne et al. (2005)	Q	
		3700	Kühne et al. (2005)	?	

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloro-1,1-difluoroethane	1.5×10^{-4}	2600	Kutsuna (2013)	M	
CH_3CF_2Cl	1.4×10^{-4}	3200	Maaßen (1995)	M	770
(R142b)	1.4×10^{-4}	3200	Reichl (1995)	M	771
[75-68-3]	1.5×10^{-4}	3000	Chang and Criddle (1995)	M	772
BHNZEZWIUMJCGF-UHFFFAOYSA-N	1.4×10^{-4}	2500	McLinden (1989)	V	
	1.9×10^{-4}		Irmann (1965)	C	295
	1.6×10^{-4}		Hayer et al. (2022)	Q	20
	1.4×10^{-4}	3200	Li et al. (2019)	Q	1
	1.5×10^{-4}		Modarresi et al. (2007)	Q	68
	8.4×10^{-5}		Yaffe et al. (2003)	Q	249, 250
	1.5×10^{-3}		Katritzky et al. (1998)	Q	
	1.5×10^{-4}		Irmann (1965)	Q	
1-chloro-1,2-difluoroethane		2900	Kühne et al. (2005)	Q	
$C_2H_3ClF_2$		3200	Kühne et al. (2005)	?	
[338-64-7]					
UOVSDUIHNGNMBZ-UHFFFAOYSA-N					
1-chloro-1,1,2-trifluoroethane		2900	Kühne et al. (2005)	Q	
$C_2H_2F_3Cl$		3500	Kühne et al. (2005)	?	
(R133b)					
[421-04-5]					
HILNUELUDBMBJQ-UHFFFAOYSA-N					
2-chloro-1,1-difluoroethene	1.7×10^{-4}	3300	Maaßen (1995)	M	773
C_2HClF_2	1.7×10^{-4}	3300	Reichl (1995)	M	774
(R1122)	1.9×10^{-4}		Hayer et al. (2022)	Q	20
[359-10-4]		2800	Kühne et al. (2005)	Q	
HTHNTJCVPNKCPZ-UHFFFAOYSA-N		3300	Kühne et al. (2005)	?	
	1.1×10^{-4}		Abraham and Weathersby (1994)	?	21
chlorotrifluoroethene	3.2×10^{-5}		HSDB (2015)	Q	100
C_2ClF_3					
[79-38-9]					
UUAGAQFQZIEFAH-UHFFFAOYSA-N					
3,3-dichloro-1,1,1,2,2-pentafluoropropane	9.8×10^{-5}	3500	Kutsuna (2013)	M	
$CF_3CF_2CHCl_2$	1.5×10^{-5}		Keshavarz et al. (2022)	Q	
(R225ca)	8.4×10^{-4}		Duchowicz et al. (2020)	Q	
[422-56-0]	9.0×10^{-5}		HSDB (2015)	Q	100
COAUHYBSXMIJDK-UHFFFAOYSA-N	2.0×10^{-5}		Zhang et al. (2010)	Q	288, 289
	3.0×10^{-4}		Zhang et al. (2010)	Q	288, 290
	1.1×10^{-4}		Zhang et al. (2010)	Q	288, 291
	3.9×10^{-5}		Zhang et al. (2010)	Q	288, 292
	2.0×10^{-5}		Duchowicz et al. (2020)	?	186, 21

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3-dichloro-1,1,2,2,3-pentafluoro-propane	1.1×10^{-4}	3100	Kutsuna (2013)	M	
$CClF_2CF_2CHClF$	3.6×10^{-6}		HSDB (2015)	Q	100
(R225cb)					
[507-55-1]					
UJIGKESMIPTWJH-UHFFFAOYSA-N					
1-chloro-2-fluorobenzene	3.1×10^{-3}		Ebert et al. (2023)	?	317
C_6H_4ClF					
[348-51-6]					
ZCJAYDKWZAWMPR-UHFFFAOYSA-N					
1-chloro-3-fluorobenzene	1.6×10^{-3}		Ebert et al. (2023)	?	317
C_6H_4ClF					
[625-98-9]					
VZHJIJZEOCBKRA-UHFFFAOYSA-N					
1-chloro-3-(trifluoromethyl)benzene	2.9×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_7H_4ClF_3$	2.8×10^{-3}		Zhang et al. (2010)	Q	288, 290
[98-15-7]	1.4×10^{-3}		Zhang et al. (2010)	Q	288, 291
YTCGOUNVIAWCMG-UHFFFAOYSA-N	1.4×10^{-4}		Zhang et al. (2010)	Q	288, 292
1-chloro-4-(trifluoromethyl)benzene	2.8×10^{-4}		HSDB (2015)	Q	100
$C_7H_4ClF_3$	2.9×10^{-4}		Zhang et al. (2010)	Q	288, 289
[98-56-6]	3.1×10^{-3}		Zhang et al. (2010)	Q	288, 290
QULYNCCPRWKEMF-UHFFFAOYSA-N	1.5×10^{-3}		Zhang et al. (2010)	Q	288, 291
	1.4×10^{-4}		Zhang et al. (2010)	Q	288, 292
3-chloro-4-fluorobenzotrifluoride	2.4×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_7H_3ClF_4$	2.5×10^{-3}		Zhang et al. (2010)	Q	288, 290
[78068-85-6]	8.6×10^{-4}		Zhang et al. (2010)	Q	288, 291
BKHVEYHSOXVAOP-UHFFFAOYSA-N	1.1×10^{-4}		Zhang et al. (2010)	Q	288, 292
3,4-dichlorobenzotrifluoride	3.8×10^{-4}		HSDB (2015)	Q	100
$C_7H_3Cl_2F_3$	3.9×10^{-4}		Zhang et al. (2010)	Q	288, 289
[328-84-7]	5.3×10^{-3}		Zhang et al. (2010)	Q	288, 290
XILPLWOGHPSJBK-UHFFFAOYSA-N	2.0×10^{-3}		Zhang et al. (2010)	Q	288, 291
	2.3×10^{-4}		Zhang et al. (2010)	Q	288, 292
chlorodifluoroethanoic acid	2.5×10^{2}	10000	Burkholder et al. (2019)	L	
$CF_2ClCOOH$	2.5×10^{2}	10000	Burkholder et al. (2015)	L	
(chlorodifluoroacetic acid)	2.5×10^{2}	10000	Sander et al. (2011)	L	
[76-04-0]	2.4×10^{2}	10000	Bowden et al. (1998a)	M	
OAWAZQITIZDJRB-UHFFFAOYSA-N	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	4.4×10^{1}		Duchowicz et al. (2020)	Q	
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	246

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.4×10^{2}		Duchowicz et al. (2020)	?	186, 21
carbonic chloride fluoride COFCl [353-49-1] OXVVNXMNLYYMOL-UHFFFAOYSA-N	9.9×10^{-2}		George et al. (1993)	X	629
trifluoroacetylchloride	2.0×10^{-2}		Mirabel et al. (1996)	M	
CF_3COCl	2.7×10^{-3}		De Bruyn et al. (1995a)	M	451
[354-32-5]	2.0×10^{-2}		George et al. (1994b)	M	632
PNQBEPDZQUOCNY-UHFFFAOYSA-N	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	9.3×10^{-3}		Duchowicz et al. (2020)	Q	300
	2.2×10^{-2}		Duchowicz et al. (2020)	?	186, 21
2,2-dichloro-1,1-difluoro-1-methoxyethane	2.9×10^{-3}	4100	Fogg and Sangster (2003)	L	
$C_3H_4Cl_2F_2O$	1.7×10^{-3}		Steward et al. (1973)	L	14
(methoxyflurane)	3.0×10^{-3}	4300	Allott et al. (1973)	L	
[76-38-0]	1.7×10^{-3}		Lerman et al. (1983)	M	14
RFKMCNOHBTXSMU-UHFFFAOYSA-N	2.9×10^{-3}	3600	Smith et al. (1981b)	M	775
	1.8×10^{-3}		Stoelting and Longshore (1972)	M	14
	2.9×10^{-2}		Keshavarz et al. (2022)	Q	
	1.7×10^{-2}		Duchowicz et al. (2020)	Q	
	4.1×10^{-3}		Hilal et al. (2008)	Q	
	1.8×10^{-2}		Modarresi et al. (2007)	Q	68
		4800	Kühne et al. (2005)	Q	
	2.7×10^{-3}		Duchowicz et al. (2020)	?	186, 21
	2.7×10^{-3}		HSDB (2015)	?	421
		4000	Kühne et al. (2005)	?	
	1.7×10^{-3}		Abraham and Weathersby (1994)	?	21
	2.7×10^{-3}		Abraham et al. (1990)	?	
2-(chlorodifluoromethoxy)-1,1,1-trifluoroethane $C_3H_2ClF_5O$ [33018-78-9] HPDPVPUXPBZBOJ-UHFFFAOYSA-N	1.7×10^{-5}		Ebert et al. (2023)	?	367
2-(chlorofluoromethoxy)-1,1,1,2-tetrafluoroethane $C_3H_2ClF_5O$ [56885-28-0] GGEBMRHBGQLKGJ-UHFFFAOYSA-N	2.2×10^{-4}		Ebert et al. (2023)	?	367

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloro-2,2,2-trifluoroethyl difluoromethyl ether	2.4×10^{-4}		Fogg and Sangster (2003)	L	
$C_3H_2ClF_5O$	2.4×10^{-4}		Steward et al. (1973)	L	14
(forane; isoflurane)	2.4×10^{-4}		Allott et al. (1973)	L	14
[26675-46-7]	2.4×10^{-4}		Lerman et al. (1983)	M	14
PIWKPBJCKXDKJR-UHFFFAOYSA-N	4.8×10^{-4}	5300	Smith et al. (1981b)	M	
	5.7×10^{-4}		Keshavarz et al. (2022)	Q	
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	185
	4.2×10^{-4}		Hilal et al. (2008)	Q	
	1.2×10^{-3}		Modarresi et al. (2007)	Q	68
		4400	Kühne et al. (2005)	Q	
	3.8×10^{-4}		Goss (2005)	Q	
	3.4×10^{-4}		Duchowicz et al. (2020)	?	186, 21
	3.4×10^{-4}		HSDB (2015)	?	421
		4500	Kühne et al. (2005)	?	
	2.4×10^{-4}		Abraham and Weathersby (1994)	?	21
	3.4×10^{-4}		Abraham et al. (1990)	?	
2-chloro-1,1,2-trifluoroethyl difluoromethyl ether	3.0×10^{-4}		Fogg and Sangster (2003)	L	
$C_3H_2ClF_5O$	3.0×10^{-4}		Allott et al. (1973)	L	14
(enflurane)	2.7×10^{-4}		Guitart et al. (1989)	M	14
[13838-16-9]	2.9×10^{-4}		Lerman et al. (1983)	M	14
JPGQOUSTVILISH-UHFFFAOYSA-N	1.3×10^{-3}		HSDB (2015)	V	
	3.0×10^{-4}		Steward et al. (1973)	C	14
	6.9×10^{-4}		Hilal et al. (2008)	Q	
	3.1×10^{-4}		Abraham and Weathersby (1994)	?	21
3-[2-chloro-4-(trifluoromethyl)phenoxy]benzoic acid	6.4×10^{2}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_8ClF_3O_3$	3.3×10^{2}		Zhang et al. (2010)	Q	288, 290
[63734-62-3]	2.1×10^{5}		Zhang et al. (2010)	Q	288, 291
ONKRUAQFUNKYAX-UHFFFAOYSA-N	2.9×10^{3}		Zhang et al. (2010)	Q	288, 292
3-(2-chloro-4-(trifluoromethyl)phenoxy)phenyl acetate	1.1		Zhang et al. (2010)	Q	288, 289
$C_{15}H_{10}ClF_3O_3$	2.4×10^{1}		Zhang et al. (2010)	Q	288, 290
[50594-77-9]	2.9×10^{1}		Zhang et al. (2010)	Q	288, 291
KNFRYRRZMRETJX-UHFFFAOYSA-N	3.6		Zhang et al. (2010)	Q	288, 292
transfluthrin $C_{15}H_{12}Cl_2F_4O_2$ [118712-89-3] DDVNRFNDOPPVQJ-HQJQHLMTSA-N	2.2×10^{-1}		Ebert et al. (2023)	?	319

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tefluthrin	6.2×10^{-3}		HSDB (2015)	V	
$C_{17}H_{14}O_2ClF_7$	5.0×10^{-3}		Maniere et al. (2011)	?	12, 166
[79538-32-2]					
ZFHGXWPMULPQSE-GPCIZFCYSA-N					
clobetasol	6.2×10^{4}		HSDB (2015)	Q	100
$C_{22}H_{28}ClFO_4$					
[25122-41-2]					
FCSHDIVRCWTZOX-DVTGEIKXSA-N					
flufenprox	2.1×10^{1}		Ebert et al. (2023)	?	319
$C_{24}H_{22}ClF_3O_3$					
[107713-58-6]					
RURQAJURNPMSSK-UHFFFAOYSA-N					
EINECS 273-236-7	1.5×10^{14}		Zhang et al. (2010)	Q	288, 289
$C_{28}H_{33}Cl_3F_6O_{11}$	6.9×10^{18}		Zhang et al. (2010)	Q	288, 290
[68954-01-8]	2.3×10^{12}		Zhang et al. (2010)	Q	288, 291
KVXVLCBFSKMBAR-UHFFFAOYSA-N	1.6×10^{15}		Zhang et al. (2010)	Q	288, 292
3,5-dichloro-2,4,6-trifluoropyridine	1.6		Zhang et al. (2010)	Q	288, 289
$C_5Cl_2F_3N$	7.7×10^{-4}		Zhang et al. (2010)	Q	288, 290
[1737-93-5]	1.6×10^{-3}		Zhang et al. (2010)	Q	288, 291
PKSORSNCSXBXOT-UHFFFAOYSA-N	2.7×10^{-2}		Zhang et al. (2010)	Q	288, 292
chlorodifluoronitrooxymethane	2.9×10^{-2}	5900	Kanakidou et al. (1995)	E	776
$CClF_2OONO_2$					
[70490-95-8]					
HWHZTSGXJYKIPK-UHFFFAOYSA-N					
1-chloro-2-nitro-4-(trifluoromethyl)-benzene	7.2×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_7H_3ClF_3NO_2$	1.2×10^{-1}		Zhang et al. (2010)	Q	288, 290
[121-17-5]	1.1×10^{-1}		Zhang et al. (2010)	Q	288, 291
TZGFQIXRVUHDLE-UHFFFAOYSA-N	1.0×10^{-2}		Zhang et al. (2010)	Q	288, 292
2-chloro-1,3-dinitro-5-(trifluoromethyl)-benzene	1.8×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_7H_2ClF_3N_2O_4$	2.8		Zhang et al. (2010)	Q	288, 290
[393-75-9]	1.7×10^{-1}		Zhang et al. (2010)	Q	288, 291
HFHAVERNVFNSHL-UHFFFAOYSA-N	9.0×10^{-1}		Zhang et al. (2010)	Q	288, 292
fluroxypyr	5.7×10^{5}		HSDB (2015)	V	
$C_7H_5Cl_2FN_2O_3$	5.9×10^{9}		Maniere et al. (2011)	?	12, 166
[69377-81-7]					
MEFQWPUMEMWTJP-UHFFFAOYSA-N					

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
fluoroimide $C_{10}H_4Cl_2FNO_2$ [41205-21-4] IPENDKRRWFURRE-UHFFFAOYSA-N	7.7×10^{-1}		Ebert et al. (2023)	?	319
norflurazon $C_{12}H_9ClF_3N_3O$ [27314-13-2] NVGOPFQZYCNLDU-UHFFFAOYSA-N	2.9×10^{4} 2.9×10^{4} 5.5×10^{3}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
fluchloralin $C_{12}H_{13}ClF_3N_3O_4$ [33245-39-5] MNFMIVVPXOGUMX-UHFFFAOYSA-N	6.6×10^{-1} 7.4×10^{-1}		HSDB (2015) Mackay et al. (2006d)	V V	
flurochloridone $C_{12}H_{10}Cl_2F_3NO$ [61213-25-0] OQZCSNDVOWYALR-UHFFFAOYSA-N	2.6×10^{2} 8.2×10^{-1} 4.2×10^{2}		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	187 166
flupyradifurone $C_{12}H_{11}ClF_2N_2O_2$ [951659-40-8] QOIYTRGFOFZNKF-UHFFFAOYSA-N	6.5×10^{6}		Ebert et al. (2023)	?	319
fluxofenim $C_{12}H_{11}NO_3ClF_3$ [88485-37-4] UKSLKNUCVPZQCQ-GZTJUZNOSA-N	2.6 5.8×10^{2}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
fluazinam $C_{13}H_4Cl_2F_6N_4O_4$ [79622-59-6] UZCGKGPEKUCDTF-UHFFFAOYSA-N	3.9×10^{-2} 3.9×10^{-2}		HSDB (2015) Maniere et al. (2011)	V ?	 12, 166
5-(2-chloro-4-(trifluoromethyl)phenoxy)-2-nitrophenol $C_{13}H_7ClF_3NO_4$ [42874-63-5] WYTRKEWETULQOA-UHFFFAOYSA-N	9.9 1.1×10^{3} 2.3×10^{6} 2.3×10^{1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
florpyrauxifen $C_{13}H_8Cl_2F_2N_2O_3$ [943832-81-3] XFZUQTKDBCOXPP-UHFFFAOYSA-N	3.2×10^{7}		Ebert et al. (2023)	?	319

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tetraconazole	2.3×10^3		HSDB (2015)	V	
$C_{13}H_{11}Cl_2F_4N_3O$	2.8×10^3		Maniere et al. (2011)	?	242, 166
[112281-77-3]					
LQDARGUHUSPFNL-UHFFFAOYSA-N					
fluopicolide	9.0×10^3		HSDB (2015)	V	
$C_{14}H_8Cl_3F_3N_2O$	2.4×10^4		Maniere et al. (2011)	?	242, 166
[239110-15-7]					
GBOYJIHYACSLGN-UHFFFAOYSA-N					
diflubenzuron	2.1×10^3		Duchowicz et al. (2020)	V	187
$C_{14}H_9ClF_2N_2O_2$	2.1×10^3		HSDB (2015)	V	
(difluron)	2.1×10^3		Mackay et al. (2006d)	V	
[35367-38-5]	2.1×10^1		Barcelo and Hennion (1997)	X	569
QQQYTWIFVNKMRW-UHFFFAOYSA-N	7.2×10^3		Duchowicz et al. (2020)	Q	
	3.3×10^1		Goodarzi et al. (2010)	Q	570
	1.7×10^3		Maniere et al. (2011)	?	166
efavirenz	1.4×10^3		HSDB (2015)	Q	100
$C_{14}H_9ClF_3NO_2$					
[154598-52-4]					
XPOQHMRABVBWPR-ZDUSSCGKSA-N					
halauxifen-methyl	8.1×10^5		Maniere et al. (2011)	?	242, 572, 166
$C_{14}H_{11}Cl_2FN_2O_3$	8.2×10^5		Maniere et al. (2011)	?	242, 495, 166
[943831-98-9]	8.3×10^5		Maniere et al. (2011)	?	242, 575, 166
KDHKOPYYWOHESS-UHFFFAOYSA-N	9.0×10^5		Maniere et al. (2011)	?	242, 166
fluroxypyr-butometyl	2.4×10^3		Ebert et al. (2023)	?	319
$C_{14}H_{19}Cl_2FN_2O_4$					
[154486-27-8]					
ZKFARSBUEBZZJT-UHFFFAOYSA-N					
teflubenzuron	6.2×10^4		Duchowicz et al. (2020)	V	187
$C_{14}H_6N_2O_2Cl_2F_4$	2.5×10^4		Duchowicz et al. (2020)	Q	
[83121-18-0]					
CJDWRQLODFKPEL-UHFFFAOYSA-N					
fluroxypyr-meptyl	3.7×10^1		Maniere et al. (2011)	?	12, 166
$C_{15}H_{21}Cl_2FN_2O_3$					
(attain A)					
[81406-37-3]					
OLZQTUCTGLHFTQ-UHFFFAOYSA-N					

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
quinoxyfen $C_{15}H_8Cl_2FNO$ [124495-18-7] WRPIRSINYZBGPK-UHFFFAOYSA-N	1.0×10^{3}		HSDB (2015)	Q	100
5-(2-chloro-4-(trifluoromethyl)phenoxy)-2-nitrophenyl acetate	2.7×10^{2}		Zhang et al. (2010)	Q	288, 289
$C_{15}H_9ClF_3NO_5$	1.5×10^{3}		Zhang et al. (2010)	Q	288, 290
[50594-44-0]	3.7×10^{4}		Zhang et al. (2010)	Q	288, 291
PSWSPFSDVZVVDC-UHFFFAOYSA-N	3.1×10^{2}		Zhang et al. (2010)	Q	288, 292
triflumuron $C_{15}H_{10}ClF_3N_2O_3$ [64628-44-0] XAIPTRIXGHTTNT-UHFFFAOYSA-N	1.1×10^{3}		Ebert et al. (2023)	?	319
oxyfluorfen	1.2×10^{1}		Duchowicz et al. (2020)	V	187
$C_{15}H_{11}ClF_3NO_4$	1.2×10^{1}		HSDB (2015)	V	
[42874-03-3]	8.3×10^{1}		Duchowicz et al. (2020)	Q	
OQMBBFQZGJFLBU-UHFFFAOYSA-N	4.2×10^{1}		Maniere et al. (2011)	?	166
pyraflufen-ethyl	1.2×10^{4}		MacBean (2012b)	X	352
$C_{15}H_{13}Cl_2F_3N_2O_4$	4.5×10^{4}		Maniere et al. (2011)	?	12, 166
[129630-19-9]					
APTZNLHMIGJTEW-UHFFFAOYSA-N					
cis-furconazole $C_{15}H_{14}Cl_2F_3N_3O_2$ [112839-32-4] ULCWZQJLFZEXCS-KGLIPLIRSA-N	3.7×10^{3}		Ebert et al. (2023)	?	319
carfentrazone ethyl	3.3×10^{3}		Duchowicz et al. (2020)	V	187
$C_{15}H_{14}Cl_2F_3N_3O_3$	3.3×10^{3}		HSDB (2015)	V	
[128639-02-1]	1.7×10^{4}		Duchowicz et al. (2020)	Q	
MLKCGVHIFJBRCD-UHFFFAOYSA-N	6.4×10^{3}		Maniere et al. (2011)	?	12, 166
triflumizole	1.9×10^{5}		Duchowicz et al. (2020)	V	187
$C_{15}H_{15}ClF_3N_3O$	2.5×10^{7}		Mackay et al. (2006d)	V	
[68694-11-1]	3.7×10^{1}		Duchowicz et al. (2020)	Q	
HSMVPDGQOIQYSR-UHFFFAOYSA-N					
diflumetorim	3.1×10^{2}		Duchowicz et al. (2020)	V	187
$C_{15}H_{16}N_3OClF_2$	2.8×10^{3}		Duchowicz et al. (2020)	Q	
[130339-07-0]					
NEKULYKCZPJMMJ-UHFFFAOYSA-N					

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-(2,4-dichlorophenyl)-6-fluoro-2-(1H-1,2,4-triazol-1-yl)-quinazolin-4(3H)-one	5.6×10^{8}		Hilal et al. (2008)	Q	
$C_{16}H_8Cl_2FN_5O$	1.4×10^{5}		Modarresi et al. (2007)	Q	68
(fluquinconazole)	4.8×10^{5}		Maniere et al. (2011)	?	242, 166
[136426-54-5]					
IJJVMEJXYNJXOJ-UHFFFAOYSA-N					
hexaflumuron	9.9×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{16}H_8Cl_2F_6N_2O_3$	9.9×10^{-1}		HSDB (2015)	V	
[86479-06-3]	4.3×10^{4}		Duchowicz et al. (2020)	Q	
RGNPBRKPHBKNKX-UHFFFAOYSA-N					
fluopyram	3.4×10^{4}		Maniere et al. (2011)	?	242, 166
$C_{16}H_{11}ClF_6N_2O$					
[658066-35-4]					
KVDJTXBXMWJJEF-UHFFFAOYSA-N					
haloxyfop-p-methyl	8.3×10^{2}		Maniere et al. (2011)	?	242, 166
$C_{16}H_{13}ClF_3NO_4$					
[72619-32-0]					
MFSWTRQUCLNFOM-SECBINFHSA-N					
flumetralin	5.2		Duchowicz et al. (2020)	V	187
$C_{16}H_{12}ClF_4N_3O_4$	4.0×10^{3}		Duchowicz et al. (2020)	Q	
[62924-70-3]					
PWNAWOCHVWERAR-UHFFFAOYSA-N					
haloxyfop-methyl	3.1×10^{1}		Duchowicz et al. (2020)	V	187
$C_{16}H_{13}ClF_3NO_4$	3.1×10^{2}		Duchowicz et al. (2020)	Q	
[69806-40-2]					
MFSWTRQUCLNFOM-UHFFFAOYSA-N					
pydiflumetofen	6.6×10^{3}		Ebert et al. (2023)	?	319
$C_{16}H_{16}Cl_3F_2N_3O_2$					
[1228284-64-7]					
DGOAXBPOVUPPEB-UHFFFAOYSA-N					
nuarimol	1.5×10^{7}		MacBean (2012a)	?	
$C_{17}H_{12}ClFN_2O$					
[63284-71-9]					
SAPGTCDSBGMXCD-UHFFFAOYSA-N					
clodinafop-propargyl	3.6×10^{3}		Duchowicz et al. (2020)	V	187
$C_{17}H_{13}ClFNO_4$	3.5×10^{3}		HSDB (2015)	V	
[105512-06-9]	2.4×10^{3}		Duchowicz et al. (2020)	Q	
JBDHZKLJNAIJNC-LLVKDONJSA-N	3.6×10^{3}		Maniere et al. (2011)	?	242, 166

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
flamprop-methyl $C_{17}H_{15}ClFNO_3$ [52756-25-9] RBNIGDFIUWJJEV-UHFFFAOYSA-N	2.2×10^{3}		MacBean (2012a)	?	
pyridalyl $C_{18}H_{14}Cl_4F_3NO_3$ [179101-81-6] UBSUICNYBBPFHD-UHFFFAOYSA-N	4.9×10^{6}		HSDB (2015)	V	
mefentrifluconazole $C_{18}H_{15}ClF_3N_3O_2$ [1417782-03-6] JERZEQUMJNCPRJ-UHFFFAOYSA-N	6.2×10^{2}		Maniere et al. (2011)	?	12, 166
bixafen $C_{18}H_{12}N_3OCl_2F_3$ [581809-46-3] LDLMOOXUCMHBMZ-UHFFFAOYSA-N	2.6×10^{4}		Maniere et al. (2011)	?	242, 166
benzovindiflupyr $C_{18}H_{15}Cl_2F_2N_3O$ [1072957-71-1] CCCGEKHKTPTUHJ-UHFFFAOYSA-N	7.7×10^{5}		Maniere et al. (2011)	?	242, 166
lactofen $C_{19}H_{15}ClF_3NO_7$ [77501-63-4] CONWAEURSVPLRM-UHFFFAOYSA-N	2.1×10^{1} 2.3×10^{1} 4.0×10^{4}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
flupoxam $C_{19}H_{14}N_4O_2ClF_5$ [119126-15-7] AOQMRUTZEYVDIL-UHFFFAOYSA-N	1.1×10^{2} 2.7×10^{7}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
flamprop-m-isopropyl $C_{19}H_{19}NO_3ClF$ [63782-90-1] IKVXBIIHQGXQRQ-CYBMUJFWSA-N	3.9×10^{2} 2.3×10^{1}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
haloxyfop-ethoxyethyl $C_{19}H_{19}ClF_3NO_5$ [87237-48-7] MIJLZGZLQLAQCM-UHFFFAOYSA-N	3.8×10^{4}		Ebert et al. (2023)	?	319
chlorfluazuron $C_{20}H_9Cl_3F_5N_3O_3$ [71422-67-8] UISUNVFOGSJSKD-UHFFFAOYSA-N	8.2×10^{6} 1.1×10^{6} 3.9×10^{8} 2.1×10^{6} 5.5×10^{6}		Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Duchowicz et al. (2020)	Q Q Q Q ?	 68 186, 21

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
fluazuron $C_{20}H_{10}N_3O_3Cl_2F_5$ [86811-58-7] YOWNVPAUWYHLQX-UHFFFAOYSA-N	$>2.3\times10^{10}$		MacBean (2012a)	?	
flufenoxuron $C_{21}H_{11}ClF_6N_2O_3$ [101463-69-8] RYLHNOVXKPXDIP-UHFFFAOYSA-N	3.8×10^{6}		HSDB (2015)	Q	100
fluoxastrobin $C_{21}H_{16}N_4O_5ClF$ [361377-29-9] UFEODZBUAFNAEU-NLRVBDNBSA-N	9.0×10^{6} 1.0×10^{7}		HSDB (2015) Maniere et al. (2011)	V ?	 12, 166
haloperidol $C_{21}H_{23}ClFNO_2$ [52-86-8] LNEPOXFFQSENCJ-UHFFFAOYSA-N	4.3×10^{8}		HSDB (2015)	Q	100
indoxacarb $C_{22}H_{17}ClF_3N_3O_7$ [173584-44-6] VBCVPMMZEGZULK-NRFANRHFSA-N	1.5×10^{4} $>1.7\times10^{4}$		HSDB (2015) Maniere et al. (2011)	V ?	 166
cyfluthrin $C_{22}H_{18}Cl_2FNO_3$ [68359-37-5] QQODLKZGRKWIFG-UHFFFAOYSA-N	3.4×10^{2} 1.1×10^{1} 1.7		HSDB (2015) Maniere et al. (2011) Maniere et al. (2011)	V ? ?	 12, 166 12, 166
cyfluthrin I $C_{22}H_{18}Cl_2FNO_3$ [86560-92-1] QQODLKZGRKWIFG-QSFXBCCZSA-N	2.2		Ebert et al. (2023)	?	319
β-cyfluthrin (cis) $C_{22}H_{18}Cl_2FNO_3$ [86560-93-2] QQODLKZGRKWIFG-XFQXTVEOSA-N	1.4×10^{2}		Ebert et al. (2023)	?	367
cyfluthrin II $C_{22}H_{18}Cl_2FNO_3$ [86560-94-3] QQODLKZGRKWIFG-BPAFIMBUSA-N	1.1×10^{2}		Ebert et al. (2023)	?	367
β-cyfluthrin (trans) $C_{22}H_{18}Cl_2FNO_3$ [86560-95-4] QQODLKZGRKWIFG-QKYXUNIQSA-N	3.6×10^{1}		Ebert et al. (2023)	?	367

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
metamifop $C_{23}H_{18}N_2O_4ClF$ [256412-89-2] ADDQHLREJDZPMT-CQSZACIVSA-N	1.6×10^{1}		MacBean (2012a)	?	12
pyriminostrobin $C_{23}H_{18}Cl_2F_3N_3O_4$ [1257598-43-8] YYXSCUSVVALMNW-FOWTUZBSSA-N	8.3×10^{3}		Ebert et al. (2023)	?	319
cyhalothrin $C_{23}H_{19}NO_3ClF_3$ [68085-85-8] ZXQYGBMAQZUVMI-BWHPXCRDSA-N	7.0×10^{-1}		HSDB (2015)	Q	100
bifenthrin $C_{23}H_{22}ClF_3O_2$ [82657-04-3] OMFRMAHOUUJSGP-UNOMPAQXSA-N	9.9 9.9 9.9 2.7×10^{-1} 4.7		Duchowicz et al. (2020) HSDB (2015) Hilal et al. (2008) Duchowicz et al. (2020) Hilal et al. (2008)	V V C Q Q	187
λ-cyhalothrin $C_{23}H_{19}ClF_3NO_3$ [91465-08-6] DFVKOWFGNASVPK-QQDHXZELSA-N	5.0×10^{1}		Maniere et al. (2011)	?	12, 166
γ-cyhalothrin $C_{23}H_{19}ClF_3NO_3$ [76703-62-3] ZXQYGBMAQZUVMI-GCMPRSNUSA-N	4.5×10^{1}		Maniere et al. (2011)	?	242, 166
flucycloxuron $C_{25}H_{20}ClF_2N_3O_3$ [94050-52-9] PCKNFPQPGUWFHO-UQRQXUALSA-N	3.8×10^{1}		MacBean (2012a)	?	
τ-fluvalinate $C_{26}H_{22}ClF_3N_2O_3$ [102851-06-9] INISTDXBRIBGOC-XMMISQBUSA-N	8.3×10^{3}		Maniere et al. (2011)	?	166
fluvalinate $C_{26}H_{22}ClF_3N_2O_3$ [69409-94-5] INISTDXBRIBGOC-UHFFFAOYSA-N	6.6×10^{2}		HSDB (2015)	Q	100

A7 Organic species with bromine (Br)

A7.1 Bromocarbons (C, H, O, N, Br)

Table A7.1: Bromocarbons (C, H, O, N, Br)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bromomethane	1.5×10^{-3}	3300	Burkholder et al. (2019)	L	777
CH_3Br	1.5×10^{-3}	3000	Burkholder et al. (2019)	L	71
(methyl bromide)	1.7×10^{-3}	3100	Burkholder et al. (2015)	L	
[74-83-9]	1.5×10^{-3}	3000	Burkholder et al. (2015)	L	71
GZUXJHMPEANEGY-UHFFFAOYSA-N	1.5×10^{-3}	3800	Brockbank (2013)	L	
	1.7×10^{-3}	3100	Sander et al. (2011)	L	
	1.7×10^{-3}	3100	Sander et al. (2006)	L	
	1.7×10^{-3}	3100	Staudinger and Roberts (2001)	L	
	1.6×10^{-3}	3100	Wilhelm et al. (1977)	L	
	1.3×10^{-3}	2800	Hiatt (2013)	M	
	2.0×10^{-3}		Thomas et al. (2006)	M	155, 705
	1.8×10^{-3}	2500	De Bruyn and Saltzman (1997)	M	778
	1.4×10^{-3}		Gan and Yates (1996)	M	295
	1.7×10^{-3}	3400	Elliott and Rowland (1993)	M	
	1.5×10^{-3}	2600	Swain and Thornton (1962)	M	
	1.6×10^{-3}	3200	Glew and Moelwyn-Hughes (1953)	M	779
	1.6×10^{-3}		Mackay et al. (2006b)	V	
	1.6×10^{-3}		Lide and Frederikse (1995)	V	
	1.6×10^{-3}		Mackay et al. (1993)	V	
	1.9×10^{-3}		Mackay and Shiu (1981)	V	12
	1.5×10^{-3}		Hine and Mookerjee (1975)	V	
	1.5×10^{-3}		Yaws (2003)	X	238
	4.4×10^{-5}	350	Goldstein (1982)	X	299
	1.8×10^{-4}		Keshavarz et al. (2022)	Q	
	3.5×10^{-3}		Duchowicz et al. (2020)	Q	185
	5.5×10^{-4}		Wang et al. (2017)	Q	81, 239
	3.8×10^{-3}		Wang et al. (2017)	Q	81, 240
	2.3×10^{-3}		Wang et al. (2017)	Q	81, 241
	3.7×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.7×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.3×10^{-3}		Modarresi et al. (2007)	Q	68
		3400	Kühne et al. (2005)	Q	
	1.9×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.8×10^{-3}		Yao et al. (2002)	Q	230
	1.2×10^{-3}		English and Carroll (2001)	Q	231, 232
	9.9×10^{-5}		Katritzky et al. (1998)	Q	
	1.5×10^{-3}		Suzuki et al. (1992)	Q	233
	3.1×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	7.9×10^{-4}		Irmann (1965)	Q	

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.3×10^{-3}		Duchowicz et al. (2020)	?	186, 21
	1.8×10^{-3}		Thomas et al. (2006)	?	155, 706
		3200	Kühne et al. (2005)	?	
	1.5×10^{-3}		Yaws (1999)	?	21
	1.7×10^{-3}		Yates and Gan (1998)	?	
	1.4×10^{-3}		Yaws and Yang (1992)	?	21
	1.6×10^{-3}		Abraham et al. (1990)	?	
dibromomethane	1.2×10^{-2}	4300	Burkholder et al. (2019)	L	1
CH_2Br_2	9.0×10^{-3}	4600	Burkholder et al. (2019)	L	71
[74-95-3]	9.0×10^{-3}	4600	Burkholder et al. (2015)	L	71
FJBFPHVGVWTDIP-UHFFFAOYSA-N	1.2×10^{-2}	4300	Brockbank (2013)	L	1, 780
	3.1×10^{-2}		Mackay and Shiu (1981)	L	
	1.2×10^{-2}	5000	Hiatt (2013)	M	
	8.9×10^{-3}	4400	Ooki and Yokouchi (2011)	M	71
	1.4×10^{-2}		Dohnal and Hovorka (1999)	M	12
	1.5×10^{-2}		Hovorka and Dohnal (1997)	M	12
	1.2×10^{-2}	4900	Kondoh and Nakajima (1997)	M	
	9.7×10^{-3}	3800	Moore et al. (1995)	M	781, 71
	1.1×10^{-2}	4000	Wright et al. (1992)	M	782
	1.1×10^{-2}	4100	Tse et al. (1992)	M	
	1.1×10^{-2}	4400	Rex (1906)	M	
	1.1×10^{-2}		Mackay et al. (2006b)	V	
	1.3×10^{-2}	4200	Fogg and Sangster (2003)	V	
	7.1×10^{-3}		Mackay et al. (1993)	V	
	1.1×10^{-2}		Hine and Mookerjee (1975)	V	
	1.1×10^{-2}		Yaws (2003)	X	238
	3.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-1}		Gharagheizi et al. (2010)	Q	247
	3.8×10^{-2}		Hilal et al. (2008)	Q	
	1.7×10^{-3}		Modarresi et al. (2007)	Q	68
		4500	Kühne et al. (2005)	Q	
	1.2×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	8.2×10^{-3}		Yao et al. (2002)	Q	230, 268
	2.7×10^{-3}		Katritzky et al. (1998)	Q	
	9.5×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.2×10^{-2}		Mackay et al. (2006b)	?	
		4300	Kühne et al. (2005)	?	
	1.1×10^{-2}		Yaws (1999)	?	21
	1.2×10^{-2}		Mackay et al. (1993)	?	
	1.1×10^{-2}		Abraham et al. (1990)	?	

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tribromomethane	1.7×10^{-2}	5200	Burkholder et al. (2019)	L	
$CHBr_3$	1.1×10^{-2}	6200	Burkholder et al. (2019)	L	71
(bromoform)	1.7×10^{-2}	5200	Burkholder et al. (2015)	L	
[75-25-2]	1.1×10^{-2}	6200	Burkholder et al. (2015)	L	71
DIKBFYAXUHHXCS-UHFFFAOYSA-N	1.8×10^{-2}	4800	Brockbank (2013)	L	
	1.7×10^{-2}	5200	Sander et al. (2011)	L	
	1.7×10^{-2}	5200	Sander et al. (2006)	L	
	1.7×10^{-2}	5200	Staudinger and Roberts (2001)	L	
	1.7×10^{-2}	5200	Staudinger and Roberts (1996)	L	
	1.6×10^{-2}		Mackay and Shiu (1981)	L	
	2.2×10^{-2}	6300	Hiatt (2013)	M	
	9.9×10^{-3}	6200	Ooki and Yokouchi (2011)	M	71
	2.0×10^{-2}		Ruiz-Bevia and Fernandez-Torres (2010)	M	
	9.6×10^{-3}		Zhang et al. (2002)	M	14
	2.3×10^{-2}		Hovorka and Dohnal (1997)	M	12
	1.4×10^{-2}	4500	Kondoh and Nakajima (1997)	M	
	1.5×10^{-2}	4300	Moore et al. (1995)	M	783, 71
	8.5×10^{-3}	1500	Khalfaoui and Newsham (1994a)	M	
	2.4×10^{-2}	4100	Wright et al. (1992)	M	784
	1.9×10^{-2}	5000	Tse et al. (1992)	M	
	1.8×10^{-2}	4700	Munz and Roberts (1987)	M	
	1.6×10^{-2}	5700	Nicholson et al. (1984)	M	
	1.9×10^{-2}		Warner et al. (1980)	M	
	1.7×10^{-2}		Mackay et al. (2006b)	V	
	1.8×10^{-2}	5300	Fogg and Sangster (2003)	V	
	1.7×10^{-2}		Mackay et al. (1993)	V	
	1.7×10^{-2}		Warner et al. (1980)	V	
	1.5×10^{-2}		Hine and Mookerjee (1975)	V	
	1.8×10^{-2}	2700	Goldstein (1982)	X	299
	1.7×10^{-2}		Ryan et al. (1988)	C	
	1.7×10^{-2}		Nicholson et al. (1984)	C	
	1.9×10^{-2}		Shen (1982)	C	
	8.8×10^{-3}		Keshavarz et al. (2022)	Q	
	1.0×10^{-2}		Duchowicz et al. (2020)	Q	
	7.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	7.3×10^{-3}		Hilal et al. (2008)	Q	
	9.8×10^{-4}		Modarresi et al. (2007)	Q	68
		5600	Kühne et al. (2005)	Q	
	1.8×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.3×10^{-2}		Yao et al. (2002)	Q	230
	1.4×10^{-2}		Katritzky et al. (1998)	Q	
	2.4×10^{-2}		Nirmalakhandan and Speece (1988)	Q	

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.8×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	2.1×10^{-2}		Mackay et al. (2006b)	?	
		5000	Kühne et al. (2005)	?	
	1.7×10^{-2}		Yaws (1999)	?	21
	2.1×10^{-2}		Mackay et al. (1993)	?	
	1.5×10^{-2}		Abraham et al. (1990)	?	
tetrabromomethane	2.0×10^{-2}		Duchowicz et al. (2020)	V	187
CBr_4	2.0×10^{-2}		HSDB (2015)	V	
[558-13-4]	1.2×10^{-2}		Fogg and Sangster (2003)	V	785, 38
HJUGFYREWKUQJT-UHFFFAOYSA-N	2.0×10^{-2}		Hilal et al. (2008)	C	
	9.8×10^{-4}		Duchowicz et al. (2020)	Q	
	2.1×10^{-3}		Hilal et al. (2008)	Q	
	2.2×10^{-4}		Modarresi et al. (2007)	Q	68
bromoethane	1.3×10^{-3}	3900	Burkholder et al. (2019)	L	
C_2H_5Br	1.3×10^{-3}	3900	Brockbank (2013)	L	
[74-96-4]	1.3×10^{-3}		Li et al. (1993)	M	
RDHPKYGYEGBMSE-UHFFFAOYSA-N	1.3×10^{-3}	3900	Rex (1906)	M	
	1.3×10^{-3}		Duchowicz et al. (2020)	V	187
			Mackay et al. (2006b)	V	685
	8.1×10^{-4}		Mackay et al. (1993)	V	
	1.4×10^{-3}		Abraham (1984)	V	
	1.3×10^{-3}		Hine and Mookerjee (1975)	V	
	1.3×10^{-3}		Yaws (2003)	X	238
	9.2×10^{-5}		Ryan et al. (1988)	C	
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	3.2×10^{-3}		Gharagheizi et al. (2012)	Q	
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
	3.4×10^{-3}		Hilal et al. (2008)	Q	
	1.2×10^{-3}		Modarresi et al. (2007)	Q	68
		3700	Kühne et al. (2005)	Q	
	1.4×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	7.7×10^{-4}		Yao et al. (2002)	Q	230
	1.1×10^{-3}		English and Carroll (2001)	Q	231, 232
	2.3×10^{-4}		Katritzky et al. (1998)	Q	
	1.1×10^{-3}		Suzuki et al. (1992)	Q	233
	1.6×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
		3800	Kühne et al. (2005)	?	
	1.3×10^{-3}		Yaws (1999)	?	21
	1.3×10^{-3}		Yaws and Yang (1992)	?	21
	1.4×10^{-3}		Abraham et al. (1990)	?	

Table A7.1: Bromocarbons (C, H, O, N, Br) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1-dibromoethane $C_2H_4Br_2$ [557-91-5] APQIUTYORBAGEZ-UHFFFAOYSA-N	7.6×10^{-3}		HSDB (2015)	Q	100
1,2-dibromoethane $C_2H_4Br_2$ (ethylene dibromide) [106-93-4] PAAZPARNPHGIKF-UHFFFAOYSA-N	1.4×10^{-2}	4300	Burkholder et al. (2019)	L	
	1.5×10^{-2}	3900	Burkholder et al. (2015)	L	
	1.4×10^{-2}	4200	Brockbank (2013)	L	
	1.7×10^{-2}	5500	Hiatt (2013)	M	
	1.9×10^{-2}		Dohnal and Hovorka (1999)	M	12
	1.3×10^{-2}		Welke et al. (1998)	M	
	1.9×10^{-2}		Hovorka and Dohnal (1997)	M	12
	1.8×10^{-2}	5500	Kondoh and Nakajima (1997)	M	
	1.1×10^{-2}	3000	Khalfaoui and Newsham (1994a)	M	33
	1.5×10^{-2}	3900	Ashworth et al. (1988)	M	279
	1.5×10^{-2}		Mackay et al. (2006b)	V	
	2.1×10^{-3}		Mackay et al. (1993)	V	
	1.4×10^{-2}		Hine and Mookerjee (1975)	V	
	1.2×10^{-2}		Yaws (2003)	X	238
	1.1×10^{-2}	1900	Goldstein (1982)	X	299
	1.5×10^{-2}		HSDB (2015)	C	
	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	3.3×10^{-3}		Duchowicz et al. (2020)	Q	185
	6.2×10^{-3}		Wang et al. (2017)	Q	81, 239
	4.6×10^{-2}		Wang et al. (2017)	Q	81, 240
	4.4×10^{-2}		Wang et al. (2017)	Q	81, 241
	2.8×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	6.5×10^{-3}		Modarresi et al. (2007)	Q	68
		4800	Kühne et al. (2005)	Q	
	1.6×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	4.1×10^{-3}		Katritzky et al. (1998)	Q	
	7.5×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.2×10^{-3}		Rumble (2021)	?	786, 787
	1.5×10^{-2}		Duchowicz et al. (2020)	?	186, 21
	1.5×10^{-2}		Mackay et al. (2006b)	?	
		4200	Kühne et al. (2005)	?	
	1.3×10^{-2}		Yaws (1999)	?	21
	1.5×10^{-2}		Mackay et al. (1993)	?	
	1.4×10^{-2}		Yaws and Yang (1992)	?	21
	2.1×10^{-2}		Abraham et al. (1990)	?	
	1.6×10^{-2}		Mackay and Yeun (1983)	?	
	1.8×10^{-2}		Chiou et al. (1980)	?	80

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-dibromoethane-d4 $C_2D_4Br_2$ (ethylene dibromide-d4) [22581-63-1] PAAZPARNPHGIKF-LNLMKGTHSA-N	1.6×10^{-2}	4800	Hiatt (2013)	M	
1,1,2-tribromoethane $C_2H_3Br_3$ [78-74-0] QUMDOMSJJIFTCA-UHFFFAOYSA-N	2.4×10^{-2}		Ebert et al. (2023)	?	317
1,1,2,2-tetrabromoethane $C_2H_2Br_4$ [79-27-6] QXSZNDIIPUOQMB-UHFFFAOYSA-N	1.4×10^{-2}	1300	Burkholder et al. (2019)	L	
	1.4×10^{-2}	1300	Brockbank (2013)	L	
	1.0×10^{-2}	840	Khalfaoui and Newsham (1994a)	M	
	7.4×10^{-1}		Duchowicz et al. (2020)	V	187
	7.6×10^{-1}		HSDB (2015)	V	
	7.3×10^{-1}		Yaws (2003)	X	238
	1.4×10^{-2}		Duchowicz et al. (2020)	Q	
	5.7×10^{-1}		Zhang et al. (2010)	Q	288, 289
	2.9×10^{-1}		Zhang et al. (2010)	Q	288, 290
	4.3×10^{-1}		Zhang et al. (2010)	Q	288, 291
	1.5×10^{-1}		Zhang et al. (2010)	Q	288, 292
	7.2×10^{-1}		Gharagheizi et al. (2010)	Q	247
	2.4×10^{-1}		Hilal et al. (2008)	Q	
	7.0×10^{-1}		Yaffe et al. (2003)	Q	249, 250
	2.3×10^{-1}		Katritzky et al. (1998)	Q	
	7.3×10^{-1}		Yaws (1999)	?	21
1-bromopropane C_3H_7Br [106-94-5] CYNYIHKIEHGYOZ-UHFFFAOYSA-N	1.1×10^{-3}	4600	Brockbank (2013)	L	
	1.1×10^{-3}		Li et al. (1993)	M	
	1.1×10^{-3}	4500	Rex (1906)	M	
	1.4×10^{-3}		HSDB (2015)	V	
	2.6×10^{-4}		Mackay et al. (2006b)	V	
	2.6×10^{-4}		Mackay et al. (1993)	V	
	1.0×10^{-3}		Abraham (1984)	V	
	1.0×10^{-3}		Hine and Mookerjee (1975)	V	
	1.3×10^{-3}		Yaws (2003)	X	238, 12
	1.5×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.8×10^{-3}		Hilal et al. (2008)	Q	
	1.2×10^{-3}		Modarresi et al. (2007)	Q	68
	1.4×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	3.9×10^{-4}		Yao et al. (2002)	Q	230
	8.4×10^{-4}		English and Carroll (2001)	Q	231, 275

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.4×10^{-4}		Katritzky et al. (1998)	Q	
	3.5×10^{-4}		Russell et al. (1992)	Q	280
	8.4×10^{-4}		Suzuki et al. (1992)	Q	233
	1.3×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.1×10^{-3}		Yaws (1999)	?	21, 12
	1.4×10^{-3}		Yaws and Yang (1992)	?	21, 12
	1.0×10^{-3}		Abraham et al. (1990)	?	
2-bromopropane	9.0×10^{-4}	3900	Brockbank (2013)	L	1
C_3H_7Br	8.4×10^{-4}		Li et al. (1993)	M	
[75-26-3]	9.0×10^{-4}	4500	Rex (1906)	M	
NAMYKGVDVNBCFQ-UHFFFAOYSA-N	9.0×10^{-4}		Duchowicz et al. (2020)	V	187
	9.0×10^{-4}		HSDB (2015)	V	
	7.9×10^{-4}		Mackay et al. (2006b)	V	
	7.9×10^{-4}		Mackay et al. (1993)	V	
	9.0×10^{-4}		Hine and Mookerjee (1975)	V	
	1.0×10^{-3}		Yaws (2003)	X	238, 12
	5.4×10^{-4}		Duchowicz et al. (2020)	Q	
	3.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	9.4×10^{-4}		Gharagheizi et al. (2010)	Q	247
	1.5×10^{-3}		Hilal et al. (2008)	Q	
	7.5×10^{-4}		Modarresi et al. (2007)	Q	68
	9.2×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	3.4×10^{-4}		Yao et al. (2002)	Q	230, 268
	6.7×10^{-4}		English and Carroll (2001)	Q	231, 232
	3.3×10^{-4}		Katritzky et al. (1998)	Q	
	7.3×10^{-4}		Suzuki et al. (1992)	Q	233
	9.2×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	8.1×10^{-4}		Yaws (1999)	?	21, 12
	1.0×10^{-3}		Yaws and Yang (1992)	?	21, 12
	9.0×10^{-4}		Abraham et al. (1990)	?	
1,2-dibromopropane	5.3×10^{-3}		Albanese et al. (1987)	M	
$C_3H_6Br_2$	6.8×10^{-3}		Duchowicz et al. (2020)	V	187
[78-75-1]	6.8×10^{-3}		HSDB (2015)	V	
XFNJYAKDBJUJAJ-UHFFFAOYSA-N	6.8×10^{-3}		Mackay et al. (2006b)	V	
	1.1×10^{-2}		Hine and Mookerjee (1975)	V	
	6.3×10^{-3}		Yaws (2003)	X	238
	1.5×10^{-3}		Duchowicz et al. (2020)	Q	
	3.5×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.6×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.9×10^{-2}		Hilal et al. (2008)	Q	
	2.8×10^{-3}		Modarresi et al. (2007)	Q	68
	6.9×10^{-3}		Yaffe et al. (2003)	Q	249, 250

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.2×10^{-3}		Katritzky et al. (1998)	Q	
	4.4×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	6.6×10^{-3}		Yaws and Yang (1992)	?	21
1,3-dibromopropane	1.1×10^{-3}		Mackay et al. (1993)	V	
$C_3H_6Br_2$	1.1×10^{-2}		Hine and Mookerjee (1975)	V	
[109-64-8]	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
VEFLKXRACNJHOV-UHFFFAOYSA-N	3.0×10^{-3}		Duchowicz et al. (2020)	Q	300
	7.2×10^{-2}		Hilal et al. (2008)	Q	
	5.0×10^{-3}		Modarresi et al. (2007)	Q	68
	1.2×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	5.6×10^{-3}		Katritzky et al. (1998)	Q	
	6.0×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.1×10^{-2}		Duchowicz et al. (2020)	?	186, 21
1-bromobutane	7.4×10^{-4}		Brockbank (2013)	L	
C_4H_9Br	4.6×10^{-4}		Hoff et al. (1993)	M	
[109-65-9]	8.2×10^{-4}		Li et al. (1993)	M	
MPPPKRYCTPRNTB-UHFFFAOYSA-N	1.1×10^{-3}		Duchowicz et al. (2020)	V	187
	1.1×10^{-3}		HSDB (2015)	V	
	8.0×10^{-4}		Abraham (1984)	V	
	8.0×10^{-4}		Hine and Mookerjee (1975)	V	
	8.0×10^{-4}		Yaws (2003)	X	238
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	9.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	7.5×10^{-4}		Gharagheizi et al. (2010)	Q	247
	2.2×10^{-3}		Hilal et al. (2008)	Q	
	8.7×10^{-4}		Modarresi et al. (2007)	Q	68
	1.1×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	2.7×10^{-4}		Yao et al. (2002)	Q	230
	6.2×10^{-4}		English and Carroll (2001)	Q	231, 232
	4.1×10^{-4}		Katritzky et al. (1998)	Q	
	5.8×10^{-4}		Russell et al. (1992)	Q	280
	6.5×10^{-4}		Suzuki et al. (1992)	Q	233
	1.0×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	8.3×10^{-4}		Haynes (2014)	?	788
	8.1×10^{-4}		Yaws (1999)	?	21
	8.1×10^{-4}		Yaws and Yang (1992)	?	21
	7.9×10^{-4}		Abraham et al. (1990)	?	
2-bromobutane	8.8×10^{-4}		Brockbank (2013)	L	
C_4H_9Br	7.7×10^{-4}		Li et al. (1993)	M	
[78-76-2]	6.2×10^{-4}		HSDB (2015)	Q	100
UPSXAPQYNGXVBF-UHFFFAOYSA-N	1.4×10^{-3}		Hilal et al. (2008)	Q	

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-bromo-2-methylpropane	4.2×10^{-4}		Hine and Mookerjee (1975)	V	
C_4H_9Br	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
[78-77-3]	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	245
HLVFKOKELQSXIQ-UHFFFAOYSA-N	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	2.0×10^{-3}		Hilal et al. (2008)	Q	
	7.7×10^{-4}		Modarresi et al. (2007)	Q	68
	4.2×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	4.0×10^{-4}		English and Carroll (2001)	Q	231, 232
	8.6×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	5.8×10^{-4}		Suzuki et al. (1992)	Q	233
	4.2×10^{-4}		Abraham et al. (1990)	?	
2-bromo-2-methylpropane	2.4×10^{-4}		Duchowicz et al. (2020)	V	187
C_4H_9Br	2.4×10^{-4}		HSDB (2015)	V	
[507-19-7]	2.0×10^{-4}		Duchowicz et al. (2020)	Q	
RKSOPLXZQNSWAS-UHFFFAOYSA-N	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	5.2×10^{-4}		Hilal et al. (2008)	Q	
	5.1×10^{-4}		Modarresi et al. (2007)	Q	68
	4.5×10^{-4}		English and Carroll (2001)	Q	231, 232
	4.2×10^{-4}		Katritzky et al. (1998)	Q	
	5.2×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	3.1×10^{-4}		Yaws and Yang (1992)	?	21, 28
	9.7×10^{-5}		Abraham et al. (1990)	?	
1-bromo-3-methylbutane	4.9×10^{-4}		Mackay et al. (1993)	V	
$C_5H_{11}Br$	2.9×10^{-4}		Hine and Mookerjee (1975)	V	
[107-82-4]	5.9×10^{-4}		Keshavarz et al. (2022)	Q	
YXZFFTJAHVMMLF-UHFFFAOYSA-N	4.5×10^{-4}		Duchowicz et al. (2020)	Q	185
	1.8×10^{-3}		Hilal et al. (2008)	Q	
	7.8×10^{-4}		Modarresi et al. (2007)	Q	68
	4.7×10^{-4}		Katritzky et al. (1998)	Q	
	7.0×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	4.5×10^{-4}		Suzuki et al. (1992)	Q	233
	2.9×10^{-4}		Duchowicz et al. (2020)	?	186, 21
1,4-dibromobutane	1.7×10^{-2}		Albanese et al. (1987)	M	
$C_4H_8Br_2$	7.3×10^{-2}		Hilal et al. (2008)	Q	
[110-52-1]	4.3×10^{-3}		Modarresi et al. (2007)	Q	68
ULTHEAFYOOPTTB-UHFFFAOYSA-N					

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-bromopentane $C_5H_{11}Br$ [110-53-2] YZWKKMVJZFACSU-UHFFFAOYSA-N	5.0×10^{-4}		Duchowicz et al. (2020)	V	187
	4.7×10^{-4}		Abraham (1984)	V	
	5.6×10^{-4}		Yaws (2003)	X	238
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	6.1×10^{-4}		Gharagheizi et al. (2012)	Q	
	5.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
	1.8×10^{-3}		Hilal et al. (2008)	Q	
	6.5×10^{-4}		Modarresi et al. (2007)	Q	68
	5.1×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	4.6×10^{-4}		English and Carroll (2001)	Q	231, 232
	5.1×10^{-4}		Katritzky et al. (1998)	Q	
	8.0×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	5.6×10^{-4}		Yaws (1999)	?	21
	5.0×10^{-4}		Yaws and Yang (1992)	?	21
	4.7×10^{-4}		Abraham et al. (1990)	?	
1-bromo-2-methylbutane $C_5H_{11}Br$ [10422-35-2] XKVLZBNEPALHIO-UHFFFAOYSA-N	8.8×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
1-bromohexane $C_6H_{13}Br$ [111-25-1] MNDIARAMWBIKFW-UHFFFAOYSA-N	3.0×10^{-4}		Duchowicz et al. (2020)	V	187
	3.0×10^{-4}		Abraham (1984)	V	
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	3.1×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.5×10^{-3}		Hilal et al. (2008)	Q	
	5.2×10^{-4}		Modarresi et al. (2007)	Q	68
	2.2×10^{-4}		Yaffe et al. (2003)	Q	249, 273
	3.4×10^{-4}		English and Carroll (2001)	Q	231, 232
	5.3×10^{-4}		Katritzky et al. (1998)	Q	
	6.2×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	3.0×10^{-4}		Abraham et al. (1990)	?	
1-bromo-3-methylpentane $C_6H_{13}Br$ [51116-73-5] MDCCBJLCTOTLKM-UHFFFAOYSA-N	2.3×10^{-4}		English and Carroll (2001)	Q	231, 232
	5.8×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
bromocyclohexane $C_6H_{11}Br$ [108-85-0] AQNQQHJNRPDOQV-UHFFFAOYSA-N	7.0×10^{-3}		Hilal et al. (2008)	Q	

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-bromoheptane	2.2×10^{-4}		Brockbank (2013)	L	
$C_7H_{15}Br$	2.2×10^{-4}		Duchowicz et al. (2020)	V	187
[629-04-9]	2.3×10^{-4}		Abraham (1984)	V	
LSXKDWGTSHCFPP-UHFFFAOYSA-N	2.2×10^{-4}		Yaws (2003)	X	238
	1.1×10^{-3}		Duchowicz et al. (2020)	Q	
	3.5×10^{-4}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	2.3×10^{-4}		Gharagheizi et al. (2010)	Q	247
	1.2×10^{-3}		Hilal et al. (2008)	Q	
	4.7×10^{-4}		Modarresi et al. (2007)	Q	68
	2.2×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	6.5×10^{-5}		Yao et al. (2002)	Q	230
	2.6×10^{-4}		English and Carroll (2001)	Q	231, 275
	5.6×10^{-4}		Katritzky et al. (1998)	Q	
	5.0×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	2.2×10^{-4}		Yaws (1999)	?	21
	2.3×10^{-4}		Abraham et al. (1990)	?	
1-bromooctane	1.7×10^{-4}		Duchowicz et al. (2020)	V	187
$C_8H_{17}Br$	2.4×10^{-4}	4600	Sarraute et al. (2004)	V	
[111-83-1]	1.7×10^{-4}		Abraham (1984)	V	
VMKOFRJSULQZRM-UHFFFAOYSA-N	1.1×10^{-3}		Duchowicz et al. (2020)	Q	
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	9.7×10^{-4}		Hilal et al. (2008)	Q	
	4.0×10^{-4}		Modarresi et al. (2007)	Q	68
	1.7×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	1.9×10^{-4}		English and Carroll (2001)	Q	231, 232
	5.6×10^{-4}		Katritzky et al. (1998)	Q	
	3.9×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	1.7×10^{-4}		Abraham et al. (1990)	?	
1,8-dibromooctane $C_8H_{16}Br_2$ [4549-32-0] DKEGCUDAFWNSSO-UHFFFAOYSA-N	1.3×10^{-2}	6900	Sarraute et al. (2006)	M	789
1,2-dibromo-4-(1,2-dibromoethyl)cyclohexane	1.7×10^{2}		HSDB (2015)	Q	100
$C_8H_{12}Br_4$	2.4×10^{-1}		Zhang et al. (2010)	Q	288, 289
[3322-93-8]	2.9		Zhang et al. (2010)	Q	288, 290
PQRRSJBLKOPVJV-UHFFFAOYSA-N	1.0×10^{1}		Zhang et al. (2010)	Q	288, 291
	2.5×10^{-1}		Zhang et al. (2010)	Q	288, 292

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-bromononane $C_9H_{19}Br$ [693-58-3] AYMUQTNXKPEMLM-UHFFFAOYSA-N	7.9×10^{-4}		Hilal et al. (2008)	Q	
1-bromodecane $C_{10}H_{21}Br$ [112-29-8] MYMSJFSOOQERIO-UHFFFAOYSA-N	1.7×10^{-4}		Ebert et al. (2023)	?	317
hexabromocyclododecane $C_{12}H_{18}Br_6$ [3194-55-6] DEIGXXQKDWULML-UHFFFAOYSA-N	2.1×10^{-1}		Duchowicz et al. (2020)	V	187
	2.1×10^{-1}		HSDB (2015)	V	
	1.6×10^{-2}		HSDB (2015)	V	
	1.3×10^{-2}		Duchowicz et al. (2020)	Q	
	5.7		Zhang et al. (2010)	Q	288, 289
	1.7×10^{2}		Zhang et al. (2010)	Q	288, 290
	5.7×10^{3}		Zhang et al. (2010)	Q	288, 291
	6.5		Zhang et al. (2010)	Q	288, 292
vinyl bromide C_2H_3Br [593-60-2] INLLPKCGLOXCIV-UHFFFAOYSA-N	7.0×10^{-4}		HSDB (2015)	Q	100
	8.0×10^{-4}		Zhang et al. (2010)	Q	288, 289
	7.7×10^{-4}		Zhang et al. (2010)	Q	288, 290
	4.8×10^{-4}		Zhang et al. (2010)	Q	288, 291
	8.2×10^{-4}		Zhang et al. (2010)	Q	288, 292
1,2-dibromoethene $C_2H_2Br_2$ [540-49-8] UWTUEMKLYAGTNQ-UHFFFAOYSA-N	1.2×10^{-2}		Duchowicz et al. (2020)	V	187
	1.2×10^{-2}		HSDB (2015)	V	
	4.8×10^{-3}		Duchowicz et al. (2020)	Q	
(*Z*)-1,2-dibromoethene $C_2H_2Br_2$ (*cis*-1,2-dibromoethene) [590-11-4] UWTUEMKLYAGTNQ-UPHRSURJSA-N	2.4×10^{-3}		Yaffe et al. (2003)	Q	249, 250
3-bromo-1-propene C_3H_5Br (allyl bromide) [106-95-6] BHELZAPQIKSEDF-UHFFFAOYSA-N	1.7×10^{-3}		Yaws (2003)	X	238
	9.0×10^{-4}		HSDB (2015)	Q	100
	3.9×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-3}		Gharagheizi et al. (2010)	Q	247
	8.6×10^{-3}		Hilal et al. (2008)	Q	
	2.6×10^{-3}		Modarresi et al. (2007)	Q	68
	1.0×10^{-3}		Yao et al. (2002)	Q	230
	1.7×10^{-3}		Yaws (1999)	?	21
	1.7×10^{-3}		Yaws and Yang (1992)	?	21
	1.7×10^{-3}		Abraham et al. (1990)	?	

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-bromo-1-propyne	8.8×10^{-3}	4000	Yates and Gan (1998)	M	1
C_3H_3Br	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
(propargyl bromide)	8.4×10^{-3}		Duchowicz et al. (2020)	Q	
[106-96-7]		3200	Kühne et al. (2005)	Q	
YORCIIVHUBAYBQ-UHFFFAOYSA-N	8.7×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4200	Kühne et al. (2005)	?	
			Fogg and Sangster (2003)	W	790
1-bromocyclohexene	2.0×10^{-3}		Hilal et al. (2008)	Q	
C_6H_9Br					
[2044-08-8]					
QBUMXSSCYUMVAW-UHFFFAOYSA-N					
1-bromo-4-methylcyclohexene	1.4×10^{-3}		Hilal et al. (2008)	Q	
$C_7H_{11}Br$					
[31053-84-6]					
LIUFYLLBQSSKQS-UHFFFAOYSA-N					
bromobenzene	4.3×10^{-3}	4500	Brockbank (2013)	L	1
C_6H_5Br	5.0×10^{-3}	4200	Fogg and Sangster (2003)	L	
[108-86-1]	4.8×10^{-3}		Mackay and Shiu (1981)	L	
QARVLSVVCXYDNA-UHFFFAOYSA-N	6.0×10^{-3}	4300	Hiatt (2013)	M	
	3.9×10^{-3}	2900	Lau et al. (2010)	M	11
	5.0×10^{-3}		de Wolf and Lieder (1998)	M	88
	4.0×10^{-3}		Shiu and Mackay (1997)	M	
	6.1×10^{-3}		Hovorka and Dohnal (1997)	M	12
	4.9×10^{-3}	4200	Kondoh and Nakajima (1997)	M	
	5.3×10^{-3}	5300	Hansen et al. (1993)	M	282
	4.4×10^{-3}		Li and Carr (1993)	M	
	4.0×10^{-3}		Mackay and Shiu (1981)	M	
	4.7×10^{-3}		Shiu and Mackay (1997)	V	
	4.7×10^{-3}		Mackay et al. (1993)	V	
	5.0×10^{-3}		Hwang et al. (1992)	V	
	4.7×10^{-3}		Hine and Mookerjee (1975)	V	
	4.6×10^{-3}		Yaws (2003)	X	238
	4.7×10^{-3}		HSDB (2015)	C	
	4.0×10^{-3}		Schüürmann (2000)	C	21
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	7.9×10^{-3}		Duchowicz et al. (2020)	Q	185
	3.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	4.2×10^{-3}		Gharagheizi et al. (2010)	Q	247
	5.2×10^{-3}		Hilal et al. (2008)	Q	
	7.7×10^{-3}		Modarresi et al. (2007)	Q	68
		4800	Kühne et al. (2005)	Q	
	4.1×10^{-3}		Yaffe et al. (2003)	Q	249, 250

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.2×10^{-3}		Yao et al. (2002)	Q	230
	5.4×10^{-3}		English and Carroll (2001)	Q	231, 232
	2.9×10^{-3}		Katritzky et al. (1998)	Q	
	5.1×10^{-3}		Suzuki et al. (1992)	Q	233
	7.3×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	4.0×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4300	Kühne et al. (2005)	?	
	4.6×10^{-3}		Yaws (1999)	?	21
	4.7×10^{-3}		Yaws and Yang (1992)	?	21
	4.7×10^{-3}		Abraham et al. (1990)	?	
bromobenzene-d5 C_6D_5Br [4165-57-5] QARVLSVVCXYDNA-RALIUCGRSA-N	6.5×10^{-3}	4200	Hiatt (2013)	M	
1,2-dibromobenzene $C_6H_4Br_2$ [583-53-9] WQONPSCCEXUXTQ-UHFFFAOYSA-N	9.5×10^{-3}		Schüürmann (2000)	V	
1,3-dibromobenzene $C_6H_4Br_2$ [108-36-1] JSRLURSZEMLAFO-UHFFFAOYSA-N	1.2×10^{-2}		Brockbank (2013)	L	
	8.0×10^{-3}		Duchowicz et al. (2020)	V	187
	5.0×10^{-3}		Mackay and Shiu (1981)	V	557
	1.2×10^{-2}		Yaws (2003)	X	238
	7.7×10^{-3}		Duchowicz et al. (2020)	Q	
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-2}		Gharagheizi et al. (2010)	Q	247
	9.0×10^{-3}		Hilal et al. (2008)	Q	
	6.4×10^{-3}		Modarresi et al. (2007)	Q	68
	7.0×10^{-3}		Yao et al. (2002)	Q	230
	4.2×10^{-2}		Katritzky et al. (1998)	Q	
	1.2×10^{-2}		Yaws (1999)	?	21
1,4-dibromobenzene $C_6H_4Br_2$ [106-37-6] SWJPEBQEEAHIGZ-UHFFFAOYSA-N	9.4×10^{-3}		Kuramochi et al. (2004)	M	
	1.1×10^{-2}		Duchowicz et al. (2020)	V	187
	1.1×10^{-2}		HSDB (2015)	V	
	4.3×10^{-3}		Schüürmann (2000)	V	
	4.8×10^{-3}		Mackay and Shiu (1981)	V	557
	2.0×10^{-2}		Hine and Mookerjee (1975)	V	
	1.1×10^{-2}		Kuramochi et al. (2004)	C	
	7.1×10^{-3}		Duchowicz et al. (2020)	Q	
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-2}		Hilal et al. (2008)	Q	

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.0×10^{-2}		Modarresi et al. (2007)	Q	68
		5600	Kühne et al. (2005)	Q	
	4.5×10^{-3}		English and Carroll (2001)	Q	231, 275
	4.1×10^{-2}		Katritzky et al. (1998)	Q	
	2.4×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
		6900	Kühne et al. (2005)	?	
1,2,4-tribromobenzene	3.1×10^{-2}		Kuramochi et al. (2004)	M	
$C_6H_3Br_3$	2.9×10^{-2}		Kuramochi et al. (2004)	C	
[615-54-3]	1.8×10^{-2}		Hilal et al. (2008)	Q	
FWAJPSIPOULHHH-UHFFFAOYSA-N					
1,3,5-tribromobenzene	1.3×10^{-2}		Duchowicz et al. (2020)	V	187
$C_6H_3Br_3$	5.8×10^{-3}		Duchowicz et al. (2020)	Q	
[626-39-1]	2.9×10^{-2}		Zhang et al. (2010)	Q	288, 289
YWDUZLFWHVQCHY-UHFFFAOYSA-N	4.0×10^{-2}		Zhang et al. (2010)	Q	288, 290
	2.5×10^{-2}		Zhang et al. (2010)	Q	288, 291
	2.6×10^{-2}		Zhang et al. (2010)	Q	288, 292
	5.1×10^{-1}		Katritzky et al. (1998)	Q	
1,2,4,5-tetrabromobenzene	2.7×10^{-3}		Kuramochi et al. (2004)	M	
$C_6H_2Br_4$	2.0×10^{-2}		Hilal et al. (2008)	Q	
[636-28-2]					
QCKHVNQHBOGZER-UHFFFAOYSA-N					
hexabromobenzene	9.3×10^{-2}		Kuramochi et al. (2004)	M	
C_6Br_6	4.1×10^{-1}		Kuramochi et al. (2014)	V	
[87-82-1]	7.1		Tittlemier et al. (2002)	V	
CAYGQBVSOZLICD-UHFFFAOYSA-N	3.5×10^{-1}		HSDB (2015)	Q	100
	4.0×10^{-1}		Xiao et al. (2012)	Q	
	4.6×10^{-1}		Zhang et al. (2010)	Q	288, 289
	4.6×10^{-1}		Zhang et al. (2010)	Q	288, 290
	6.0×10^{-2}		Zhang et al. (2010)	Q	288, 291
	6.7×10^{-1}		Zhang et al. (2010)	Q	288, 292
	1.2×10^{-2}		Hilal et al. (2008)	Q	
(bromomethyl)-benzene	1.4×10^{-3}		HSDB (2015)	Q	100
C_7H_7Br	5.4×10^{-2}		Hilal et al. (2008)	Q	
(benzyl bromide)	2.2×10^{-2}		Abraham et al. (1990)	?	
[100-39-0]					
AGEZXYOZHKGVCM-UHFFFAOYSA-N					
p-bromobenzyl bromide	3.6×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_7H_6Br_2$	2.7×10^{-1}		Zhang et al. (2010)	Q	288, 290
[589-15-1]	2.0×10^{-1}		Zhang et al. (2010)	Q	288, 291
YLRBJYMANQKEAW-UHFFFAOYSA-N	2.4×10^{-2}		Zhang et al. (2010)	Q	288, 292

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-bromo-2-methylbenzene	4.1×10^{-3}		HSDB (2015)	Q	100
$BrC_6H_4CH_3$	5.3×10^{-3}		Hilal et al. (2008)	Q	
(*o*-bromotoluene)					
[95-46-5]					
QSSXJPIWXQTSIX-UHFFFAOYSA-N					
1-bromo-3-methylbenzene	1.5×10^{-3}		Duchowicz et al. (2020)	V	187
$BrC_6H_4CH_3$	1.5×10^{-3}		HSDB (2015)	V	
(*m*-bromotoluene)	4.0×10^{-3}		Duchowicz et al. (2020)	Q	
[591-17-3]	5.2×10^{-3}		Hilal et al. (2008)	Q	
WJIFKOVZNJTSGO-UHFFFAOYSA-N	4.8×10^{-3}		Modarresi et al. (2007)	Q	68
	1.5×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	7.9×10^{-3}		Katritzky et al. (1998)	Q	
1-bromo-4-methylbenzene	3.6×10^{-3}	4800	Brockbank (2013)	L	
$BrC_6H_4CH_3$	3.4×10^{-3}	4600	Brockbank et al. (2013)	M	
(*p*-bromotoluene)	4.2×10^{-3}		Hine and Mookerjee (1975)	V	
[106-38-7]	5.3×10^{-2}		Keshavarz et al. (2022)	Q	
ZBTMRBYMKUEVEU-UHFFFAOYSA-N	4.0×10^{-3}		Duchowicz et al. (2020)	Q	300
	4.2×10^{-3}		Li et al. (2014)	Q	242
	5.6×10^{-3}		Hilal et al. (2008)	Q	
	5.5×10^{-3}		Modarresi et al. (2007)	Q	68
	4.5×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	3.4×10^{-3}		English and Carroll (2001)	Q	231, 232
	8.0×10^{-3}		Katritzky et al. (1998)	Q	
	5.2×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	3.6×10^{-3}		Suzuki et al. (1992)	Q	233
	5.2×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	4.2×10^{-3}		Duchowicz et al. (2020)	?	186, 21
	4.2×10^{-3}		Abraham et al. (1990)	?	
3,5-dibromotoluene	1.7×10^{-2}	4800	Hiatt (2013)	M	
$C_7H_6Br_2$					
[1611-92-3]					
DPKKOVGCHDUSAI-UHFFFAOYSA-N					
pentabromotoluene	4.0×10^{-1}		Xiao et al. (2012)	Q	
$C_7H_3Br_5$					
[87-83-2]					
OZHJEQVYCBTHJT-UHFFFAOYSA-N					
1-bromo-2-ethylbenzene	3.0×10^{-3}		Hine and Mookerjee (1975)	V	
C_8H_9Br	4.3×10^{-3}		Hilal et al. (2008)	Q	
[1973-22-4]	2.8×10^{-3}		English and Carroll (2001)	Q	231, 232
HVRUGFJYCAFAAN-UHFFFAOYSA-N	2.9×10^{-3}		Suzuki et al. (1992)	Q	233
	4.5×10^{-3}		Nirmalakhandan and Speece (1988)	Q	

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-bromo-4-ethylbenzene	3.1×10^{-3}		Zhang et al. (2010)	Q	288, 289
C_8H_9Br	6.1×10^{-3}		Zhang et al. (2010)	Q	288, 290
[1585-07-5]	4.2×10^{-3}		Zhang et al. (2010)	Q	288, 291
URFPRAHGGBYNPW-UHFFFAOYSA-N	5.2×10^{-3}		Zhang et al. (2010)	Q	288, 292
1-(bromomethyl)-2-methylbenzene	1.3×10^{-2}		HSDB (2015)	Q	100
C_8H_9Br					
(*o*-xylyl bromide)					
[89-92-9]					
WGVYCXYGPNNUQA-UHFFFAOYSA-N					
1-(bromomethyl)-3-methylbenzene	1.3×10^{-2}		HSDB (2015)	Q	100
C_8H_9Br					
(*m*-xylyl bromide)					
[620-13-3]					
FWLWTILKTABGKQ-UHFFFAOYSA-N					
1-(bromomethyl)-4-methylbenzene	1.3×10^{-2}		HSDB (2015)	Q	100
C_8H_9Br					
(*p*-xylyl bromide)					
[104-81-4]					
WZRKSPFYXUXINF-UHFFFAOYSA-N					
(2-bromoethyl)-benzene	6.5×10^{-3}		Duchowicz et al. (2020)	V	187
C_8H_9Br	6.5×10^{-3}		HSDB (2015)	V	
[103-63-9]	7.9×10^{-3}		Duchowicz et al. (2020)	Q	
WMPPDTMATNBGJN-UHFFFAOYSA-N	2.2×10^{-2}		Modarresi et al. (2007)	Q	68
	6.9×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.3×10^{-2}		Katritzky et al. (1998)	Q	
2-bromostyrene	9.0×10^{-3}		Zhang et al. (2010)	Q	288, 289
C_8H_7Br	9.5×10^{-3}		Zhang et al. (2010)	Q	288, 290
[125904-11-2]	7.3×10^{-3}		Zhang et al. (2010)	Q	288, 291
SSZOCHFYWWVSAI-UHFFFAOYSA-N	1.5×10^{-2}		Zhang et al. (2010)	Q	288, 292
(2-bromoethenyl)benzene	1.8×10^{-2}		HSDB (2015)	Q	100
C_8H_7Br					
[103-64-0]					
YMOONIIMQBGTDU-VOTSOKGWSA-N					
2,3,4,5,6-pentabromoethylbenzene	1.2×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_8H_5Br_5$	3.6×10^{-1}		Zhang et al. (2010)	Q	288, 290
[85-22-3]	3.3×10^{-2}		Zhang et al. (2010)	Q	288, 291
FIAXCDIQXHJNIX-UHFFFAOYSA-N	9.7×10^{-2}		Zhang et al. (2010)	Q	288, 292
1-bromo-2-(2-propyl)-benzene	1.7×10^{-3}		Hine and Mookerjee (1975)	V	
$BrC_6H_4C_3H_7$	2.5×10^{-3}		Hilal et al. (2008)	Q	
(*o*-bromocumene)	2.0×10^{-3}		Suzuki et al. (1992)	Q	233
[7073-94-1]	3.1×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
LECYCYNAEJDSIL-UHFFFAOYSA-N					

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-bromonaphthalene	3.5×10^{-2}		Duchowicz et al. (2020)	V	187
$C_{10}H_7Br$	5.0×10^{-2}		Yaws (2003)	X	238, 295
[90-11-9]	3.0×10^{-2}		Duchowicz et al. (2020)	Q	
DLKQHBOKULLWDQ-UHFFFAOYSA-N	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	247
	8.2×10^{-2}		Hilal et al. (2008)	Q	
	3.7×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.8×10^{-2}		Katritzky et al. (1998)	Q	
	3.5×10^{-2}		Yaws (1999)	?	21, 295
2-bromonaphthalene	4.3×10^{-2}		Ebert et al. (2023)	?	319
$C_{10}H_7Br$					
[580-13-2]					
APSMUYYLXZULMS-UHFFFAOYSA-N					
1,4-dibromonaphthalene	5.8×10^{-2}		Ebert et al. (2023)	?	317
$C_{10}H_6Br_2$					
[83-53-4]					
IBGUDZMIAZLJNY-UHFFFAOYSA-N					
decabromobiphenyl	2.3×10^{2}		HSDB (2015)	Q	100
$C_{12}Br_{10}$	2.4×10^{2}		Zhang et al. (2010)	Q	288, 289
[13654-09-6]	3.0×10^{2}		Zhang et al. (2010)	Q	288, 290
AQPHBYQUCKHJLT-UHFFFAOYSA-N	2.3×10^{2}		Zhang et al. (2010)	Q	288, 291
	5.0×10^{2}		Zhang et al. (2010)	Q	288, 292
4-bromo-1,1'-biphenyl	6.0×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_9Br$	6.9×10^{-2}		Zhang et al. (2010)	Q	288, 290
[92-66-0]	1.7×10^{-1}		Zhang et al. (2010)	Q	288, 291
PKJBWOWQJHHAHG-UHFFFAOYSA-N	3.5×10^{-1}		Zhang et al. (2010)	Q	288, 292
octabromobiphenyl	4.1×10^{3}		HSDB (2015)	V	
$C_{12}H_2Br_8$					
[27858-07-7]					
NDRKXFLZSRHAJE-UHFFFAOYSA-N					
2,2',4,4',5,5'-hexabromobiphenyl	2.3		HSDB (2015)	V	
$C_{12}H_4Br_6$					
[59080-40-9]					
HMBBJSKXDBUNNT-UHFFFAOYSA-N					
1,2-bis(pentabromophenyl) ethane	1.5×10^{2}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_4Br_{10}$	8.8×10^{2}		Zhang et al. (2010)	Q	288, 290
[84852-53-9]	8.6×10^{1}		Zhang et al. (2010)	Q	288, 291
BZQKBFHEWDPQHD-UHFFFAOYSA-N	1.7×10^{2}		Zhang et al. (2010)	Q	288, 292
1,3,6,8-tetrabromopyrene	4.7×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_6Br_4$	4.4×10^{1}		Zhang et al. (2010)	Q	288, 290
[128-63-2]	6.2×10^{-1}		Zhang et al. (2010)	Q	288, 291
ZKBKRTZIYOKNRG-UHFFFAOYSA-N	6.5×10^{1}		Zhang et al. (2010)	Q	288, 292

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
6-bromobenzo[*a*]pyrene $C_{20}H_{11}Br$ [21248-00-0] MJSYSGSEEADMTK-UHFFFAOYSA-N	1.2×10^{2}		HSDB (2015)	Q	100
bromomethanol	4.1		Wang et al. (2017)	Q	81, 239
CH_2BrOH	3.2×10^{1}		Wang et al. (2017)	Q	81, 240
[50398-29-3]	2.5×10^{2}		Wang et al. (2017)	Q	81, 241
OEDMOCYNWLHUDP-UHFFFAOYSA-N	2.0×10^{1}		Krysztofiak et al. (2012)	Q	
dibromomethanol $CHBr_2OH$ [166600-78-8] WICMSCLXMMZMFF-UHFFFAOYSA-N	1.7×10^{2}		Krysztofiak et al. (2012)	Q	
tribromomethanol CBr_3OH [5405-30-1] ACRXLLXANWELLX-UHFFFAOYSA-N	1.5×10^{3}		Krysztofiak et al. (2012)	Q	
formyl bromide	4.5×10^{-1}		Wang et al. (2017)	Q	81, 239
CHBrO	3.2×10^{-2}		Wang et al. (2017)	Q	81, 240
[7726-11-6]	3.7×10^{-3}		Wang et al. (2017)	Q	81, 241
AIFARXRIYKCEEV-UHFFFAOYSA-N	7.3×10^{-1}		Krysztofiak et al. (2012)	Q	
carbonyl bromide CBr_2O [593-95-3] MOIPGXQKZSZOQX-UHFFFAOYSA-N	2.1×10^{-1}		Krysztofiak et al. (2012)	Q	
bromomethyl peroxide	3.7×10^{1}		Wang et al. (2017)	Q	81, 239
CH_2BrO_2H	1.3×10^{2}		Wang et al. (2017)	Q	81, 240
WXVCUAGYVVWQBP-UHFFFAOYSA-N	3.0×10^{1}		Wang et al. (2017)	Q	81, 241
	2.5×10^{1}		Krysztofiak et al. (2012)	Q	
dibromomethyl peroxide $CHBr_2O_2H$ JBKQCSQVMCXDPZ-UHFFFAOYSA-N	2.2×10^{2}		Krysztofiak et al. (2012)	Q	
tribromomethyl peroxide CBr_3O_2H WJYKCADCZNTKBI-UHFFFAOYSA-N	1.9×10^{3}		Krysztofiak et al. (2012)	Q	
bromoethanoic acid	1.5×10^{3}	9300	Burkholder et al. (2019)	L	
$CH_2BrCOOH$	1.5×10^{3}	9300	Burkholder et al. (2015)	L	
(bromoacetic acid)	1.5×10^{3}	9300	Sander et al. (2011)	L	
[79-08-3]	1.5×10^{3}	9300	Bowden et al. (1998a)	M	
KDPAWGWELVVRCH-UHFFFAOYSA-N	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	1.5×10^{2}		Duchowicz et al. (2020)	Q	185
	4.2×10^{2}		Wang et al. (2017)	Q	81, 239
	5.6×10^{3}		Wang et al. (2017)	Q	81, 240

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.5×10^{2}		Wang et al. (2017)	Q	81, 241
	2.0×10^{3}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{3}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	246
		8800	Kühne et al. (2005)	Q	
	1.5×10^{3}		Duchowicz et al. (2020)	?	186, 21
		9300	Kühne et al. (2005)	?	
dibromoethanoic acid	2.3×10^{3}	8900	Burkholder et al. (2019)	L	
$CHBr_2COOH$	2.3×10^{3}	8900	Burkholder et al. (2015)	L	
(dibromoacetic acid)	2.3×10^{3}	8900	Sander et al. (2011)	L	
[631-64-1]	2.2×10^{3}	8900	Bowden et al. (1998a)	M	
SIEILFNCEFEENQ-UHFFFAOYSA-N	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	4.9×10^{2}		Duchowicz et al. (2020)	Q	185
	3.9×10^{3}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{3}		Raventos-Duran et al. (2010)	Q	246
		9900	Kühne et al. (2005)	Q	
	2.2×10^{3}		Duchowicz et al. (2020)	?	186, 21
		9000	Kühne et al. (2005)	?	
tribromoethanoic acid	3.0×10^{3}	9000	Burkholder et al. (2019)	L	
CBr_3COOH	3.0×10^{3}	9000	Burkholder et al. (2015)	L	
(tribromoacetic acid)	3.0×10^{3}	9000	Sander et al. (2011)	L	
[75-96-7]	2.9×10^{3}	9000	Bowden et al. (1998a)	M	
QIONYIKHPASLHO-UHFFFAOYSA-N	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	3.5×10^{2}		Duchowicz et al. (2020)	Q	
	2.0×10^{3}		Raventos-Duran et al. (2010)	Q	272, 244
	9.9		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{4}		Raventos-Duran et al. (2010)	Q	246
	3.0×10^{3}		Duchowicz et al. (2020)	?	186, 21
MCM:BRETO3H	4.5×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_3O_3Br$	1.4×10^{2}		Wang et al. (2017)	Q	81, 240
RGXORGOPJDPEIK-UHFFFAOYSA-N	9.8×10^{-1}		Wang et al. (2017)	Q	81, 241
MCM:DIBRETO2H	5.4×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_4O_2Br_2$	2.2×10^{2}		Wang et al. (2017)	Q	81, 240
ZXSZEFURCAPOPD-UHFFFAOYSA-N	9.6×10^{1}		Wang et al. (2017)	Q	81, 241
MCM:DIBRETOH	1.1×10^{2}		Wang et al. (2017)	Q	81, 239
$C_2H_4OBr_2$	1.1×10^{2}		Wang et al. (2017)	Q	81, 240
IYJYRKYSUOTLAE-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:BRETAL	4.1×10^{-1}		Wang et al. (2017)	Q	81, 239
C_2H_3OBr	6.0		Wang et al. (2017)	Q	81, 240
NMPVEAUIHMEAQP-UHFFFAOYSA-N	2.5×10^{-1}		Wang et al. (2017)	Q	81, 241

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-bromopropanol C_3H_7BrO [627-18-9] RQFUZUMFPRMVDX-UHFFFAOYSA-N	8.2		Modarresi et al. (2007)	Q	68
2,3-dibromopropanol $C_3H_6Br_2O$ [96-13-9] QWVCIORZLNBIIC-UHFFFAOYSA-N	1.6×10^{2} 1.6×10^{2} 1.1×10^{2} 1.2×10^{1} 1.4×10^{1}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	100 288, 289 288, 290 288, 291 288, 292
bromoacetone C_3H_5BrO [598-31-2] VQFAIAKCILWQPZ-UHFFFAOYSA-N	1.7		HSDB (2015)	Q	100
(bromomethyl)oxirane C_3H_5BrO (epibromohydrin) [3132-64-7] GKIPXFAANLTWBM-UHFFFAOYSA-N	4.1		HSDB (2015)	Q	100
2,3-dibromobutane-1,4-diol $C_4H_8Br_2O_2$ [90801-18-6] OXYNQEOLHRWEPE-QWWZWVQMSA-N	3.2×10^{3} 1.0×10^{5} 1.5×10^{6} 4.7×10^{4}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
bromoacetic acid, ethyl ester $C_4H_7BrO_2$ [105-36-2] PQJJJMRNHATNKG-UHFFFAOYSA-N	3.7×10^{-1}		HSDB (2015)	Q	100
brometone $C_4H_7Br_3O$ (1,1,1-tribromo-2-methyl-2-propanol) [76-08-4] JUGRTVJQTFZHOM-UHFFFAOYSA-N	1.0×10^{3}		HSDB (2015)	Q	100
2,2-bis(bromomethyl)-1,3-propanediol $C_5H_{10}Br_2O_2$ [3296-90-0] CHUGKEQJSLOLHL-UHFFFAOYSA-N	2.4×10^{3}		HSDB (2015)	Q	100
trisbromoneopentyl alcohol $C_5H_9Br_3O$ [36483-57-5] HQWKMYFWGMCJSW-UHFFFAOYSA-N	7.7×10^{2} 7.5 1.1×10^{1} 1.0		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-bromophenol HOC_6H_4Br [95-56-7] VADKRMSMGWJZCF-UHFFFAOYSA-N	4.5×10^{1}		HSDB (2015)	Q	100
	4.2		Hilal et al. (2008)	Q	
3-bromophenol HOC_6H_4Br [591-20-8] MNOJRWOWILAHAV-UHFFFAOYSA-N	4.5×10^{1}		HSDB (2015)	Q	100
	2.3×10^{1}		Hilal et al. (2008)	Q	
4-bromophenol HOC_6H_4Br [106-41-2] GZFGOTFRPZRKDS-UHFFFAOYSA-N	6.7×10^{1}		Abraham et al. (1994a)	R	
	6.8×10^{1}	8200	Parsons et al. (1971)	T	419
	4.3		Keshavarz et al. (2022)	Q	
	1.5×10^{2}		Duchowicz et al. (2020)	Q	
	6.5×10^{1}		Li et al. (2014)	Q	242
	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	243, 244
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	246
	1.6×10^{1}		Hilal et al. (2008)	Q	
	2.3×10^{1}		Modarresi et al. (2007)	Q	68
	6.5×10^{1}		Yaffe et al. (2003)	Q	249, 250
	3.5×10^{1}		English and Carroll (2001)	Q	231, 232
	1.3×10^{2}		Katritzky et al. (1998)	Q	
	3.0×10^{2}		Nirmalakhandan et al. (1997)	Q	
	3.3×10^{1}		Nirmalakhandan and Speece (1988)	Q	
	6.5×10^{1}		Duchowicz et al. (2020)	?	186, 21
	6.9×10^{1}		Abraham et al. (1990)	?	
2,4-dibromophenol $C_6H_4Br_2O$ [615-58-7] FAXWFCTVSHEODL-UHFFFAOYSA-N	1.1×10^{2}		HSDB (2015)	Q	100
2,6-dibromophenol $C_6H_4Br_2O$ [608-33-3] SSIZLKDLDKIHEV-UHFFFAOYSA-N	1.1×10^{2}		HSDB (2015)	Q	100
2,4,6-tribromophenol $C_6H_3Br_3O$ [118-79-6] BSWWXRFVMJHFBN-UHFFFAOYSA-N	2.1×10^{2}		HSDB (2015)	Q	100
	2.8×10^{2}		Zhang et al. (2010)	Q	288, 289
	1.5×10^{-1}		Zhang et al. (2010)	Q	288, 290
	6.2		Zhang et al. (2010)	Q	288, 291
	7.7		Zhang et al. (2010)	Q	288, 292
2,3,4,6-tetrabromophenol $C_6H_2Br_4O$ [14400-94-3] CXPJZISGVIVNEL-UHFFFAOYSA-N	7.0×10^{2}		HSDB (2015)	Q	100

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pentabromophenol C_6HBr_5O [608-71-9] SVHOVVJFOWGYJO-UHFFFAOYSA-N	1.8×10^{3} 1.8×10^{3} 1.2 2.2×10^{1} 1.3×10^{2}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	100 288, 289 288, 290 288, 291 288, 292
1-bromo-2-methoxybenzene C_7H_7BrO (2-bromoanisole) [578-57-4] HTDQSWDEWGSAMN-UHFFFAOYSA-N	2.9×10^{-2}		Pfeifer et al. (2001)	M	733
1-bromo-3-methoxybenzene C_7H_7BrO (3-bromoanisole) [2398-37-0] PLDWAJLZAAHOGG-UHFFFAOYSA-N	7.2×10^{-3}		Pfeifer et al. (2001)	M	733
1-bromo-4-methoxybenzene C_7H_7BrO (4-bromoanisole) [104-92-7] QJPJQTDYNZXKQF-UHFFFAOYSA-N	1.1×10^{-2}		Pfeifer et al. (2001)	M	733
1,5-dibromo-2-methoxybenzene $C_7H_6Br_2O$ (2,4-dibromoanisole) [21702-84-1] XGXUGXPKRBQINS-UHFFFAOYSA-N	8.1×10^{-2}		Pfeifer et al. (2001)	M	733
1,3-dibromo-2-methoxybenzene $C_7H_6Br_2O$ (2,6-dibromoanisole) [38603-09-7] BMZVDHQOAJUZJL-UHFFFAOYSA-N	3.7×10^{-2}		Pfeifer et al. (2001)	M	733
1,2,3-tribromo-4-methoxybenzene $C_7H_5Br_3O$ (2,3,4-tribromoanisole) [95970-13-1] NKWYZAWFQZLPSU-UHFFFAOYSA-N	9.9×10^{-3}		Ebert et al. (2023)	?	791
1,3,4-tribromo-2-methoxybenzene $C_7H_5Br_3O$ (2,3,6-tribromoanisole) [95970-19-7] XZYCSFIRWAPGJV-UHFFFAOYSA-N	5.2×10^{-3}	2800	Diaz et al. (2005)	M	792

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3,5-tribromo-2-methoxybenzene	1.9×10^{-2}	6400	Diaz et al. (2005)	M	
$C_7H_5Br_3O$	1.3×10^{-2}		Pfeifer et al. (2001)	M	733
(2,4,6-tribromoanisole)	3.1×10^{-2}		HSDB (2015)	Q	100
[607-99-8]					
YXTRCOAFNXQTKL-UHFFFAOYSA-N					
pentabromomethoxybenzene	1.0		Pfeifer et al. (2001)	M	733
$C_7H_3Br_5O$					
(pentabromoanisole)					
[1825-26-9]					
VEFNQGLEDJPUJF-UHFFFAOYSA-N					
1,3,5-tribromo-2-methoxy-4-methylbenzene	4.4×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_8H_7Br_3O$	2.0×10^{-1}		Zhang et al. (2010)	Q	288, 290
[41424-36-6]	3.2×10^{-1}		Zhang et al. (2010)	Q	288, 291
NMPPAMFEYWGNCI-UHFFFAOYSA-N	1.9×10^{-1}		Zhang et al. (2010)	Q	288, 292
4,5,6,7-tetrabromo-1,3-isobenzofurandione	6.1×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_8Br_4O_3$	4.4×10^{5}		Zhang et al. (2010)	Q	288, 290
[632-79-1]	2.4×10^{2}		Zhang et al. (2010)	Q	288, 291
QHWKHLYUUZGSCW-UHFFFAOYSA-N	8.0×10^{2}		Zhang et al. (2010)	Q	288, 292
allyl 2,4,6-tribromophenyl ether	3.8×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_9H_7Br_3O$	1.3×10^{-1}		Zhang et al. (2010)	Q	288, 290
[3278-89-5]	2.0×10^{-1}		Zhang et al. (2010)	Q	288, 291
RZLLIOPGUFOWOD-UHFFFAOYSA-N	6.2×10^{-1}		Zhang et al. (2010)	Q	288, 292
2,4-dibromo-6-methylphenyl glycidyl ether	8.2×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_{10}H_{10}Br_2O_2$	7.0		Zhang et al. (2010)	Q	288, 290
[75150-13-9]	5.2×10^{1}		Zhang et al. (2010)	Q	288, 291
XQTJZNGNEJLXTR-UHFFFAOYSA-N	5.4		Zhang et al. (2010)	Q	288, 292
2-(2,4,6-tribromophenoxy)ethyl acrylate	2.9×10^{2}		Zhang et al. (2010)	Q	288, 289
$C_{11}H_9Br_3O_3$	1.6×10^{1}		Zhang et al. (2010)	Q	288, 290
[7347-19-5]	4.3×10^{3}		Zhang et al. (2010)	Q	288, 291
AMBJXYFIMKHOQE-UHFFFAOYSA-N	1.3×10^{2}		Zhang et al. (2010)	Q	288, 292
2,3,7,8-tetrabromodibenzo-*p*-dioxin	3.0		Ebert et al. (2023)	?	319
$C_{12}H_4Br_4O_2$					
[50585-41-6]					
JZLQUWSWOJPCAK-UHFFFAOYSA-N					

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
octabromodibenzo-*p*-dioxin $C_{12}Br_8O_2$ [2170-45-8] XAHTWKGGNHXJRP-UHFFFAOYSA-N	5.1×10^{1}		Ebert et al. (2023)	?	319
4,4'-methylenebis(2,6-dibromophenol)	7.5×10^{7}		Zhang et al. (2010)	Q	288, 289
$C_{13}H_8Br_4O_2$	9.0×10^{1}		Zhang et al. (2010)	Q	288, 290
[21825-03-6]	1.3×10^{4}		Zhang et al. (2010)	Q	288, 291
WPZJSWWEEJJSIZ-UHFFFAOYSA-N	3.4×10^{3}		Zhang et al. (2010)	Q	288, 292
1,1'-[1,2-ethanediylbis(oxy)]bis pentabromobenzene	5.3×10^{4}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_4Br_{10}O_2$	8.6×10^{2}		Zhang et al. (2010)	Q	288, 290
[61262-53-1]	2.2×10^{2}		Zhang et al. (2010)	Q	288, 291
JJEPQBZQAGCZTH-UHFFFAOYSA-N	1.1×10^{3}		Zhang et al. (2010)	Q	288, 292
4,4'-dibromobenzil	8.0×10^{3}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_8Br_2O_2$	2.6×10^{3}		Zhang et al. (2010)	Q	288, 290
[35578-47-3]	1.9×10^{2}		Zhang et al. (2010)	Q	288, 291
NYCBYBDDECLFPE-UHFFFAOYSA-N	1.3×10^{5}		Zhang et al. (2010)	Q	288, 292
1,2-bis(2,4,6-tribromophenoxy)ethane	1.8×10^{1}		Kuramochi et al. (2014)	V	
$C_{14}H_8Br_6O_2$	2.3×10^{1}		HSDB (2015)	Q	100
(BTBPE)	6.4×10^{1}		Xiao et al. (2012)	Q	
[37853-59-1]	1.3×10^{3}		Zhang et al. (2010)	Q	288, 289
YATIGPZCMOYEGE-UHFFFAOYSA-N	7.3×10^{1}		Zhang et al. (2010)	Q	288, 290
	1.1×10^{3}		Zhang et al. (2010)	Q	288, 291
	1.0×10^{3}		Zhang et al. (2010)	Q	288, 292
2-ethylhexyl-2,3,4,5-tetrabromobenzoate $C_{15}H_{18}Br_4O_2$ (EHTeBB) [183658-27-7] HVDXCGSGEQKWGB-UHFFFAOYSA-N	1.6		Xiao et al. (2012)	Q	
tribromobisphenol A $C_{15}H_{13}Br_3O_2$ [6386-73-8] WYBOEVJIVYIEJL-UHFFFAOYSA-N	1.1×10^{2}		HSDB (2015)	Q	449
4,4'-(1-methylethylidene)bis(2,6-dibromophenol)	2.4×10^{2}		HSDB (2015)	V	
$C_{15}H_{12}Br_4O_2$	4.2×10^{7}		Zhang et al. (2010)	Q	288, 289
[79-94-7]	3.9×10^{1}		Zhang et al. (2010)	Q	288, 290
VEORPZCZECFIRK-UHFFFAOYSA-N	8.0×10^{4}		Zhang et al. (2010)	Q	288, 291
	1.6×10^{3}		Zhang et al. (2010)	Q	288, 292

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-[2-[2,6-bis(bromanyl)-4-oxidanyl-phenyl]propan-2-yl]-3,5-bis(bromanyl)phenol	4.2×10^{7}		Zhang et al. (2010)	Q	288, 289
$C_{15}H_{12}Br_4O_2$	2.0×10^{7}		Zhang et al. (2010)	Q	288, 290
[94334-64-2]	2.2×10^{7}		Zhang et al. (2010)	Q	288, 291
KIZJVNGSIWXYTL-UHFFFAOYSA-N	1.7×10^{8}		Zhang et al. (2010)	Q	288, 292
2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl 3,4,5,6-tetrabromophthalate	3.6×10^{10}		Zhang et al. (2010)	Q	288, 289
$C_{15}H_{16}Br_4O_7$	1.5×10^{11}		Zhang et al. (2010)	Q	288, 290
[20566-35-2]	3.1×10^{13}		Zhang et al. (2010)	Q	288, 291
OQHHASWHOGRCRC-UHFFFAOYSA-N	5.7×10^{10}		Zhang et al. (2010)	Q	288, 292
bromopropylate	2.1×10^{1}		Duchowicz et al. (2020)	V	187
$C_{17}H_{16}Br_2O_3$	2.1×10^{1}		HSDB (2015)	V	
[18181-80-1]	4.2×10^{2}		Duchowicz et al. (2020)	Q	
FOANIXZHAMJWOI-UHFFFAOYSA-N					
1,2,4,5-tetrabromo-3,6-bis(pentabromophenoxy)benzene	1.5×10^{6}		Zhang et al. (2010)	Q	288, 289
$C_{18}O_2Br_{14}$	4.1×10^{5}		Zhang et al. (2010)	Q	288, 290
[58965-66-5]	2.1×10^{6}		Zhang et al. (2010)	Q	288, 291
YMIUHIAWWDYGGU-UHFFFAOYSA-N	6.7×10^{5}		Zhang et al. (2010)	Q	288, 292
2,2-bis(3,5-dibromo-4-(2-hydroxyethoxy)phenyl)propane	5.6×10^{7}		Zhang et al. (2010)	Q	288, 289
$C_{19}H_{20}Br_4O_4$	1.5×10^{8}		Zhang et al. (2010)	Q	288, 290
[4162-45-2]	6.1×10^{9}		Zhang et al. (2010)	Q	288, 291
RVHUMFJSCJBNGS-UHFFFAOYSA-N	2.5×10^{8}		Zhang et al. (2010)	Q	288, 292
metrafenone $C_{19}H_{21}BrO_5$ [220899-03-6] AMSPWOYQQAWRRM-UHFFFAOYSA-N	7.6		Maniere et al. (2011)	?	12, 166
solvent red 43	4.4×10^{12}		Zhang et al. (2010)	Q	288, 289
$C_{20}H_8Br_4O_5$	1.5×10^{8}		Zhang et al. (2010)	Q	288, 290
[15086-94-9]	2.7×10^{10}		Zhang et al. (2010)	Q	288, 291
DBZJJPROPLPMSN-UHFFFAOYSA-N	2.9×10^{8}		Zhang et al. (2010)	Q	288, 292
2,2-bis[4-(2,3-dibromopropoxy)-3,5-dibromophenyl]-propane	2.4×10^{5}		Zhang et al. (2010)	Q	288, 289
$C_{21}H_{20}Br_8O_2$	4.0×10^{4}		Zhang et al. (2010)	Q	288, 290
[21850-44-2]	1.7×10^{5}		Zhang et al. (2010)	Q	288, 291
LXIZRZRTWSDLKK-UHFFFAOYSA-N	8.6×10^{4}		Zhang et al. (2010)	Q	288, 292

Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2-bis(4-allyloxy-3,5-dibromophenyl)propane	7.7×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_{21}H_{20}Br_4O_2$	1.3×10^{1}		Zhang et al. (2010)	Q	288, 290
[25327-89-3]	1.7×10^{2}		Zhang et al. (2010)	Q	288, 291
PWXTUWQHMIFLKL-UHFFFAOYSA-N	1.9×10^{2}		Zhang et al. (2010)	Q	288, 292
AC1MJ2TG	1.3×10^{8}		Zhang et al. (2010)	Q	288, 289
$C_{21}H_{24}Br_4O_4$	4.7×10^{6}		Zhang et al. (2010)	Q	288, 290
[33294-14-3]	9.2×10^{6}		Zhang et al. (2010)	Q	288, 291
UTMWVHZWNKBNKF-UHFFFAOYSA-N	1.2×10^{6}		Zhang et al. (2010)	Q	288, 292
tetrabromophenolphthalein, ethyl ester	1.0×10^{11}		Zhang et al. (2010)	Q	288, 289
$C_{22}H_{14}Br_4O_4$	1.2×10^{7}		Zhang et al. (2010)	Q	288, 290
[1176-74-5]	3.1×10^{10}		Zhang et al. (2010)	Q	288, 291
SQFXATUXPUCFFO-UHFFFAOYSA-N	3.5×10^{8}		Zhang et al. (2010)	Q	288, 292
4,10-dibromodibenzo[*def*, *mno*]chrysene-6,12-dione	5.8×10^{6}		Zhang et al. (2010)	Q	288, 289
$C_{22}H_8Br_2O_2$	2.7×10^{5}		Zhang et al. (2010)	Q	288, 290
[4378-61-4]	4.1×10^{6}		Zhang et al. (2010)	Q	288, 291
HTENFZMEHKCNMD-UHFFFAOYSA-N	1.1×10^{8}		Zhang et al. (2010)	Q	288, 292
bis(2-ethylhexyl)-3,4,5,6-tetrabromophthalate $C_{24}H_{34}Br_4O_4$ (TBPH) [26040-51-7] UUEDINPOVKWVAZ-UHFFFAOYSA-N	4.0×10^{2}		Xiao et al. (2012)	Q	
bromadiolone	1.1×10^{6}		HSDB (2015)	V	
$C_{30}H_{23}BrO_4$	1.1×10^{6}		Maniere et al. (2011)	?	242, 166
[28772-56-7] OWNRRUFOJXFKCU-UHFFFAOYSA-N					
brodifacoum $C_{31}H_{23}BrO_3$ [56073-10-0] VEUZZDOCACZPRY-UHFFFAOYSA-N	4.6×10^{2}		Rubbiani (2013)	?	

A7.2 Polybrominated diphenyl ethers (PBDEs)

Table A7.2: Polybrominated diphenyl ethers (PBDEs)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-bromodiphenyl ether $C_{12}H_9BrO$ (PBDE-1) [36563-47-0] RRWFUWRLNIZICP-UHFFFAOYSA-N	2.3×10^{-2}	7400	Long et al. (2017)	Q	288
3-bromodiphenyl ether $C_{12}H_9BrO$ (PBDE-2) [6876-00-2] AHDAKFFMKLQPTD-UHFFFAOYSA-N	2.3×10^{-2}	7400	Long et al. (2017)	Q	288
4-bromodiphenyl ether $C_{12}H_9BrO$ (PBDE-3) [101-55-3] JDUYPUMQALQRCN-UHFFFAOYSA-N	5.0×10^{-2} 4.3×10^{-2} 5.8×10^{-2} 9.6×10^{-2} 1.4×10^{-2} 8.2×10^{-2}	 5500 7400 	Lau et al. (2006) Lau et al. (2006) Charles and Destaillats (2005) Mackay et al. (1993) Long et al. (2017) HSDB (2015)	M M M V Q Q	721 722 288 100
2,2'-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-4) [51452-87-0] JMSKYMHFNWGUJG-UHFFFAOYSA-N	9.5×10^{-2}	7400	Long et al. (2017)	Q	288
2,3-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-5) [446254-14-4] JTYRXXKXOULVAP-UHFFFAOYSA-N	5.1×10^{-2}	7400	Long et al. (2017)	Q	288
2,3'-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-6) [147217-72-9] GODQTPRKFHOLPH-UHFFFAOYSA-N	9.4×10^{-2}	7400	Long et al. (2017)	Q	288
2,4-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-7) [171977-44-9] JMCIHKKTRDLVCO-UHFFFAOYSA-N	6.9×10^{-2}	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4'-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-8) [147217-71-8] RJQLQJZMLISKRJ-UHFFFAOYSA-N	5.8×10^{-2}	7400	Long et al. (2017)	Q	288
2,5-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-9) [337513-66-3] URDWJMUOJJSXAE-UHFFFAOYSA-N	8.0×10^{-2}	7400	Long et al. (2017)	Q	288
2,6-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-10) [51930-04-2] MUVDKHMQIZJFTC-UHFFFAOYSA-N	8.3×10^{-2}	7400	Long et al. (2017)	Q	288
3,3'-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-11) [6903-63-5] ALSVFJIXSNRBLE-UHFFFAOYSA-N	7.8×10^{-2}	7400	Long et al. (2017)	Q	288
3,4-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-12) [189084-59-1] SUUJFDKVPDCZQZ-UHFFFAOYSA-N	3.3×10^{-2}	7400	Long et al. (2017)	Q	288
3,4'-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-13) [83694-71-7] BGPOVBPKODCMMN-UHFFFAOYSA-N	5.5×10^{-2}	7400	Long et al. (2017)	Q	288
3,5-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-14) [46438-88-4] FOXBZJLXVUHYQZ-UHFFFAOYSA-N	9.9×10^{-2}	7400	Long et al. (2017)	Q	288
4,4'-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-15) [2050-47-7] YAWIAFUBXXPJMQ-UHFFFAOYSA-N	8.3×10^{-2}		Lau et al. (2006)	M	721
	7.1×10^{-2}		Lau et al. (2006)	M	722
	7.3×10^{-2}	4500	Charles and Destaillats (2005)	M	
	4.8×10^{-2}		Tittlemier et al. (2002)	V	
	2.4×10^{-1}		Wania and Dugani (2003)	R	
	3.9×10^{-2}	7400	Long et al. (2017)	Q	288
	9.0×10^{-2}		Hilal et al. (2008)	Q	

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-16) [147217-74-1] VRNGWCVCSHJUEJ-UHFFFAOYSA-N	2.2×10^{-1}	7400	Long et al. (2017)	Q	288
2,2',4-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-17) [147217-75-2] VYBFILXLBMWOLI-UHFFFAOYSA-N	2.3×10^{-1}	7400	Long et al. (2017)	Q	288
2,2',5-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-18) [407606-55-7] FAZLXBWRNJAGSV-UHFFFAOYSA-N	2.4×10^{-1}	7400	Long et al. (2017)	Q	288
2,2',6-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-19) [147217-73-0] YDFQHBRKURQGAH-UHFFFAOYSA-N	3.6×10^{-1}	7400	Long et al. (2017)	Q	288
2,3,3'-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-20) [147217-76-3] RQJUBSPXDSGLRB-UHFFFAOYSA-N	1.8×10^{-1}	7400	Long et al. (2017)	Q	288
2,3,4-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-21) [337513-67-4] RXWRVYYPLRPDOS-UHFFFAOYSA-N	1.0×10^{-1}	7400	Long et al. (2017)	Q	288
2,3,4'-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-22) [446254-15-5] WZHNIFQVNBINLF-UHFFFAOYSA-N	1.2×10^{-1}	7400	Long et al. (2017)	Q	288
2,3,5-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-23) [446254-16-6] XQHLKDAUZRXBGC-UHFFFAOYSA-N	2.3×10^{-1}	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,6-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-24) [218304-36-0] GFLRHBRMAZDOIG-UHFFFAOYSA-N	1.8×10^{-1}	7400	Long et al. (2017)	Q	288
2,3',4-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-25) [147217-77-4] AURKEOPYVUYTLO-UHFFFAOYSA-N	2.3×10^{-1}	7400	Long et al. (2017)	Q	288
2,3',5-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-26) [337513-75-4] VUOBKVBAFJQQDB-UHFFFAOYSA-N	2.5×10^{-1}	7400	Long et al. (2017)	Q	288
2,3',6-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-27) [337513-53-8] JUPZALSVNWJHII-UHFFFAOYSA-N	3.4×10^{-1}	7400	Long et al. (2017)	Q	288
2,4,4'-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-28) [41318-75-6] UPNBETHEXPIWQX-UHFFFAOYSA-N	1.6×10^{-1} 1.1×10^{-1} 7.7×10^{-2} 1.8×10^{-1} 1.2×10^{-1} 2.0×10^{-1} 5.2×10^{-1} 1.8×10^{-1} 1.4×10^{-1}	8100 7400 12000 7400 	Long et al. (2017) Lau et al. (2006) Lau et al. (2006) Cetin and Odabasi (2005) Charles and Destaillats (2005) Tittlemier et al. (2002) Wania and Dugani (2003) Long et al. (2017) Hilal et al. (2008)	M M M M M V R Q Q	288 721 722 33 288
2,4,5-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-29) [337513-56-1] LTMKAFUXYKEDLR-UHFFFAOYSA-N	1.6×10^{-1}	7400	Long et al. (2017)	Q	288
2,4,6-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-30) [155999-95-4] TVZAPPGLBLTACB-UHFFFAOYSA-N	3.4×10^{-1}	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4',5-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-31) [65075-08-3] PURZBWMLFRWRMG-UHFFFAOYSA-N	1.9×10^{-1}	7400	Long et al. (2017)	Q	288
2,4',6-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-32) [189084-60-4] TYDVYKIQSZGUMV-UHFFFAOYSA-N	1.6×10^{-1}	7400	Long et al. (2017)	Q	288
2,3',4'-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-33) [49690-94-0] BUQBQEYUVAKJQK-UHFFFAOYSA-N	1.3×10^{-1}	7400	Long et al. (2017)	Q	288
2,3',5'-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-34) [446254-17-7] XMNXHCHZIPYCNA-UHFFFAOYSA-N	4.2×10^{-1}	7400	Long et al. (2017)	Q	288
3,3',4-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-35) [147217-80-9] CDVYKQPKJYPWRO-UHFFFAOYSA-N	1.2×10^{-1}	7400	Long et al. (2017)	Q	288
3,3',5-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-36) [147217-79-6] XUKPJLVONRTECE-UHFFFAOYSA-N	2.8×10^{-1}	7400	Long et al. (2017)	Q	288
3,4,4'-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-37) [147217-81-0] YALAYFVVZFORPV-UHFFFAOYSA-N	9.0×10^{-2}	7400	Long et al. (2017)	Q	288
3,4,5-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-38) [337513-54-9] DPGVQKLGQZZLMI-UHFFFAOYSA-N	9.9×10^{-2}	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4',5-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-39) [407606-57-9] UFFNOPDHJNQYKD-UHFFFAOYSA-N	2.0×10^{-1}	7400	Long et al. (2017)	Q	288
2,2',3,3'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-40) [337513-77-6] SXSUUFZWSVMTRL-UHFFFAOYSA-N	4.8×10^{-1}	7400	Long et al. (2017)	Q	288
2,2',3,4-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-41) [337513-68-5] UAEBSKBXZAIRMX-UHFFFAOYSA-N	3.2×10^{-1}	7400	Long et al. (2017)	Q	288
2,2',3,4'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-42) [446254-18-8] HQDQKPAHIDGGMH-UHFFFAOYSA-N	5.2×10^{-1}	7400	Long et al. (2017)	Q	288
2,2',3,5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-43) [446254-19-9] LKMQHSYDVDIECC-UHFFFAOYSA-N	6.6×10^{-1}	7400	Long et al. (2017)	Q	288
2,2',3,5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-44) [446254-20-2] VBGBGTYMDIVKNK-UHFFFAOYSA-N	5.7×10^{-1}	7400	Long et al. (2017)	Q	288
2,2',3,6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-45) [446254-21-3] VTFWUBIOZQCMQS-UHFFFAOYSA-N	7.3×10^{-1}	7400	Long et al. (2017)	Q	288
2,2',3,6'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-46) [446254-22-4] GBUUKJRFSKCMTB-UHFFFAOYSA-N	1.1	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',4,4'-tetrabromodiphenyl ether	9.1×10^{-1}	7400	Long et al. (2017)	M	288
$C_{12}H_6Br_4O$	1.6×10^{-1}		Lau et al. (2006)	M	721
(PBDE-47)	1.7×10^{-1}		Lau et al. (2006)	M	722
[5436-43-1]	8.7×10^{-1}	7300	Cetin and Odabasi (2005)	M	
XYBSIYMGXVUVGY-UHFFFAOYSA-N	1.7×10^{-1}	620	Charles and Destaillats (2005)	M	42
	9.3×10^{-1}		Kuramochi et al. (2014)	V	
	6.7×10^{-1}		Tittlemier et al. (2002)	V	
	9.0×10^{-1}		Wania and Dugani (2003)	R	
	8.5×10^{-1}	7400	Long et al. (2017)	Q	288
	2.2×10^{-1}		Hilal et al. (2008)	Q	
2,2',4,5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-48) [337513-55-0] FJGDNHOVDFREMP-UHFFFAOYSA-N	4.8×10^{-1}	7400	Long et al. (2017)	Q	288
2,2',4,5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-49) [243982-82-3] QWVDUBDYUPHNHY-UHFFFAOYSA-N	8.6×10^{-1}	7400	Long et al. (2017)	Q	288
2,2',4,6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-50) [446254-23-5] FXUAKFRJBKFDSY-UHFFFAOYSA-N	1.1	7400	Long et al. (2017)	Q	288
2,2',4,6'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-51) [189084-57-9] WKBBBTLDLKYGBI-UHFFFAOYSA-N	1.3	7400	Long et al. (2017)	Q	288
2,2',5,5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-52) [446254-24-6] CDTHXJORUCZHMD-UHFFFAOYSA-N	8.9×10^{-1}	7400	Long et al. (2017)	Q	288
2,2',5,6'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-53) [446254-25-7] SDVQGIMOFXMKHR-UHFFFAOYSA-N	1.4	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',6,6'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-54) [446254-26-8] WCDCHQGVTZHVSO-UHFFFAOYSA-N	1.7	7400	Long et al. (2017)	Q	288
2,3,3',4-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-55) [446254-27-9] VIHUMJGEWQPWOT-UHFFFAOYSA-N	3.0×10^{-1}	7400	Long et al. (2017)	Q	288
2,3,3',4'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-56) [446254-28-0] NFOIVCGFYJIYIB-UHFFFAOYSA-N	2.8×10^{-1}	7400	Long et al. (2017)	Q	288
2,3,3',5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-57) [337513-82-3] CSIFWDKYUJLQEB-UHFFFAOYSA-N	6.2×10^{-1}	7400	Long et al. (2017)	Q	288
2,3,3',5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-58) [446254-29-1] SWOYBZHGPZIRHS-UHFFFAOYSA-N	1.3	7400	Long et al. (2017)	Q	288
2,3,3',6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-59) [446254-30-4] DMAMJZQQOWYEHT-UHFFFAOYSA-N	6.5×10^{-1}	7400	Long et al. (2017)	Q	288
2,3,4,4'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-60) [446254-31-5] ARERIMFZYPFJAV-UHFFFAOYSA-N	2.3×10^{-1}	7400	Long et al. (2017)	Q	288
2,3,4,5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-61) [446254-32-6] NDRSXNBQWAOQPP-UHFFFAOYSA-N	3.2×10^{-1}	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4,6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-62) [446254-33-7] YIQYWYZZLOZVRM-UHFFFAOYSA-N	5.5×10^{-1}	7400	Long et al. (2017)	Q	288
2,3,4',5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-63) [446254-34-8] HNICYXFGCWPYGC-UHFFFAOYSA-N	5.0×10^{-1}	7400	Long et al. (2017)	Q	288
2,3,4',6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-64) [446254-35-9] LDCXVFJUWKKBNY-UHFFFAOYSA-N	3.3×10^{-1}	7400	Long et al. (2017)	Q	288
2,3,5,6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-65) [446254-36-0] HPEUYVBOPJQVPN-UHFFFAOYSA-N	4.8×10^{-1}	7400	Long et al. (2017)	Q	288
2,3',4,4'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-66) [189084-61-5] DHUMTYRHKMCVAG-UHFFFAOYSA-N	2.0 4.7×10^{-1}	7400	Tittlemier et al. (2002) Long et al. (2017)	V Q	288
2,3',4,5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-67) [446254-37-1] OARGWSONVLGXQA-UHFFFAOYSA-N	4.7×10^{-1}	7400	Long et al. (2017)	Q	288
2,3',4,5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-68) [446254-38-2] UFWGRLCUOLLWAO-UHFFFAOYSA-N	1.6	7400	Long et al. (2017)	Q	288
2,3',4,6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-69) [327185-09-1] NHZNRCYNZJADTG-UHFFFAOYSA-N	9.8×10^{-1}	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3',4',5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-70) [446254-39-3] GHQMTYWQVJZWAR-UHFFFAOYSA-N	5.2×10^{-1}	7400	Long et al. (2017)	Q	288
2,3',4',6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-71) [189084-62-6] COPAGYRSCJVION-UHFFFAOYSA-N	5.2×10^{-1}	7400	Long et al. (2017)	Q	288
2,3',5,5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-72) [446254-40-6] GBBNZKQTOOZGIS-UHFFFAOYSA-N	9.6×10^{-1}	7400	Long et al. (2017)	Q	288
2,3',5',6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-73) [446254-41-7] WQFLVWXBCRJAQN-UHFFFAOYSA-N	1.7	7400	Long et al. (2017)	Q	288
2,4,4',5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-74) [446254-42-8] LXCFDVVDUVPAGR-UHFFFAOYSA-N	3.9×10^{-1}	7400	Long et al. (2017)	Q	288
2,4,4',6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-75) [189084-63-7] BWCNKMFFUGBFGB-UHFFFAOYSA-N	6.3×10^{-1}	7400	Long et al. (2017)	Q	288
2,3',4',5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-76) [446254-43-9] NCSWBJSFVPJPPK-UHFFFAOYSA-N	4.7×10^{-1}	7400	Long et al. (2017)	Q	288
3,3',4,4'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-77) [93703-48-1] RYGLOWMCGZHYRQ-UHFFFAOYSA-N	8.3×10^{-1} 2.3×10^{-1}	7400	Tittlemier et al. (2002) Long et al. (2017)	V Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3',4,5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-78) [446254-45-1] HWOBLTZZSVXBOJ-UHFFFAOYSA-N	2.9×10^{-1}	7400	Long et al. (2017)	Q	288
3,3',4,5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-79) [446254-48-4] LELQGHJEUVRPEV-UHFFFAOYSA-N	4.7×10^{-1}	7400	Long et al. (2017)	Q	288
3,3',5,5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-80) [103173-66-6] HFIOZJQRZKNPKJ-UHFFFAOYSA-N	1.1	7400	Long et al. (2017)	Q	288
3,4,4',5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-81) [446254-50-8] ULFOIXCXIWHJDS-UHFFFAOYSA-N	2.4×10^{-1}	7400	Long et al. (2017)	Q	288
2,2',3,3',4-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-82) [327185-11-5] RQMSPGJESCCPQX-UHFFFAOYSA-N	7.1×10^{-1}	7400	Long et al. (2017)	Q	288
2,2',3,3',5-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-83) [446254-51-9] XAHYSNUYJLNDBX-UHFFFAOYSA-N	1.4	7400	Long et al. (2017)	Q	288
2,2',3,3',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-84) [446254-52-0] PPIZNRAVQHNLJM-UHFFFAOYSA-N	1.8	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,4'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-85) [182346-21-0] DMLQSUZPTTUUDP-UHFFFAOYSA-N	9.1		Tittlemier et al. (2002)	V	
	1.3	7400	Long et al. (2017)	Q	288
2,2',3,4,5-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-86) [446254-53-1] YMVWYUWOUOQCQP-UHFFFAOYSA-N	9.2×10^{-1}	7400	Long et al. (2017)	Q	288
2,2',3,4,5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-87) [446254-54-2] WKYQUGCIKNOXFW-UHFFFAOYSA-N	1.1×10^{2}	7400	Long et al. (2017)	Q	288
2,2',3,4,6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-88) [446254-55-3] OPZUHBCVIZNZFB-UHFFFAOYSA-N	1.2	7400	Long et al. (2017)	Q	288
2,2',3,4,6'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-89) [446254-56-4] XGFLJLJXVIMCNR-UHFFFAOYSA-N	1.8	7400	Long et al. (2017)	Q	288
2,2',3,4',5-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-90) [446254-57-5] BATFXMGTVIESIQ-UHFFFAOYSA-N	2.3	7400	Long et al. (2017)	Q	288
2,2',3,4',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-91) [446254-58-6] HWNJTZKDPNZUSO-UHFFFAOYSA-N	1.7	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,5,5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-92) [446254-59-7] QWSQOVAGRDRZLM-UHFFFAOYSA-N	1.9	7400	Long et al. (2017)	Q	288
2,2',3,5,6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-93) [446254-60-0] BRTPVPJQMWLDNO-UHFFFAOYSA-N	1.5	7400	Long et al. (2017)	Q	288
2,2',3,5,6'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-94) [446254-61-1] JOPASNJHCFYVHD-UHFFFAOYSA-N	3.8	7400	Long et al. (2017)	Q	288
2,2',3,5',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-95) [446254-62-2] BZDYRALIEYVMEP-UHFFFAOYSA-N	1.8	7400	Long et al. (2017)	Q	288
2,2',3,6,6'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-96) [446254-63-3] ZFCJNRDWGBZUED-UHFFFAOYSA-N	3.9	7400	Long et al. (2017)	Q	288
2,2',3,4',5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-97) [446254-64-4] MAGYDGJRSCULJL-UHFFFAOYSA-N	1.0	7400	Long et al. (2017)	Q	288
2,2',3,4',6'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-98) [38463-82-0] OCLWEJVGAUFXQU-UHFFFAOYSA-N	3.5	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',4,4',5-pentabromodiphenyl ether	1.5	8900	Long et al. (2017)	M	288
$C_{12}H_5Br_5O$	6.2×10^{-1}		Lau et al. (2006)	M	721
(PBDE-99)	3.3×10^{-1}		Lau et al. (2006)	M	722
[60348-60-9]	1.5	8800	Cetin and Odabasi (2005)	M	
WHPVYXDFIXRKLN-UHFFFAOYSA-N	2.7×10^{-1}	-6700	Charles and Destaillats (2005)	M	42
	2.1		Kuramochi et al. (2014)	V	
	4.3		Tittlemier et al. (2002)	V	
	1.9		Wania and Dugani (2003)	R	
	1.6	7400	Long et al. (2017)	Q	288
	8.4		Zhang et al. (2010)	Q	288, 289
	3.7		Zhang et al. (2010)	Q	288, 290
	1.2×10^{2}		Zhang et al. (2010)	Q	288, 291
	2.4×10^{1}		Zhang et al. (2010)	Q	288, 292
	4.3×10^{-1}		Hilal et al. (2008)	Q	
2,2',4,4',6-pentabromodiphenyl ether	3.6	7300	Long et al. (2017)	M	288
$C_{12}H_5Br_5O$	3.3×10^{-1}		Lau et al. (2006)	M	721
(PBDE-100)	3.2×10^{-1}		Lau et al. (2006)	M	722
[189084-64-8]	3.8	6800	Cetin and Odabasi (2005)	M	
NSKIRYMHNFTRLR-UHFFFAOYSA-N	1.9×10^{-1}	12	Charles and Destaillats (2005)	M	42
	1.4×10^{1}		Tittlemier et al. (2002)	V	
	2.6		Wania and Dugani (2003)	R	
	3.9	7400	Long et al. (2017)	Q	288
	3.7×10^{-1}		Hilal et al. (2008)	Q	
2,2',4,5,5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-101) [446254-65-5] QUZWDWNIWWAQDI-UHFFFAOYSA-N	1.4	7400	Long et al. (2017)	Q	288
2,2',4,5,6'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-102) [446254-66-6] JHFMCUVMAIQWRI-UHFFFAOYSA-N	2.8	7400	Long et al. (2017)	Q	288
2,2',4,5',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-103) [446254-67-7] RJEMKRNASVHYKR-UHFFFAOYSA-N	3.4	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',4,6,6'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-104) [446254-68-8] CRSCWEYUPUKHPI-UHFFFAOYSA-N	6.7	7400	Long et al. (2017)	Q	288
2,3,3',4,4'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-105) [373594-78-6] LBPWAGZGYNOKAM-UHFFFAOYSA-N	6.1×10^{-1}	7400	Long et al. (2017)	Q	288
2,3,3',4,5-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-106) [446254-69-9] KLQKWMYXEWUAFP-UHFFFAOYSA-N	8.5×10^{-1}	7400	Long et al. (2017)	Q	288
2,3,3',4',5-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-107) [446254-70-2] OMGVAMFMRSETEG-UHFFFAOYSA-N	1.9	7400	Long et al. (2017)	Q	288
2,3,3',4,5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-108) [446254-71-3] VBKPKHVLHGOKOJ-UHFFFAOYSA-N	2.0	7400	Long et al. (2017)	Q	288
2,3,3',4,6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-109) [446254-72-4] FXXXWTMLIQLDRP-UHFFFAOYSA-N	1.2	7400	Long et al. (2017)	Q	288
2,3,3',4',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-110) [446254-73-5] LESZGJVTZILBTK-UHFFFAOYSA-N	9.4×10^{-1}	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',5,5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-111) [446254-74-6] PCHDCOXHJBWEPW-UHFFFAOYSA-N	2.1	7400	Long et al. (2017)	Q	288
2,3,3',5,6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-112) [446254-75-7] MFBMNSFADPTAKZ-UHFFFAOYSA-N	1.7	7400	Long et al. (2017)	Q	288
2,3,3',5',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-113) [446254-76-8] OGZHLJXRGZFVLI-UHFFFAOYSA-N	3.1	7400	Long et al. (2017)	Q	288
2,3,4,4',5-pentabromodiphenyl ether	6.2×10^{-1}		Lau et al. (2006)	M	721
$C_{12}H_5Br_5O$	7.7×10^{-1}		Lau et al. (2006)	M	722
(PBDE-114)	8.8×10^{-1}	4000	Charles and Destaillats (2005)	M	42
[446254-77-9]	7.5×10^{-1}	7400	Long et al. (2017)	Q	288
SFNAUTSNWPPDSY-UHFFFAOYSA-N					
2,3,4,4',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-115) [446254-78-0] BKTLDVXDOVSTEV-UHFFFAOYSA-N	9.8×10^{-1}	7400	Long et al. (2017)	Q	288
2,3,4,5,6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-116) [189084-65-9] ACRQLFSHISNWRY-UHFFFAOYSA-N	6.1×10^{-1}	7400	Long et al. (2017)	Q	288
2,3,4',5,6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-117) [446254-79-1] SOJBOGWFDBDWEG-UHFFFAOYSA-N	8.6×10^{-1}	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3',4,4',5-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-118) [446254-80-4] VTMFEPLDDHZBGI-UHFFFAOYSA-N	9.2×10^{-1}	7400	Long et al. (2017)	Q	288
2,3',4,4',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-119) [189084-66-0] KXEOYBYEJCRPGB-UHFFFAOYSA-N	1.8	7400	Long et al. (2017)	Q	288
2,3',4,5,5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-120) [417727-71-0] AKSBEUHDCRZJAN-UHFFFAOYSA-N	1.7	7400	Long et al. (2017)	Q	288
2,3',4,5',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-121) [446254-81-5] GVGNVZBJVFDAAO-UHFFFAOYSA-N	5.9	7400	Long et al. (2017)	Q	288
2,3,3',4',5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-122) [446254-82-6] CDNHGSPFIUITTN-UHFFFAOYSA-N	7.2×10^{-1}	7400	Long et al. (2017)	Q	288
2,3',4,4',5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-123) [446254-83-7] SBKMUEQNZNDYFW-UHFFFAOYSA-N	1.2	7400	Long et al. (2017)	Q	288
2,3',4',5,5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-124) [446254-84-8] FGHJTAAHIFEHLT-UHFFFAOYSA-N	1.1	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3',4',5',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-125) [446254-85-9] SESXKFPOVUVGLR-UHFFFAOYSA-N	1.3	7400	Long et al. (2017)	Q	288
3,3',4,4',5-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-126) [366791-32-4] SJNIIWPIAVQNRK-UHFFFAOYSA-N	5.6×10^{-1}	7400	Long et al. (2017)	Q	288
3,3',4,5,5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-127) [446254-86-0] RATMRXKBPDCKCZ-UHFFFAOYSA-N	1.1	7400	Long et al. (2017)	Q	288
2,2',3,3',4,4'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-128) [182677-28-7] WFLVELCLEGVBIH-UHFFFAOYSA-N	2.1	7400	Long et al. (2017)	Q	288
2,2',3,3',4,5-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-129) [446254-87-1] PRNCVYAUCSGSOE-UHFFFAOYSA-N	1.9	7400	Long et al. (2017)	Q	288
2,2',3,3',4,5'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-130) [446254-88-2] YURCHLXPAGSJHU-UHFFFAOYSA-N	3.7	7400	Long et al. (2017)	Q	288
2,2',3,3',4,6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-131) [446254-89-3] MGKVPJFIGGBCBA-UHFFFAOYSA-N	1.0×10^{1}	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-132) [446254-90-6] FFEKBOKDYRZGRV-UHFFFAOYSA-N	4.0	7400	Long et al. (2017)	Q	288
2,2',3,3',5,5'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-133) [446254-91-7] XTBFPFHQPGZZJX-UHFFFAOYSA-N	6.3	7400	Long et al. (2017)	Q	288
2,2',3,3',5,6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-134) [446254-92-8] MIBDGPWSGDWIQR-UHFFFAOYSA-N	4.8	7400	Long et al. (2017)	Q	288
2,2',3,3',5,6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-135) [446254-93-9] AMGHASDTWACNCS-UHFFFAOYSA-N	8.6	7400	Long et al. (2017)	Q	288
2,2',3,3',6,6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-136) [446254-94-0] NTWGDSLWLUPCDW-UHFFFAOYSA-N	7.8	7400	Long et al. (2017)	Q	288
2,2',3,4,4',5-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-137) [446254-95-1] HSTYYNPYXZYIAG-UHFFFAOYSA-N	3.0	7400	Long et al. (2017)	Q	288
2,2',3,4,4',5'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-138) [182677-30-1] IZFQCEZFGCMHOM-UHFFFAOYSA-N	2.7	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,4',6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-140) [243982-83-4] FLRODCDHJZNIGA-UHFFFAOYSA-N	7.7	7400	Long et al. (2017)	Q	288
2,2',3,4,5,5'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-141) [446254-97-3] XTXIYMGRRUJOIT-UHFFFAOYSA-N	2.6	7400	Long et al. (2017)	Q	288
2,2',3,4,5,6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-142) [446254-98-4] LJDGJCNHVGGOFW-UHFFFAOYSA-N	1.4	7400	Long et al. (2017)	Q	288
2,2',3,4,5,6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-143) [446254-99-5] RQLZDUSZXOOBTM-UHFFFAOYSA-N	5.1	7400	Long et al. (2017)	Q	288
2,2',3,4,5',6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-144) [446255-00-1] ZMSJCQOCTPYCQP-UHFFFAOYSA-N	5.2	7400	Long et al. (2017)	Q	288
2,2',3,4,6,6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-145) [446255-01-2] BTKLHMBWCRVCLC-UHFFFAOYSA-N	1.0×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,4',5,5'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-146) [446255-02-3] HGXPYDNHBUCRTR-UHFFFAOYSA-N	5.3	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4',5,6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-147) [116995-33-6] OWBKWMDBTWHGHS-UHFFFAOYSA-N	5.1	7400	Long et al. (2017)	Q	288
2,2',3,4',5,6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-148) [446255-03-4] OJMHGSMSQZEBFH-UHFFFAOYSA-N	1.2×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,4',5',6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-149) [446255-04-5] UJOUSZKYGGTPFQ-UHFFFAOYSA-N	5.1	7400	Long et al. (2017)	Q	288
2,2',3,4',6,6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-150) [446255-05-6] SQNOZOVDXXSLSG-UHFFFAOYSA-N	1.7×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,5,5',6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-151) [446255-06-7] NGOQQUYCSISZMY-UHFFFAOYSA-N	4.4	7400	Long et al. (2017)	Q	288
2,2',3,5,6,6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-152) [446255-07-8] BYBJJARTBKUIJD-UHFFFAOYSA-N	9.4	7400	Long et al. (2017)	Q	288
2,2',4,4',5,5'-hexabromodiphenyl ether	3.7	7200	Long et al. (2017)	M	288
$C_{12}H_4Br_6O$	3.5	7800	Cetin and Odabasi (2005)	M	
(PBDE-153)	6.1		Kuramochi et al. (2014)	V	
[68631-49-2]	1.5×10^{1}		Tittlemier et al. (2002)	V	
RZXIRSKYBISPGF-UHFFFAOYSA-N	2.9		Wania and Dugani (2003)	R	
	3.9	7400	Long et al. (2017)	Q	288
	8.4×10^{-1}		Hilal et al. (2008)	Q	

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',4,4',5,6'-hexabromodiphenyl ether	7.1	6800	Long et al. (2017)	M	288
$C_{12}H_4Br_6O$	7.3	6800	Cetin and Odabasi (2005)	M	
(PBDE-154)	4.2		Tittlemier et al. (2002)	V	
[207122-15-4]	1.1×10^{1}	7400	Long et al. (2017)	Q	288
VHNPZYZQKWIWOD-UHFFFAOYSA-N	7.2×10^{-1}		Hilal et al. (2008)	Q	
2,2',4,4',6,6'-hexabromodiphenyl ether	2.5×10^{1}	7400	Long et al. (2017)	Q	288
$C_{12}H_4Br_6O$					
(PBDE-155)					
[35854-94-5]					
HRSCBOSGEKXXSI-UHFFFAOYSA-N					
2,3,3',4,4',5-hexabromodiphenyl ether	1.5	7400	Long et al. (2017)	Q	288
$C_{12}H_4Br_6O$					
(PBDE-156)					
[405237-85-6]					
JSDPCMJWYRDQEV-UHFFFAOYSA-N					
2,3,3',4,4',5'-hexabromodiphenyl ether	1.9	7400	Long et al. (2017)	Q	288
$C_{12}H_4Br_6O$					
(PBDE-157)					
[446255-08-9]					
JUOAMVUIJQJZSZ-UHFFFAOYSA-N					
2,3,3',4,4',6-hexabromodiphenyl ether	2.7	7400	Long et al. (2017)	Q	288
$C_{12}H_4Br_6O$					
(PBDE-158)					
[446255-09-0]					
KRYHHTVQOOJNHQ-UHFFFAOYSA-N					
2,3,3',4,5,5'-hexabromodiphenyl ether	3.0	7400	Long et al. (2017)	Q	288
$C_{12}H_4Br_6O$					
(PBDE-159)					
[446255-10-3]					
IDYFFNCFLRCOPZ-UHFFFAOYSA-N					
2,3,3',4,5,6-hexabromodiphenyl ether	2.8	7400	Long et al. (2017)	Q	288
$C_{12}H_4Br_6O$					
(PBDE-160)					
[446255-11-4]					
OCVOYHGOXIIONK-UHFFFAOYSA-N					

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',4,5',6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-161) [446255-12-5] WEYWRBBPPKSRGU-UHFFFAOYSA-N	9.0	7400	Long et al. (2017)	Q	288
2,3,3',4',5,5'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-162) [446255-13-6] UKPNCLHMNJCGCJ-UHFFFAOYSA-N	2.7	7400	Long et al. (2017)	Q	288
2,3,3',4',5,6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-163) [446255-14-7] NUEAHMLXQFHEJN-UHFFFAOYSA-N	2.3	7400	Long et al. (2017)	Q	288
2,3,3',4',5',6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-164) [446255-15-8] UJVYVXIHTJOJBZ-UHFFFAOYSA-N	3.1	7400	Long et al. (2017)	Q	288
2,3,3',5,5',6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-165) [446255-16-9] KXERERDGMTWBGZ-UHFFFAOYSA-N	7.9	7400	Long et al. (2017)	Q	288
2,3,4,4',5,6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-166) [189084-58-0] KVYODBMKQYVNEK-UHFFFAOYSA-N	1.2	7400	Long et al. (2017)	Q	288
2,3',4,4',5,5'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-167) [446255-17-0] NMUPLZRHSXJCJQ-UHFFFAOYSA-N	3.1	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3',4,4',5',6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-168) [53551-87-4] HWZAPXGFMVEGPW-UHFFFAOYSA-N	5.0	7400	Long et al. (2017)	Q	288
3,3',4,4',5,5'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-169) [446255-18-1] JKFBMDHBJYKFKL-UHFFFAOYSA-N	1.2	7400	Long et al. (2017)	Q	288
2,2',3,3',4,4',5-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-170) [327185-13-7] DLPNCMQTNWLTHD-UHFFFAOYSA-N	4.9	7400	Long et al. (2017)	Q	288
2,2',3,3',4,4',6-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-171) [446255-19-2] FRMMMROUUPQUMZ-UHFFFAOYSA-N	1.2×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,3',4,5,5'-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-172) [407606-59-1] DSRRSKFMOJQETR-UHFFFAOYSA-N	1.6×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,3',4,5,6-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-173) [446255-20-5] NLBLNZDNOSSGPW-UHFFFAOYSA-N	6.7	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,5,6'- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-174) [446255-21-6] VUUWOHUOYUGBEO-UHFFFAOYSA-N	1.2×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,3',4,5',6- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-175) [6255-22-7] YATZWTXATDYQCK-UHFFFAOYSA-N	1.7×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,3',4,6,6'- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-176) [407606-61-5] SWUALKCOTZOSMY-UHFFFAOYSA-N	2.5×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,3',4,5',6'- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-177) [446255-23-8] ZHUHLPXIJIBQBJ-UHFFFAOYSA-N	9.9	7400	Long et al. (2017)	Q	288
2,2',3,3',5,5',6- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-178) [446255-24-9] UWUVZUPEEORCRG-UHFFFAOYSA-N	1.3×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,3',5,6,6'- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-179) [446255-25-0] COVXWWKOLMNRQE-UHFFFAOYSA-N	2.2×10^{1}	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,4',5,5'- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-180) [446255-26-1] STMBXVOJNOJRPZ-UHFFFAOYSA-N	7.3	7400	Long et al. (2017)	Q	288
2,2',3,4,4',5,6- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-181) [189084-67-1] GVNRIAPLVGNZPL-UHFFFAOYSA-N	8.9	7400	Long et al. (2017)	Q	288
2,2',3,4,4',5,6'- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-182) [442690-45-1] ZYHDTADADSNMLV-UHFFFAOYSA-N	1.9×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,4,4',5',6- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-183) [207122-16-5] ILPSCQCLBHQUEM-UHFFFAOYSA-N	1.4×10^{2} 1.3×10^{1}	 7400	Tittlemier et al. (2002) Long et al. (2017)	V Q	 288
2,2',3,4,4',6,6'- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-184) [117948-63-7] JHDCZVAQPRXHEL-UHFFFAOYSA-N	3.7×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,4,5,5',6- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-185) [405237-86-7] YRNMIFAQDSUFTR-UHFFFAOYSA-N	5.1	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,5,6,6'- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-186) [446255-27-2] WUFQDCMRKKDNSF-UHFFFAOYSA-N	1.4×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,4',5,5',6- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-187) [446255-28-3] RFZPXOBFDARWHV-UHFFFAOYSA-N	9.4	7400	Long et al. (2017)	Q	288
2,2',3,4',5,6,6'- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-188) [116995-32-5] YGYDHFDPVGAMTL-UHFFFAOYSA-N	3.5×10^{1}	7400	Long et al. (2017)	Q	288
2,3,3',4,4',5,5'- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-189) [259087-35-9] CQVLRTUESBMMJW-UHFFFAOYSA-N	4.4	7400	Long et al. (2017)	Q	288
2,3,3',4,4',5,6- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-190) [189084-68-2] OUEYHQIMJGHOQN-UHFFFAOYSA-N	4.0	7400	Long et al. (2017)	Q	288
2,3,3',4,4',5',6- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-191) [446255-30-7] BNBFKFHSIPERIM-UHFFFAOYSA-N	8.4	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',4,5,5',6-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-192) [407578-53-4] ABLZOLAUBUSUHT-UHFFFAOYSA-N	1.3×10^{1}	7400	Long et al. (2017)	Q	288
2,3,3',4',5,5',6-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-193) [446255-34-1] AUFJSWANTKXCFZ-UHFFFAOYSA-N	7.3	7400	Long et al. (2017)	Q	288
2,2',3,3',4,4',5,5'-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-194) [32536-52-0] ORYGKUIDIMIRNN-UHFFFAOYSA-N	1.3×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,3',4,4',5,6-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-195) [446255-38-5] GPQLSLKPHQEEOP-UHFFFAOYSA-N	1.6×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,3',4,4',5,6'-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-196) [446255-39-6] IEWFKOVTVJNWFF-UHFFFAOYSA-N	3.7×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,3',4,4',6,6'-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-197) [117964-21-3] AAFUUKPTSPVXJH-UHFFFAOYSA-N	7.1×10^{1}	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,5,5',6-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-198) [446255-42-1] IBKRHVDFFHQOSC-UHFFFAOYSA-N	1.8×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,3',4,5,5',6'-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-199) [446255-43-2] JNSLJYRXDGBNBE-UHFFFAOYSA-N	3.3×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,3',4,5,6,6'-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-200) [446255-46-5] JWMXGEPFVCRXQR-UHFFFAOYSA-N	3.7×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,3',4,5',6,6'-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-201) [446255-50-1] HQWFMMKREWXIGN-UHFFFAOYSA-N	6.8×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,3',5,5',6,6'-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-202) [67797-09-5] AHNZLQAZTWRRDW-UHFFFAOYSA-N	5.7×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,4,4',5,5',6-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-203) [337513-72-1] RTUZOQFRIPIWPS-UHFFFAOYSA-N	2.0×10^{1}	7400	Long et al. (2017)	Q	288

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,4',5,6,6'-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-204) [446255-54-5] YZABCBOJTHQTSX-UHFFFAOYSA-N	6.2×10^{1}	7400	Long et al. (2017)	Q	288
2,3,3',4,4',5,5',6-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-205) [446255-56-7] CVMKCYDBEYHNBM-UHFFFAOYSA-N	1.8×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,3',4,4',5,5',6-nonabromodiphenyl ether $C_{12}HBr_9O$ (PBDE-206) [63387-28-0] CYRHBNRLQMLULE-UHFFFAOYSA-N	4.7×10^{1}	7400	Long et al. (2017)	Q	288
2,2',3,3',4,4',5,6,6'-nonabromodiphenyl ether $C_{12}HBr_9O$ (PBDE-207) [437701-79-6] IEEVDIAVLGLVOW-UHFFFAOYSA-N	1.2×10^{2}	7400	Long et al. (2017)	Q	288
2,2',3,3',4,5,5',6,6'-nonabromodiphenyl ether $C_{12}HBr_9O$ (PBDE-208) [437701-78-5] ASGZXYIDLFWXID-UHFFFAOYSA-N	1.1×10^{2}	7400	Long et al. (2017)	Q	288
decabromodiphenyl ether $C_{12}Br_{10}O$ (PBDE-209) [1163-19-5] WHHGLZMJPXIBIX-UHFFFAOYSA-N	1.8×10^{1}	7600	Long et al. (2017)	M	288
	1.8×10^{1}	7900	Cetin and Odabasi (2005)	M	
	2.7×10^{1}	7400	Long et al. (2017)	Q	288
	8.2×10^{2}		HSDB (2015)	Q	100
	8.2×10^{2}		Zhang et al. (2010)	Q	288, 289
	4.1×10^{2}		Zhang et al. (2010)	Q	288, 290
	1.3×10^{3}		Zhang et al. (2010)	Q	288, 291
	6.7×10^{2}		Zhang et al. (2010)	Q	288, 292

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dibromoacetonitrile C_2HBr_2N [3252-43-5] NDSBDLSWTGLNQA-UHFFFAOYSA-N	2.4×10^{1}		HSDB (2015)	Q	100
bromoacetonitrile C_2H_2BrN [590-17-0] REXUYBKPWIPONM-UHFFFAOYSA-N	2.8		HSDB (2015)	Q	449
2-bromopyridine C_5H_4BrN [109-04-6] IMRWILPUOVGIMU-UHFFFAOYSA-N	1.3 1.8×10^{-1}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
3-bromopyridine C_5H_4BrN [626-55-1] NYPYPOZNGOXYSU-UHFFFAOYSA-N	8.3×10^{-1}		Ebert et al. (2023)	?	317
1,2-dibromo-2,4-dicyanobutane $C_6H_6Br_2N_2$ [35691-65-7] DHVLDKHFGIVEIP-UHFFFAOYSA-N	1.2×10^{3}		HSDB (2015)	V	
4-bromobenzenamine C_6H_6BrN [106-40-1] WDFQBORIUYODSI-UHFFFAOYSA-N	1.1×10^{1}		HSDB (2015)	Q	449
2,4,6-tribromobenzenamine $C_6H_4Br_3N$ [147-82-0] GVPODVKBTHCGFU-UHFFFAOYSA-N	8.2×10^{1} 2.6 6.0×10^{-1} 1.2×10^{2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
N,N'-dimethyl-3,3',4,4',5,5'-hexabromo-2,2'-bipyrrole $C_{10}H_6Br_6N_2$ (DBP-Br6) [253798-63-9] BUKWTHPBLJVYMZ-UHFFFAOYSA-N	5.0×10^{2} 5.1×10^{1}		Tittlemier et al. (2004) Hilal et al. (2008)	V Q	
1,1'-ethylene 2,2'-dipyridylium dibromide $C_{12}H_{12}N_2Br$ (diquat dibromide) [85-00-7] JXEXEPZXXFNEHA-UHFFFAOYSA-M	7.0×10^{7}		HSDB (2015)	Q	100

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tralomethrin $C_{22}H_{19}NO_3Br_4$ [66841-25-6] YWSCPYYRJXKUDB-KAKFPZCNSA-N	2.5×10^{4} 2.5×10^{4} 1.2×10^{3}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
bromomethyl peroxynitrate $CH_2BrO_2NO_2$ JTAFUKGUWIYDNI-UHFFFAOYSA-N	3.5×10^{-1}		Krysztofiak et al. (2012)	Q	
dibromomethyl peroxynitrate $CHBr_2O_2NO_2$ CRBGJNSRTFAVGH-UHFFFAOYSA-N	3.0		Krysztofiak et al. (2012)	Q	
tribromomethyl peroxynitrate $CBr_3O_2NO_2$ BVMOLEXBJGZUAI-UHFFFAOYSA-N	4.0		Krysztofiak et al. (2012)	Q	
MCM:BRETPAN $C_2H_2NO_5Br$ OOFSXJVGALRPLK-UHFFFAOYSA-N	2.0×10^{1} 8.7×10^{1} 3.3×10^{-3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
2,2-dibromo-2-cyanoacetamide $C_3H_2Br_2N_2O$ (2,2-dibromo-3-nitrilopropionamide) [10222-01-2] UUIVKBHZENILKB-UHFFFAOYSA-N	5.2×10^{2} 5.2×10^{2} 8.5×10^{3}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
bronopol $C_3H_6BrNO_4$ [52-51-7] LVDKZNITIUWNER-UHFFFAOYSA-N	7.6×10^{5}		HSDB (2015)	V	
2,6-dibromo-4-nitroaniline $C_6H_4Br_2N_2O_2$ [827-94-1] YMZIFDLWYUSZCC-UHFFFAOYSA-N	8.2×10^{3} 1.7×10^{2} 1.9×10^{3} 5.7×10^{3}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
2-bromo-4,6-dinitroaniline $C_6H_4BrN_3O_4$ [1817-73-8] KWMDHCLJYMVBNS-UHFFFAOYSA-N	3.9×10^{4} 2.7×10^{2} 1.8×10^{3} 5.7×10^{4}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
3-bromonitrobenzene $C_6H_4BrNO_2$ (*m*-bromonitrobenzene) [585-79-5] FWIROFMBWVMWLB-UHFFFAOYSA-N	5.3 5.4 1.8		Duchowicz et al. (2020) Schüürmann (2000) Duchowicz et al. (2020)	V V Q	187

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-bromonitrobenzene $C_6H_4BrNO_2$ (*p*-bromonitrobenzene) [586-78-7] ZDFBKZUDCQQKAC-UHFFFAOYSA-N	2.2×10^{-1}		Li et al. (2014)	Q	242
3,5-dibromo-4-hydroxy-benzonitrile	7.4×10^{2}		Mackay et al. (2006d)	V	
$C_7H_3Br_2NO$	1.0×10^{6}		Maniere et al. (2011)	?	242, 575, 166
(bromoxynil)	2.2×10^{3}		Maniere et al. (2011)	?	242, 579, 166
[1689-84-5]	1.1×10^{6}		Maniere et al. (2011)	?	242, 495, 166
UPMXNNIRAGDFEH-UHFFFAOYSA-N					
2,6-dibromo-3-methyl-4-nitroanisole	4.5×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_8H_7Br_2NO_3$	3.5×10^{1}		Zhang et al. (2010)	Q	288, 290
[62265-99-0]	4.7		Zhang et al. (2010)	Q	288, 291
RBAJFFLBHVZCDY-UHFFFAOYSA-N	9.7		Zhang et al. (2010)	Q	288, 292
bromacil	7.6×10^{4}		HSDB (2015)	V	
$C_9H_{13}BrN_2O_2$	7.8×10^{4}		Mackay et al. (2006d)	V	
[314-40-9]	5.3×10^{2}		Suntio et al. (1988)	V	12
CTSLUCNDVMMDHG-UHFFFAOYSA-N	5.2		Barcelo and Hennion (1997)	X	569
	2.1×10^{1}		Goodarzi et al. (2010)	Q	570
N'-(4-bromophenyl)-N-methoxy-N-methylurea	3.2×10^{3}		HSDB (2015)	V	
$C_9H_{11}BrN_2O$	3.2×10^{3}		Mackay et al. (2006d)	V	
(metobromuron)	3.2×10^{1}		Barcelo and Hennion (1997)	X	569
[3060-89-7]	8.5		Goodarzi et al. (2010)	Q	570
WLFDQEVORAMCIM-UHFFFAOYSA-N	8.8×10^{3}		Maniere et al. (2011)	?	12, 166
bromuron $C_9H_{11}BrN_2O$ [3408-97-7] GSNZNZUNAJCHDO-UHFFFAOYSA-N	2.0×10^{4}		MacBean (2012a)	?	
bromoxynil butyrate $C_{11}H_9Br_2NO_2$ [3861-41-4] PGMZYNZXIYOOHJ-UHFFFAOYSA-N	5.6×10^{1}		Maniere et al. (2011)	?	12, 166

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tris(2,3-dibromopropyl)isocyanurate	8.2×10^{12}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_{15}Br_6N_3O_3$	6.5×10^{7}		Zhang et al. (2010)	Q	288, 290
[52434-90-9]	2.7×10^{8}		Zhang et al. (2010)	Q	288, 291
NZUPFZNVGSWLQC-UHFFFAOYSA-N	1.2×10^{10}		Zhang et al. (2010)	Q	288, 292
bromofenoxim	3.1×10^{-3}		Barcelo and Hennion (1997)	X	569
$C_{13}H_7Br_2N_3O_6$	8.1×10^{-4}		Goodarzi et al. (2010)	Q	570, 571
[13181-17-4]	1.3×10^{5}		MacBean (2012a)	?	12
VTQWKUZUPOTXEH-UHFFFAOYSA-N					
tribromsalan	9.7×10^{5}		Zhang et al. (2010)	Q	288, 289
$C_{13}H_8Br_3NO_2$	1.2×10^{6}		Zhang et al. (2010)	Q	288, 290
[87-10-5]	1.6×10^{6}		Zhang et al. (2010)	Q	288, 291
KVSKGMLNBAPGKH-UHFFFAOYSA-N	1.2×10^{6}		Zhang et al. (2010)	Q	288, 292
bromoxynil heptanoate $C_{14}H_{15}Br_2NO_2$ [56634-95-8] BHZWBQPHPLFZSV-UHFFFAOYSA-N	5.3		Maniere et al. (2011)	?	12, 166
1-amino-2,4-dibromo-9,10-anthracenedione $C_{14}H_7Br_2NO_2$ (1-amino-2,4-dibromoanthraquinone) [81-49-2] ZINRVIQBCHAZMM-UHFFFAOYSA-N	5.5×10^{7}		HSDB (2015)	Q	100
2,6-dibromo-4-cyanophenyl octanoate	3.1×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{15}H_{17}BrNO_2$	3.1×10^{-1}		HSDB (2015)	V	
[1689-99-2]	4.1×10^{1}		Duchowicz et al. (2020)	Q	
DQKWXTIYGWPGOO-UHFFFAOYSA-N	<5.3		Maniere et al. (2011)	?	12, 166
bromobutide $C_{15}H_{22}BrNO$ [74712-19-9] WZDDLAZXUYIVMU-UHFFFAOYSA-N	1.9×10^{2}		Ebert et al. (2023)	?	319
(2*E*)-N,N'-bis(2,4,6-tribromophenyl)-2-butenediamide	9.0×10^{9}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_8Br_6N_2O_2$	5.1×10^{8}		Zhang et al. (2010)	Q	288, 290
[92484-07-6]	6.2×10^{9}		Zhang et al. (2010)	Q	288, 291
IJUNKLAVMFKPCX-OWOJBTEDSA-N	7.2×10^{13}		Zhang et al. (2010)	Q	288, 292

Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
SAYTEX BT 93	2.7×10^{15}		HSDB (2015)	Q	100
$C_{18}H_4Br_8N_2O_4$	2.7×10^{15}		Zhang et al. (2010)	Q	288, 289
[32588-76-4]	2.3×10^{11}		Zhang et al. (2010)	Q	288, 290
DYIZJUDNMOIZQO-UHFFFAOYSA-N	3.5×10^{9}		Zhang et al. (2010)	Q	288, 291
	2.3×10^{13}		Zhang et al. (2010)	Q	288, 292
SAYTEX BN 451	2.5×10^{15}		Zhang et al. (2010)	Q	288, 289
$C_{20}H_{20}Br_4N_2O_4$	1.4×10^{11}		Zhang et al. (2010)	Q	288, 290
[52907-07-0]	5.7×10^{11}		Zhang et al. (2010)	Q	288, 291
WOFYQUJNULCFLN-UHFFFAOYSA-N	1.6×10^{15}		Zhang et al. (2010)	Q	288, 292
deltamethrin	2.0		Duchowicz et al. (2020)	V	187
$C_{22}H_{19}Br_2NO_3$	2.0		HSDB (2015)	V	
[52918-63-5]	4.0×10^{-1}		Mackay et al. (2006d)	V	
OWZREIFADZCYQD-NSHGMRRFSA-N	2.0		Siebers and Mattusch (1996)	V	12
	1.0×10^{3}		Duchowicz et al. (2020)	Q	
	3.2×10^{1}		Maniere et al. (2011)	?	166
2,2'-(methylenedi-4,1-phenylene)bis(4,5,6,7-tetrabromo-1H-isoindole-1,3(2H)-dione	5.3×10^{14}		Zhang et al. (2010)	Q	288, 289
$C_{29}H_{10}N_2O_4Br_8$	1.7×10^{14}		Zhang et al. (2010)	Q	288, 290
[32588-74-2]	9.5×10^{9}		Zhang et al. (2010)	Q	288, 291
RHFKNNBDKARGKL-UHFFFAOYSA-N	4.7×10^{15}		Zhang et al. (2010)	Q	288, 292

A7.3 Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br)

Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bromotrifluoromethane	2.0×10^{-5}		Hine and Mookerjee (1975)	V	
CF_3Br	2.0×10^{-5}		Yaws (2003)	X	238
[75-63-8]	2.0×10^{-5}		Irmann (1965)	C	
RJCQBQGAPKAMLL-UHFFFAOYSA-N	6.4×10^{-6}		Keshavarz et al. (2022)	Q	
	5.3×10^{-5}		Duchowicz et al. (2020)	Q	300
	4.7×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.8×10^{-5}		Gharagheizi et al. (2010)	Q	247
	3.2×10^{-5}		Hilal et al. (2008)	Q	
	1.1×10^{-5}		Modarresi et al. (2007)	Q	68
	2.7×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	5.6×10^{-6}		Irmann (1965)	Q	
	2.0×10^{-5}		Duchowicz et al. (2020)	?	186, 21
	2.1×10^{-5}		Yaws (1999)	?	21
dibromodifluoromethane	3.3×10^{-4}		HSDB (2015)	Q	100
CBr_2F_2					
[75-61-6]					
AZSZCFSOHXEJQE-UHFFFAOYSA-N					
1-bromo-1,2,2,2-tetrafluoroethane	1.7×10^{-4}	2700	Allott et al. (1973)	L	
C_2HBrF_4	1.2×10^{-4}		Edelist et al. (1964)	M	14
(teflurane)	1.4×10^{-4}		Keshavarz et al. (2022)	Q	
[124-72-1]	1.5×10^{-3}		Duchowicz et al. (2020)	Q	
RZXZIZDRFQFCTA-UHFFFAOYSA-N	2.1×10^{-4}		Hilal et al. (2008)	Q	
	6.7×10^{-5}		Modarresi et al. (2007)	Q	68
	1.7×10^{-4}		Duchowicz et al. (2020)	?	186, 21
	1.3×10^{-4}		Abraham and Weathersby (1994)	?	21
	1.7×10^{-4}		Abraham et al. (1990)	?	
1,2-dibromotetrafluoroethane	2.7×10^{-7}		Duchowicz et al. (2020)	V	187
$C_2Br_2F_4$	2.7×10^{-7}		HSDB (2015)	V	
[124-73-2]	2.4×10^{-4}		Duchowicz et al. (2020)	Q	
KVBKAPANDHPRDG-UHFFFAOYSA-N					
1-bromo-2-fluorobenzene	4.1×10^{-3}		Ebert et al. (2023)	?	317
C_6H_4BrF					
[1072-85-1]					
IPWBFGUBXWMIPR-UHFFFAOYSA-N					
1-bromo-3-fluorobenzene	2.9×10^{-3}		Ebert et al. (2023)	?	317
C_6H_4BrF					
[1073-06-9]					
QDFKKJYEIFBEFC-UHFFFAOYSA-N					

Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-bromo-4-fluorobenzene C_6H_4BrF [460-00-4] AITNMTXHTIIIBB-UHFFFAOYSA-N	5.3×10^{-3}	4400	Hiatt (2013)	M	
bromopentafluorobenzene C_6BrF_5 [344-04-7] XEKTVXADUPBFOA-UHFFFAOYSA-N	2.1×10^{-3}		Zhang et al. (2010)	Q	288, 289
	1.6×10^{-4}		Zhang et al. (2010)	Q	288, 290
	1.4×10^{-4}		Zhang et al. (2010)	Q	288, 291
	6.7×10^{-4}		Zhang et al. (2010)	Q	288, 292
halfenprox $C_{24}H_{23}BrF_2O_3$ [111872-58-3] WIFXJBMOTMKRMM-UHFFFAOYSA-N	1.9×10^{1}		Ebert et al. (2023)	?	319
bromethalin $C_{14}H_7Br_3F_3N_3O_4$ [63333-35-7] USMZPYXTVKAYST-UHFFFAOYSA-N	2.5×10^{3}		HSDB (2015)	Q	100
brofluthrinate $C_{26}H_{22}BrF_2NO_4$ [160791-64-0] BUHNCQOJJZAOMJ-UHFFFAOYSA-N	1.6×10^{1}		Ebert et al. (2023)	?	317
bromochloromethane CH_2BrCl [74-97-5] JPOXNPPZZKNXOV-UHFFFAOYSA-N	6.6×10^{-3}	4700	Hiatt (2013)	M	
	7.8×10^{-3}	4600	Kondoh and Nakajima (1997)	M	
	6.8×10^{-3}		HSDB (2015)	V	
	5.8×10^{-3}		Mackay et al. (2006b)	V	
	5.8×10^{-3}		Mackay et al. (1993)	V	
	6.2×10^{-3}		Yaws (2003)	X	238
	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-2}		Gharagheizi et al. (2010)	Q	247
	5.7×10^{-3}		Yao et al. (2002)	Q	230
	5.3×10^{-3}		Katritzky et al. (1998)	Q	
	6.2×10^{-3}		Yaws (1999)	?	21
			Fogg and Sangster (2003)	W	793
bromodichloromethane $CHCl_2Br$ [75-27-4] FMWLUWPQPKEARP-UHFFFAOYSA-N	4.0×10^{-3}	5200	Burkholder et al. (2019)	L	
	3.9×10^{-3}	4900	Burkholder et al. (2019)	L	71
	4.0×10^{-3}	5200	Burkholder et al. (2015)	L	
	3.9×10^{-3}	4900	Burkholder et al. (2015)	L	71
	4.0×10^{-3}	5200	Sander et al. (2011)	L	
	4.0×10^{-3}	5200	Sander et al. (2006)	L	
	4.8×10^{-3}	3700	Fogg and Sangster (2003)	L	
	4.0×10^{-3}	5200	Staudinger and Roberts (2001)	L	
	4.0×10^{-3}	5200	Staudinger and Roberts (1996)	L	
	5.2×10^{-3}	4700	Hiatt (2013)	M	

Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.8×10^{-3}		Ruiz-Bevia and Fernandez-Torres (2010)	M	
	2.9×10^{-3}		Zhang et al. (2002)	M	14
	5.4×10^{-3}	4400	Kondoh and Nakajima (1997)	M	
	3.9×10^{-3}	4800	Moore et al. (1995)	M	794, 71
	4.8×10^{-3}	4200	Tse et al. (1992)	M	
	4.7×10^{-3}	5200	Nicholson et al. (1984)	M	
	3.5×10^{-3}	5200	Ervin et al. (1980)	M	
	4.7×10^{-3}		Warner et al. (1980)	M	
	4.1×10^{-3}		Mackay et al. (2006b)	V	
	4.1×10^{-3}		Mackay et al. (1993)	V	
	4.6×10^{-3}	1200	Goldstein (1982)	X	299
	7.7×10^{-3}		Hilal et al. (2008)	C	
	4.3×10^{-3}		Nicholson et al. (1984)	C	
	4.7×10^{-3}		Nicholson et al. (1984)	C	12
	4.7×10^{-3}		Shen (1982)	C	
	8.8×10^{-3}		Keshavarz et al. (2022)	Q	
	9.4×10^{-3}		Duchowicz et al. (2020)	Q	185
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	3.9×10^{-3}		Hilal et al. (2008)	Q	
	2.4×10^{-3}		Modarresi et al. (2007)	Q	68
		4100	Kühne et al. (2005)	Q	
	4.8×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	3.2×10^{-3}		Katritzky et al. (1998)	Q	
	4.7×10^{-3}		Duchowicz et al. (2020)	?	186, 21
	6.2×10^{-3}		Mackay et al. (2006b)	?	
		3800	Kühne et al. (2005)	?	
	6.2×10^{-3}		Mackay et al. (1993)	?	
bromotrichloromethane $CBrCl_3$ [75-62-7] XNNQFQFUQLJSQT-UHFFFAOYSA-N	2.7×10^{-2}		HSDB (2015)	Q	100
dibromochloromethane $CHClBr_2$ [124-48-1] GATVIKZLVQHOMN-UHFFFAOYSA-N	8.6×10^{-3}	5500	Burkholder et al. (2019)	L	
	7.2×10^{-3}	5200	Burkholder et al. (2019)	L	71
	8.6×10^{-3}	5500	Burkholder et al. (2015)	L	
	7.2×10^{-3}	5200	Burkholder et al. (2015)	L	71
	8.6×10^{-3}	5500	Sander et al. (2011)	L	
	8.6×10^{-3}	5500	Sander et al. (2006)	L	
	8.7×10^{-3}	4400	Fogg and Sangster (2003)	L	
	8.6×10^{-3}	5500	Staudinger and Roberts (2001)	L	
	8.5×10^{-3}	5500	Staudinger and Roberts (1996)	L	
	1.1×10^{-2}	5300	Hiatt (2013)	M	

Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^{-2}		Ruiz-Bevia and Fernandez-Torres (2010)	M	
	4.6×10^{-3}		Zhang et al. (2002)	M	14
	9.8×10^{-3}	5100	Kondoh and Nakajima (1997)	M	
	7.4×10^{-3}	4600	Moore et al. (1995)	M	795, 71
	9.3×10^{-3}	4600	Tse et al. (1992)	M	
	8.5×10^{-3}	6400	Ashworth et al. (1988)	M	279
	8.6×10^{-3}	5200	Nicholson et al. (1984)	M	
	8.5×10^{-3}	5000	Ervin et al. (1980)	M	
	1.3×10^{-2}		Warner et al. (1980)	M	
	1.2×10^{-2}		Mackay et al. (2006b)	V	
	1.2×10^{-2}		Goldstein (1982)	X	448
	1.2×10^{-2}	2500	Goldstein (1982)	X	299
	1.2×10^{-2}		Nicholson et al. (1984)	C	
	1.1×10^{-2}		Nicholson et al. (1984)	C	12
	1.3×10^{-2}		Shen (1982)	C	
	5.4×10^{-3}		Hilal et al. (2008)	Q	
	2.2×10^{-3}		Modarresi et al. (2007)	Q	68
		4800	Kühne et al. (2005)	Q	
	1.3×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.6×10^{-2}		Katritzky et al. (1998)	Q	
		4600	Kühne et al. (2005)	?	
	1.2×10^{-2}		Mackay et al. (1993)	?	
1-chloro-2-bromoethane C_2H_4BrCl [107-04-0] IBYHHJPAARCAIE-UHFFFAOYSA-N	1.1×10^{-2}		Hine and Mookerjee (1975)	V	
	1.1×10^{-2}		Sieg et al. (2008)	C	
	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	3.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.8×10^{-2}		Hilal et al. (2008)	Q	
	5.5×10^{-3}		Modarresi et al. (2007)	Q	68
	1.2×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	1.7×10^{-2}		Katritzky et al. (1998)	Q	
	3.7×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.1×10^{-2}		Duchowicz et al. (2020)	?	186, 21
1,2-dibromo-1,1-dichloroethane $C_2H_2Br_2Cl_2$ [75-81-0] FIYBYNHDEOSJPL-UHFFFAOYSA-N	6.2×10^{-2}		HSDB (2015)	Q	100
1-bromo-3-chloropropane C_3H_6BrCl [109-70-6] MFESCIUQSIBMSM-UHFFFAOYSA-N	3.9×10^{-2}		HSDB (2015)	Q	100

Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-dibromo-3-chloropropane	9.7×10^{-2}	7100	Hiatt (2013)	M	
$C_3H_5Br_2Cl$	5.0×10^{-1}	10000	Kondoh and Nakajima (1997)	M	
[96-12-8]	6.6×10^{-2}		HSDB (2015)	V	
WBEJYOJJBDISQU-UHFFFAOYSA-N	6.7×10^{-2}		Meylan and Howard (1991)	V	
	9.0×10^{-2}		Hilal et al. (2008)	Q	
	1.1×10^{-2}		Modarresi et al. (2007)	Q	68
	6.4×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.1×10^{-1}		Katritzky et al. (1998)	Q	
	1.6×10^{-2}		Meylan and Howard (1991)	Q	
	4.0×10^{-2}		MacBean (2012a)	?	
1,2,3,4,5-pentabromo-6-chlorocyclohexane	1.0×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_6H_6Br_5Cl$	1.1×10^{2}		Zhang et al. (2010)	Q	288, 290
[87-84-3]	1.8×10^{3}		Zhang et al. (2010)	Q	288, 291
UZOSVZSBPTTWIG-UHFFFAOYSA-N	1.2×10^{1}		Zhang et al. (2010)	Q	288, 292
1,2,3,4-tetrabromo-5,6-dichlorocyclohexane	3.4		Zhang et al. (2010)	Q	288, 289
$C_6H_6Br_4Cl_2$	6.2×10^{1}		Zhang et al. (2010)	Q	288, 290
GABFTOZBVQIDBB-UHFFFAOYSA-N	9.9×10^{2}		Zhang et al. (2010)	Q	288, 291
	6.2		Zhang et al. (2010)	Q	288, 292
1,2,3-tribromo-4,5,6-trichlorocyclohexane	1.1		Zhang et al. (2010)	Q	288, 289
$C_6H_6Br_3Cl_3$	3.6×10^{1}		Zhang et al. (2010)	Q	288, 290
ZDEQCIGFZLZXBZ-UHFFFAOYSA-N	4.1×10^{2}		Zhang et al. (2010)	Q	288, 291
	3.0		Zhang et al. (2010)	Q	288, 292
1-bromo-4-chlorobenzene	6.8×10^{-3}		Duchowicz et al. (2020)	V	187
C_6H_4BrCl	6.8×10^{-3}		Mackay and Shiu (1981)	V	
[106-39-8]	7.7×10^{-3}		Duchowicz et al. (2020)	Q	
NHDODQWIKUYWMW-UHFFFAOYSA-N	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	9.0×10^{-3}		Hilal et al. (2008)	Q	
	6.8×10^{-3}		Modarresi et al. (2007)	Q	68
	6.9×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	3.3×10^{-2}		Katritzky et al. (1998)	Q	
1,2,4-tribromo-3,5,6-trichlorobenzene $C_6Br_3Cl_3$ [13075-01-9] XAIKFWSNTFEXDC-UHFFFAOYSA-N	4.1×10^{-2}		HSDB (2015)	Q	100

Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-(bromomethyl)-2-chlorobenzene C_7H_6BrCl [611-17-6] PURSZYWBIQIANP-UHFFFAOYSA-N	1.9×10^{-2}		HSDB (2015)	Q	449
2-bromo-4-chloro-1-methoxybenzene C_7H_6BrClO (2-bromo-4-chloroanisole) [60633-25-2] YJEMGEBDXDPBSP-UHFFFAOYSA-N	1.8×10^{-2}		Pfeifer et al. (2001)	M	733
2-bromo-6-chloro-1-methoxybenzene C_7H_6BrClO (2-bromo-6-chloroanisole) [174913-10-1] NWOYYECMNBWCNK-UHFFFAOYSA-N	1.4×10^{-2}		Pfeifer et al. (2001)	M	733
4-bromo-2-chloro-1-methoxybenzene C_7H_6BrClO (4-bromo-2-chloroanisole) [50638-47-6] FPIQNBOUYZLESW-UHFFFAOYSA-N	1.3×10^{-2}		Pfeifer et al. (2001)	M	733
2-bromo-3,5-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (2-bromo-3,5-dichloroanisole) [73931-43-8] LCHJNNXHVDDVAT-UHFFFAOYSA-N	1.1×10^{-2}		Pfeifer et al. (2001)	M	733
2-bromo-4,6-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (2-bromo-4,6-dichloroanisole) [60633-26-3] OEYKUHBCPJRXGZ-UHFFFAOYSA-N	8.2×10^{-3} 1.2×10^{-2}	3100	Diaz et al. (2005) Pfeifer et al. (2001)	M M	 733
4-bromo-2,3-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (4-bromo-2,3-dichloroanisole) [109803-52-3] BTRCDLZQISXWHZ-UHFFFAOYSA-N	1.1×10^{-2}		Pfeifer et al. (2001)	M	733

Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-bromo-2,6-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (4-bromo-2,6-dichloroanisole) [19240-91-6] OAYSFAKCFYRCRU-UHFFFAOYSA-N	1.2×10^{-2}	4900	Diaz et al. (2005)	M	
	1.2×10^{-2}		Pfeifer et al. (2001)	M	733
4-bromo-3,5-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (4-bromo-3,5-dichloroanisole) [174913-20-3] SVEZPKVUIXAEOX-UHFFFAOYSA-N	1.1×10^{-2}		Pfeifer et al. (2001)	M	733
3-bromo-2,4-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (3-bromo-2,4-dichloroanisole) [174913-16-7] OXINPOQPENRUHL-UHFFFAOYSA-N	1.2×10^{-2}		Ebert et al. (2023)	?	791
3-bromo-2,6-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (3-bromo-2,6-dichloroanisole) [174913-18-9] ANLVZYYGYBXMIX-UHFFFAOYSA-N	1.1×10^{-2}	2700	Diaz et al. (2005)	M	792
5-bromo-2,4-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (5-bromo-2,4-dichloroanisole) [174913-22-5] SJIIFORJBWPNPM-UHFFFAOYSA-N	1.1×10^{-2}		Pfeifer et al. (2001)	M	733
6-bromo-2,3-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (6-bromo-2,3-dichloroanisole) [174913-23-6] PNLDDSLZYVNPQW-UHFFFAOYSA-N	1.1×10^{-2}		Pfeifer et al. (2001)	M	733
6-bromo-2,5-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (6-bromo-2,5-dichloroanisole) [174913-14-5] BVSOVPUWHJWGEP-UHFFFAOYSA-N	7.7×10^{-3}	3000	Diaz et al. (2005)	M	

Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-bromo-3,4,5-trichloro-1-methoxybenzene $C_7H_4BrCl_3O$ (2-bromo-3,4,5-trichloroanisole) JIVCPRHFBFVZQL-UHFFFAOYSA-N	9.8×10^{-3}		Pfeifer et al. (2001)	M	733
3-bromo-2,4,6-trichloro-1-methoxybenzene $C_7H_4BrCl_3O$ (3-bromo-2,4,6-trichloroanisole) [174913-28-1] OIHHRLYOSUNYTC-UHFFFAOYSA-N	1.0×10^{-2}		Pfeifer et al. (2001)	M	733
3-bromo-2,5,6-trichloro-1-methoxybenzene $C_7H_4BrCl_3O$ (3-bromo-2,5,6-trichloroanisole) [78647-93-5] ZUXVGCIQOSXRJN-UHFFFAOYSA-N	1.0×10^{-2}		Pfeifer et al. (2001)	M	733
4-bromo-2,3,6-trichloro-1-methoxybenzene $C_7H_4BrCl_3O$ (4-bromo-2,3,6-trichloroanisole) [78647-87-7] VZRSUQWPXPUWCS-UHFFFAOYSA-N	1.0×10^{-2}		Pfeifer et al. (2001)	M	733
6-bromo-2,3,4-trichloro-1-methoxybenzene $C_7H_4BrCl_3O$ (6-bromo-2,3,4-trichloroanisole) GVCDCZPXMGMNTR-UHFFFAOYSA-N	1.1×10^{-2}		Pfeifer et al. (2001)	M	733
4-bromo-2,3,5,6-tetrachloro-1-methoxybenzene $C_7H_3BrCl_4O$ (4-bromo-2,3,5,6-tetrachloroanisole) [174913-33-8] YSVAURKXNCNUNS-UHFFFAOYSA-N	9.2×10^{-3}		Pfeifer et al. (2001)	M	733
2,4-dibromo-3-chloro-1-methoxybenzene $C_7H_5Br_2ClO$ (2,4-dibromo-3-chloroanisole) YXYRJAVLYYNRCE-UHFFFAOYSA-N	1.0×10^{-2}		Ebert et al. (2023)	?	791

Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4-dibromo-5-chloro-1-methoxybenzene $C_7H_5Br_2ClO$ (2,4-dibromo-5-chloroanisole) [174913-38-3] OTZRCEAVEJYZQS-UHFFFAOYSA-N	1.0×10^{-2}		Ebert et al. (2023)	?	791
2,6-dibromo-3-chloro-1-methoxybenzene $C_7H_5Br_2ClO$ (2,6-dibromo-3-chloroanisole) AHBGIHFKTBTQJP-UHFFFAOYSA-N	7.4×10^{-3}	770	Diaz et al. (2005)	M	792
2,6-dibromo-4-chloro-1-methoxybenzene $C_7H_5Br_2ClO$ (2,6-dibromo-4-chloroanisole) [174913-44-1] WHRDPXDGAMJNGH-UHFFFAOYSA-N	2.0×10^{-2} 1.1×10^{-2}	6700	Diaz et al. (2005) Pfeifer et al. (2001)	M M	 733
2,4-dibromo-3,5-dichloro-1-methoxybenzene $C_7H_4Br_2Cl_2O$ (2,4-dibromo-3,5-dichloroanisole) [174913-52-1] YZMXEWDTXSTFIJ-UHFFFAOYSA-N	9.1×10^{-3}		Pfeifer et al. (2001)	M	733
2,4-dibromo-5,6-dichloro-1-methoxybenzene $C_7H_4Br_2Cl_2O$ (2,4-dibromo-5,6-dichloroanisole) MUUDTVDSRYEMBU-UHFFFAOYSA-N	9.8×10^{-3}		Pfeifer et al. (2001)	M	733
2,3-dibromo-5,6-dichloro-1-methoxybenzene $C_7H_4Br_2Cl_2O$ (2,3-dibromo-5,6-dichloroanisole) WDRCOFFEZVLCLX-UHFFFAOYSA-N	9.1×10^{-3}		Pfeifer et al. (2001)	M	733
2,6-dibromo-3,4,5-trichloro-1-methoxybenzene $C_7H_3Br_2Cl_3O$ (2,6-dibromo-3,4,5-trichloroanisole) RFUGYJHXLQAXOX-UHFFFAOYSA-N	8.6×10^{-3}		Pfeifer et al. (2001)	M	733

Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4,6-tribromo-3-chloro-1-methoxybenzene $C_7H_4Br_3ClO$ (2,4,6-tribromo-3-chloroanisole) [174913-78-1] FWKUBDOTUFVPBX-UHFFFAOYSA-N	9.1×10^{-3}		Pfeifer et al. (2001)	M	733
2,3-dibromo-7,8-dichlorodibenzo-*p*-dioxin $C_{12}H_4Br_2Cl_2O_2$ [50585-40-5] SBSJXPIUKNBZND-UHFFFAOYSA-N	3.2		Ebert et al. (2023)	?	319
2',4',5',7'-tetrabromo-3,4,5,6-tetrachlorofluorescein	1.5×10^{13}		Zhang et al. (2010)	Q	288, 289
$C_{20}H_4Br_4Cl_4O_5$	1.9×10^{8}		Zhang et al. (2010)	Q	288, 290
[13473-26-2]	8.0×10^{10}		Zhang et al. (2010)	Q	288, 291
ZYIBVBKZZZDFOY-UHFFFAOYSA-N	2.2×10^{8}		Zhang et al. (2010)	Q	288, 292
bromochloroacetonitrile $C_2HBrClN$ [83463-62-1] BMWPPNAUMLRKML-UHFFFAOYSA-N	8.2		HSDB (2015)	Q	100
N,N'-dimethyl-3,3',4-tribromo-4,5,5'-trichloro-2,2'-bipyrrole	7.1		Tittlemier et al. (2004)	V	
$C_{10}H_6Br_3Cl_3N_2$ (DBP-Br3Cl3a) [400766-93-0] JSQYFPHYSOZLPT-UHFFFAOYSA-N	9.5		Hilal et al. (2008)	Q	
N,N'-dimethyl- 3,4,4'-tribromo-3',5,5'-trichloro-2,2'-bipyrrole	3.3×10^{1}		Tittlemier et al. (2004)	V	
$C_{10}H_6Br_3Cl_3N_2$ (DBP-Br3Cl3b) [666856-68-4] GUWAXPTVCYBOMV-UHFFFAOYSA-N	9.5		Hilal et al. (2008)	Q	
N,N'-dimethyl-3,3',4,4'-tetrabromo-5,5'-dichloro-2,2'-bipyrrole	2.8×10^{1}		Tittlemier et al. (2004)	V	
$C_{10}H_6Br_4Cl_2N_2$ (DBP-Br4Cl2) [253798-64-0] FQGSQKFVAAJWFY-UHFFFAOYSA-N	1.8×10^{1}		Hilal et al. (2008)	Q	

Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N,N'-dimethyl-3,3',4,4',5-pentabromo-5'-chloro-2,2'-bipyrrole $C_{10}H_6Br_5ClN_2$ (DBP-Br5Cl) [400767-00-2] LIYSVIAQQQEQBT-UHFFFAOYSA-N	1.5×10^{2}		Tittlemier et al. (2004)	V	
	3.0×10^{1}		Hilal et al. (2008)	Q	
1-bromo-3-chloro-5,5-dimethylhydantoin $C_5H_6BrClN_2O_2$ [16079-88-2] PIEXCQIOSMOEOU-UHFFFAOYSA-N	1.2×10^{1}		HSDB (2015)	Q	100
3-(4-bromo-3-chlorophenyl)-1-methoxy-1-methylurea $C_9H_{10}BrClN_2O_2$ (chlorbromuron) [13360-45-7] NLYNUTMZTCLNOO-UHFFFAOYSA-N	2.2×10^{3}		HSDB (2015)	V	
	3.2×10^{3}		Mackay et al. (2006d)	V	
	2.5×10^{3}		MacBean (2012a)	?	
N-(4-bromo-2,6-dichloro-3-methylphenyl)acetamide $C_9H_8BrCl_2NO$ [68399-95-1] MRPNWLPYJSSISQ-UHFFFAOYSA-N	6.7×10^{3}		Zhang et al. (2010)	Q	288, 289
	6.2×10^{2}		Zhang et al. (2010)	Q	288, 290
	2.1×10^{4}		Zhang et al. (2010)	Q	288, 291
	6.5×10^{3}		Zhang et al. (2010)	Q	288, 292
halacrinate $C_{12}H_7NO_2BrCl$ [34462-96-9] YDNLKBDXQCHOTH-UHFFFAOYSA-N	2.4×10^{2}		MacBean (2012a)	?	
bromuconazole $C_{13}H_{12}BrCl_2N_3O$ [116255-48-2] HJJVPARKXDDIQD-UHFFFAOYSA-N	3.3×10^{4}		Duchowicz et al. (2020)	V	187
	1.2×10^{5}		HSDB (2015)	V	
	1.4×10^{2}		Duchowicz et al. (2020)	Q	
	1.1×10^{5}		Maniere et al. (2011)	?	12, 166
(±)-(2*R**,4*S**)-bromuconazole $C_{13}H_{12}BrCl_2N_3O$ [114544-80-8]	6.4×10^{4}		Ebert et al. (2023)	?	367
(±)-(2*R**,4*R**)-bromuconazole $C_{13}H_{12}BrCl_2N_3O$ [114544-81-9]	9.5×10^{4}		Ebert et al. (2023)	?	367

Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5,7-dibromo-2-(5-bromo-7-chloro-1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one	4.2×10^{9}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_6Br_3ClN_2O_2$	3.3×10^{15}		Zhang et al. (2010)	Q	288, 290
[85702-64-3]	2.4×10^{5}		Zhang et al. (2010)	Q	288, 291
UOWUGDPSFZLTMZ-BUHFOSPRSA-N	8.8×10^{9}		Zhang et al. (2010)	Q	288, 292
chlorantraniliprole	7.0×10^{15}		HSDB (2015)	Q	100
$C_{18}H_{14}BrCl_2N_5O_2$	3.1×10^{8}		Maniere et al. (2011)	?	242, 166
[500008-45-7]					
IZCBNTYXTMZSDP-UHFFFAOYSA-N					
cyantraniliprole	5.9×10^{12}		Maniere et al. (2011)	?	242, 166
$C_{19}H_{14}BrClN_6O_2$					
[736994-63-1]					
DVBUIBGJRQBEDP-UHFFFAOYSA-N					
tribromofluoromethane	1.5×10^{-3}		Fogg and Sangster (2003)	V	
CBr_3F					
[353-54-8]					
IHZAEIHJPNTART-UHFFFAOYSA-N					
bromochlorodifluoromethane	6.1×10^{-5}		Yaws (2003)	X	238, 154
$CBrClF_2$	1.0×10^{-4}		HSDB (2015)	Q	100
[353-59-3]	2.6×10^{-4}		Gharagheizi et al. (2012)	Q	
MEXUFEQDCXZEON-UHFFFAOYSA-N	6.4×10^{-5}		Gharagheizi et al. (2010)	Q	247
	8.6×10^{-5}		Hilal et al. (2008)	Q	
	6.0×10^{-5}		Yaws (1999)	?	21, 154
1-bromo-1-chloro-2,2,2-trifluoroethane	5.6×10^{-4}	4700	Fogg and Sangster (2003)	L	
$C_2HBrClF_3$	3.1×10^{-4}		Steward et al. (1973)	L	14
(halothane)	5.3×10^{-4}	4200	Allott et al. (1973)	L	
[151-67-7]	2.8×10^{-4}		Guitart et al. (1989)	M	14
BCQZXOMGPXTTIC-UHFFFAOYSA-N	3.3×10^{-4}		Lerman et al. (1983)	M	14
	5.3×10^{-4}	5000	Smith et al. (1981b)	M	
	3.2×10^{-4}		Stoelting and Longshore (1972)	M	14
	3.4×10^{-4}		Saidman et al. (1966)	M	14
	4.9×10^{-4}		Yaws (2003)	X	238, 80
	4.2×10^{-4}		Keshavarz et al. (2022)	Q	
	2.7×10^{-3}		Duchowicz et al. (2020)	Q	185
	4.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
	8.8×10^{-4}		Hilal et al. (2008)	Q	
	1.7×10^{-4}		Modarresi et al. (2007)	Q	68
		4100	Kühne et al. (2005)	Q	
	1.0×10^{-3}		English and Carroll (2001)	Q	231, 232
	4.9×10^{-4}		Duchowicz et al. (2020)	?	186, 21
	4.9×10^{-4}		HSDB (2015)	?	421

Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		5000	Kühne et al. (2005)	?	
	4.7×10^{-4}		Yaws (1999)	?	21, 80
	3.4×10^{-4}		Abraham and Weathersby (1994)	?	21
	4.8×10^{-4}		Abraham et al. (1990)	?	
tralopyril $C_{12}H_5BrClF_3N_2$ [122454-29-9] XNFIRYXKTXAHAC-UHFFFAOYSA-N	4.5×10^{3}		Ebert et al. (2023)	?	317
chlorfenapyr $C_{15}H_{11}BrClF_3N_2O$ [122453-73-0] CWFOCCVIPCEQCK-UHFFFAOYSA-N	1.7×10^{3}		HSDB (2015)	Q	100
fluazolate $C_{15}H_{12}N_2O_2BrClF_4$ [174514-07-9] FKLQIONHGSFYJY-UHFFFAOYSA-N	1.3×10^{1}		MacBean (2012a)	?	

A8 Organic species with iodine (I)

A8.1 Iodocarbons (C, H, O, Cl, I)

Table A8.1: Iodocarbons (C, H, O, Cl, I)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
iodomethane	2.0×10^{-3}	3200	Burkholder et al. (2019)	L	1
CH_3I	1.5×10^{-3}	3900	Burkholder et al. (2019)	L	71
(methyl iodide)	2.0×10^{-3}	3600	Burkholder et al. (2015)	L	
[74-88-4]	1.5×10^{-3}	3900	Burkholder et al. (2015)	L	71
INQOMBQAUSQDDS-UHFFFAOYSA-N	2.0×10^{-3}	3100	Brockbank (2013)	L	1
	2.0×10^{-3}	3600	Sander et al. (2011)	L	
	2.0×10^{-3}	3600	Sander et al. (2006)	L	
	2.0×10^{-3}	3600	Staudinger and Roberts (2001)	L	
	1.8×10^{-3}	3200	Hiatt (2013)	M	
	1.4×10^{-3}	3900	Ooki and Yokouchi (2011)	M	71
	1.9×10^{-3}		Gan and Yates (1996)	M	295
	1.4×10^{-3}	4100	Moore et al. (1995)	M	796, 71
	2.0×10^{-3}	3700	Elliott and Rowland (1993)	M	
	1.9×10^{-3}	3800	Hunter-Smith et al. (1983)	M	660
	2.0×10^{-3}	3100	Balls (1980)	M	
	1.8×10^{-3}	3000	Swain and Thornton (1962)	M	
	1.9×10^{-3}	3000	Glew and Moelwyn-Hughes (1953)	M	797
	1.9×10^{-3}	3700	Rex (1906)	M	
	1.8×10^{-3}		Mackay et al. (2006b)	V	
	1.9×10^{-3}	3600	Fogg and Sangster (2003)	V	
	1.8×10^{-3}		Mackay et al. (1993)	V	
	1.8×10^{-3}		Abraham (1984)	V	
	1.8×10^{-3}		Hine and Mookerjee (1975)	V	
	3.5×10^{-3}		Yaws (2003)	X	238
	1.7×10^{-3}		Liss and Slater (1974)	C	
	8.8×10^{-3}		Keshavarz et al. (2022)	Q	
	3.7×10^{-3}		Duchowicz et al. (2020)	Q	
	7.4×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	3.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.1×10^{-3}		Hilal et al. (2008)	Q	
	6.8×10^{-4}		Modarresi et al. (2007)	Q	68
		3800	Kühne et al. (2005)	Q	
	1.9×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	2.1×10^{-4}		English and Carroll (2001)	Q	231, 232
	8.8×10^{-4}		Katritzky et al. (1998)	Q	
	1.8×10^{-3}		Suzuki et al. (1992)	Q	233
	3.6×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.9×10^{-3}		Duchowicz et al. (2020)	?	186, 21
	1.8×10^{-3}		Mackay et al. (2006b)	?	

Table A8.1: Iodocarbons (C, H, O, Cl, I) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		3700	Kühne et al. (2005)	?	
	3.5×10^{-3}		Yaws (1999)	?	21
	1.8×10^{-3}		Mackay et al. (1993)	?	
	3.5×10^{-3}		Yaws and Yang (1992)	?	21
diiodomethane	2.3×10^{-2}	5300	Burkholder et al. (2019)	L	71
CH_2I_2	2.3×10^{-2}	5300	Burkholder et al. (2015)	L	71
[75-11-6]	2.4×10^{-2}	4700	Moore et al. (1995)	M	798, 71
NZZFYRREKKOMAT-UHFFFAOYSA-N	3.2×10^{-2}		Mackay et al. (1993)	V	
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	246
	7.3×10^{-2}		Hilal et al. (2008)	Q	
	1.3×10^{-3}		Modarresi et al. (2007)	Q	68
	2.7×10^{-2}		Yao et al. (2002)	Q	230
	3.1×10^{-2}		Katritzky et al. (1998)	Q	
	2.9×10^{-2}		Yaws (1999)	?	21
	2.8×10^{-2}		Yaws and Yang (1992)	?	21
	2.8×10^{-2}		Abraham et al. (1990)	?	
triiodomethane	6.2×10^{-3}		Fogg and Sangster (2003)	V	
CHI_3	4.3×10^{-3}		Yaws (2003)	X	238
(iodoform)	3.2×10^{-6}		HSDB (2015)	Q	100
[75-47-8]	4.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
OKJPEAGHQZHRQV-UHFFFAOYSA-N	1.3×10^{-3}		Hilal et al. (2008)	Q	
	3.4×10^{-3}		Yaws and Yang (1992)	?	21
iodoethane	1.4×10^{-3}	4800	Burkholder et al. (2019)	L	71
C_2H_5I	1.4×10^{-3}	4800	Burkholder et al. (2015)	L	71
[75-03-6]	1.5×10^{-3}	3600	Brockbank (2013)	L	1
HVTICUPFWKNHNG-UHFFFAOYSA-N	1.5×10^{-3}	4200	Fogg and Sangster (2003)	L	799
	1.4×10^{-3}	4800	Ooki and Yokouchi (2011)	M	71
	1.4×10^{-3}		Li et al. (1993)	M	
	1.5×10^{-3}	4000	Rex (1906)	M	
	1.4×10^{-3}		Duchowicz et al. (2020)	V	187
	1.4×10^{-3}		Mackay et al. (2006b)	V	
	1.9×10^{-3}		Mackay et al. (1993)	V	
	1.4×10^{-3}		Abraham (1984)	V	
	1.4×10^{-3}		Hine and Mookerjee (1975)	V	
	1.7×10^{-3}		Yaws (2003)	X	238, 12
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	1.7×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.9×10^{-3}		Hilal et al. (2008)	Q	
		4200	Kühne et al. (2005)	Q	

Table A8.1: Iodocarbons (C, H, O, Cl, I) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^{-3}		Yaffe et al. (2003)	Q	249, 273
	4.2×10^{-3}		Yao et al. (2002)	Q	230, 268
	2.2×10^{-4}		English and Carroll (2001)	Q	231, 232
	1.2×10^{-3}		Katritzky et al. (1998)	Q	
	1.3×10^{-3}		Suzuki et al. (1992)	Q	233
	1.2×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
		4100	Kühne et al. (2005)	?	
	1.4×10^{-3}		Yaws (1999)	?	21, 12
	1.1×10^{-3}		Abraham and Weathersby (1994)	?	21
	1.8×10^{-3}		Yaws and Yang (1992)	?	21, 12
	1.4×10^{-3}		Abraham et al. (1990)	?	
(*E*)-1,2-diiodoethene $C_2H_2I_2$ [590-27-2] CVOGMKGEVNGRSK-OWOJBTEDSA-N	3.5×10^{-3}		Duchowicz et al. (2020)	V	187
	5.9×10^{-3}		Duchowicz et al. (2020)	Q	
1-iodopropane C_3H_7I (propyl iodide) [107-08-4] PVWOIHVRPOBWPI-UHFFFAOYSA-N	1.1×10^{-3}	4500	Brockbank (2013)	L	
	1.1×10^{-3}		Li et al. (1993)	M	
	1.0×10^{-3}	4600	Rex (1906)	M	
	1.1×10^{-3}		Duchowicz et al. (2020)	V	187
	1.1×10^{-3}		Mackay et al. (2006b)	V	
	1.1×10^{-3}		Mackay et al. (1993)	V	
	9.9×10^{-4}		Abraham (1984)	V	
	1.1×10^{-3}		Hine and Mookerjee (1975)	V	
	1.2×10^{-3}		Yaws (2003)	X	238, 80
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	2.9×10^{-3}		Gharagheizi et al. (2012)	Q	
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	272, 244
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.6×10^{-3}		Hilal et al. (2008)	Q	
	2.4×10^{-4}		Modarresi et al. (2007)	Q	68
		4500	Kühne et al. (2005)	Q	
	1.1×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.9×10^{-3}		Yao et al. (2002)	Q	230
	1.1×10^{-3}		English and Carroll (2001)	Q	231, 232
	1.1×10^{-3}		Katritzky et al. (1998)	Q	
	9.9×10^{-4}		Suzuki et al. (1992)	Q	233
	9.5×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
		4500	Kühne et al. (2005)	?	
	1.1×10^{-3}		Yaws (1999)	?	21, 80
	1.2×10^{-3}		Yaws and Yang (1992)	?	21, 80
	9.9×10^{-4}		Abraham et al. (1990)	?	

Table A8.1: Iodocarbons (C, H, O, Cl, I) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-iodopropane	8.5×10^{-4}	4700	Brockbank (2013)	L	
C_3H_7I	8.5×10^{-4}	4500	Rex (1906)	M	
(isopropyl iodide)	1.4×10^{-3}		Duchowicz et al. (2020)	V	187
[75-30-9]	8.8×10^{-4}		Hine and Mookerjee (1975)	V	
FMKOJHQHASLBPH-UHFFFAOYSA-N	1.1×10^{-3}		Yaws (2003)	X	238, 12
	5.7×10^{-4}		Duchowicz et al. (2020)	Q	
	6.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
	7.9×10^{-4}		Hilal et al. (2008)	Q	
	1.7×10^{-4}		Modarresi et al. (2007)	Q	68
		4500	Kühne et al. (2005)	Q	
	1.5×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.8×10^{-3}		Yao et al. (2002)	Q	230
	7.9×10^{-4}		English and Carroll (2001)	Q	231, 232
	9.7×10^{-4}		Katritzky et al. (1998)	Q	
	8.6×10^{-4}		Suzuki et al. (1992)	Q	233
	5.4×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
		4700	Kühne et al. (2005)	?	
	8.7×10^{-4}		Yaws (1999)	?	21, 12
	1.1×10^{-3}		Yaws and Yang (1992)	?	21, 12
1-iodobutane	6.9×10^{-4}		Brockbank (2013)	L	
C_4H_9I	5.9×10^{-4}		Duchowicz et al. (2020)	V	187
[542-69-8]	5.4×10^{-4}		Mackay et al. (2006b)	V	
KMGBZBJJOKUPIA-UHFFFAOYSA-N	5.4×10^{-4}		Mackay et al. (1993)	V	
	6.1×10^{-4}		Abraham (1984)	V	
	6.2×10^{-4}		Hine and Mookerjee (1975)	V	
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	1.2×10^{-3}		Hilal et al. (2008)	Q	
	1.8×10^{-4}		Modarresi et al. (2007)	Q	68
	6.7×10^{-4}		Yaffe et al. (2003)	Q	249, 250
	7.9×10^{-4}		English and Carroll (2001)	Q	231, 232
	1.1×10^{-3}		Katritzky et al. (1998)	Q	
	7.5×10^{-4}		Suzuki et al. (1992)	Q	233
	7.5×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	6.1×10^{-4}		Abraham et al. (1990)	?	

Table A8.1: Iodocarbons (C, H, O, Cl, I) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-iodobutane	5.0×10^{-4}		Duchowicz et al. (2020)	V	187
C_4H_9I	5.7×10^{-4}		Duchowicz et al. (2020)	Q	
[513-48-4]	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
IQRUSQUYPCHEKN-UHFFFAOYSA-N	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	7.0×10^{-4}		Hilal et al. (2008)	Q	
1-iodopentane	5.9×10^{-4}		Keshavarz et al. (2022)	Q	
$C_5H_{11}I$	1.2×10^{-3}		Duchowicz et al. (2020)	Q	185
[628-17-1]	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
BLXSFCHWMBESKV-UHFFFAOYSA-N	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	9.9×10^{-4}		Hilal et al. (2008)	Q	
	1.4×10^{-4}		Modarresi et al. (2007)	Q	68
	5.8×10^{-4}		English and Carroll (2001)	Q	231, 232
	5.7×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	5.1×10^{-4}		Duchowicz et al. (2020)	?	186, 21
	5.1×10^{-4}		Abraham et al. (1990)	?	
1-iodohexane	3.4×10^{-4}		Brockbank (2013)	L	
$C_6H_{13}I$	8.0×10^{-4}		Keshavarz et al. (2022)	Q	
[638-45-9]	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
ANOOTOPTCJRUPK-UHFFFAOYSA-N	8.2×10^{-4}		Hilal et al. (2008)	Q	
	1.2×10^{-4}		Modarresi et al. (2007)	Q	68
	4.2×10^{-4}		English and Carroll (2001)	Q	231, 261
	4.5×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	3.5×10^{-4}		Duchowicz et al. (2020)	?	186, 21
	3.5×10^{-4}		Abraham et al. (1990)	?	
1-iodoheptane	2.6×10^{-4}		Abraham (1984)	V	
$C_7H_{15}I$	1.1×10^{-3}		Keshavarz et al. (2022)	Q	
[4282-40-0]	1.2×10^{-3}		Duchowicz et al. (2020)	Q	185
LMHCYRULPLGEEZ-UHFFFAOYSA-N	3.1×10^{-4}		Raventos-Duran et al. (2010)	Q	243, 244
	3.1×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-4}		Raventos-Duran et al. (2010)	Q	246
	6.7×10^{-4}		Hilal et al. (2008)	Q	
	9.7×10^{-5}		Modarresi et al. (2007)	Q	68
	3.1×10^{-4}		English and Carroll (2001)	Q	231, 232
	3.5×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	2.5×10^{-4}		Duchowicz et al. (2020)	?	186, 21
	2.5×10^{-4}		Abraham et al. (1990)	?	
iodocyclohexane	3.9×10^{-3}		Hilal et al. (2008)	Q	
$C_6H_{11}I$					
[626-62-0]					
FUCOMWZKWIEKRK-UHFFFAOYSA-N					

Table A8.1: Iodocarbons (C, H, O, Cl, I) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-iodo-1-propene C_3H_5I [556-56-9] HFEHLDPGIKPNKL-UHFFFAOYSA-N	3.8×10^{-3}		Hilal et al. (2008)	Q	
1-iodocyclohexene C_6H_9I [17497-53-9] CAROGICRCNKEOD-UHFFFAOYSA-N	4.1×10^{-3}		Hilal et al. (2008)	Q	
iodobenzene C_6H_5I [591-50-4] SNHMUERNLJLMHN-UHFFFAOYSA-N	7.7×10^{-3}		Mackay and Shiu (1981)	L	
	7.6×10^{-3}		Li and Carr (1993)	M	
	1.2×10^{-2}		Duchowicz et al. (2020)	V	187
	1.2×10^{-2}		HSDB (2015)	V	
	7.9×10^{-3}		Schüürmann (2000)	V	
	1.3×10^{-2}		Mackay et al. (1993)	V	
	6.9×10^{-3}		Yaws (2003)	X	238
	8.6×10^{-3}		Duchowicz et al. (2020)	Q	
	7.7×10^{-3}		Li et al. (2014)	Q	242
	8.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	243, 244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	6.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.4×10^{-2}		Hilal et al. (2008)	Q	
	6.9×10^{-3}		Modarresi et al. (2007)	Q	68
	7.7×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	8.3×10^{-3}		Yao et al. (2002)	Q	230
	2.3×10^{-3}		English and Carroll (2001)	Q	231, 232
	6.4×10^{-3}		Katritzky et al. (1998)	Q	
	3.8×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	7.0×10^{-3}		Yaws (1999)	?	21
	7.4×10^{-3}		Yaws and Yang (1992)	?	21
	7.7×10^{-3}		Abraham et al. (1990)	?	
			Brockbank (2013)	W	800
iodoacetic acid $C_2H_3IO_2$ [64-69-7] JDNTWHVOXJZDSN-UHFFFAOYSA-N	2.4×10^{2}		HSDB (2015)	Q	100
2-iodophenol C_6H_5IO [533-58-4] KQDJTBPASNJQFQ-UHFFFAOYSA-N	1.4×10^{1}		Abraham et al. (1994a)	R	
	6.9		Hilal et al. (2008)	Q	
	1.4×10^{1}		Yaffe et al. (2003)	Q	249, 250
	1.5×10^{1}		English and Carroll (2001)	Q	231, 232
	1.6×10^{2}		Nirmalakhandan et al. (1997)	Q	

Table A8.1: Iodocarbons (C, H, O, Cl, I) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-iodophenol C_6H_5IO [626-02-8] FXTKWBZFNQHAAO-UHFFFAOYSA-N	7.0×10^{1}		Hilal et al. (2008)	Q	
4-iodophenol C_6H_5IO [540-38-5] VSMDINRNYYEDRN-UHFFFAOYSA-N	4.6×10^{1}		Hilal et al. (2008)	Q	
erythrosine $C_{20}H_8I_4O_5$ [16423-68-0] OALHHIHQOFIMEF-UHFFFAOYSA-N	3.9×10^{13} 2.3×10^{8} 8.6×10^{10} 5.1×10^{9}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
4-hydroxy-3,5-diiodo-benzonitrile $C_7H_3I_2NO$ (ioxynil) [1689-83-4] NRXQIUSYPAHGNM-UHFFFAOYSA-N	1.3×10^{2} 1.8×10^{4}		Mackay et al. (2006d) HSDB (2015)	V Q	 100
3-iodo-2-propynyl butylcarbamate $C_8H_{12}INO_2$ [55406-53-6] WYVVKGNFXHOCQV-UHFFFAOYSA-N	8.2×10^{1}		HSDB (2015)	V	
diatrizoic acid $C_{11}H_9I_3N_2O_4$ [117-96-4] YVPYQUNUQOZFHG-UHFFFAOYSA-N	3.5×10^{12} 5.4×10^{8} 1.2×10^{17} 3.3×10^{16}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
iothalamic acid $C_{11}H_9I_3N_2O_4$ [2276-90-6] UXIGWFXRQKWHHA-UHFFFAOYSA-N	4.4×10^{12} 4.8×10^{9} 4.2×10^{16} 1.9×10^{16}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
benodanil $C_{13}H_{10}INO$ [15310-01-7] LJOZMWRYMKECFF-UHFFFAOYSA-N	6.2×10^{5} $>2.3\times10^{10}$		Mackay et al. (2006d) MacBean (2012a)	V ?	
proquinazid $C_{14}H_{17}IN_2O_2$ [189278-12-4] FLVBXVXXXMLMOX-UHFFFAOYSA-N	3.3×10^{1}		Maniere et al. (2011)	?	166
iopamidol $C_{17}H_{22}I_3N_3O_8$ [60166-93-0] XQZXYNRDCRIARQ-LURJTMIESA-N	9.0×10^{19}		HSDB (2015)	Q	100

Table A8.1: Iodocarbons (C, H, O, Cl, I) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ioxaglic acid	2.7×10^{35}		Zhang et al. (2010)	Q	288, 289
$C_{24}H_{21}I_6N_5O_8$	1.4×10^{27}		Zhang et al. (2010)	Q	288, 290
[59017-64-0]	2.0×10^{29}		Zhang et al. (2010)	Q	288, 291
TYYBFXNZMFNZJT-UHFFFAOYSA-N	7.2×10^{38}		Zhang et al. (2010)	Q	288, 292
perfluorohexyl iodide	4.6×10^{-4}	8200	Abusallout et al. (2022)	M	
$C_6F_{13}I$					
[355-43-1]					
BULLJMKUVKYZDJ-UHFFFAOYSA-N					
1,1,1,2,2,3,3-heptafluoro-5-iodopentane	4.6×10^{-6}		Zhang et al. (2010)	Q	288, 289
$C_5H_4F_7I$	1.2×10^{-4}		Zhang et al. (2010)	Q	288, 290
[68188-12-5]	3.8×10^{-4}		Zhang et al. (2010)	Q	288, 291
TZNRRNKRZXHADL-UHFFFAOYSA-N	5.0×10^{-6}		Zhang et al. (2010)	Q	288, 292
1-fluoro-4-iodobenzene	4.5×10^{-3}		Ebert et al. (2023)	?	317
C_6H_4FI					
[352-34-1]					
KGNQDBQYEBMPFZ-UHFFFAOYSA-N					
5-diethylamiloride	8.8×10^{-7}		Zhang et al. (2010)	Q	288, 289
$C_6H_4F_9I$	5.6×10^{-5}		Zhang et al. (2010)	Q	288, 290
[2043-55-2]	1.9×10^{-4}		Zhang et al. (2010)	Q	288, 291
CXHFIVFPHDGZIS-UHFFFAOYSA-N	1.0×10^{-6}		Zhang et al. (2010)	Q	288, 292
1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-8-iodooctane	1.3×10^{-3}		Abusallout et al. (2022)	M	
$C_8H_4F_{13}I$	3.2×10^{-8}		Zhang et al. (2010)	Q	288, 289
[2043-57-4]	3.4×10^{-6}		Zhang et al. (2010)	Q	288, 290
NVVZEKTVIXIUKW-UHFFFAOYSA-N	5.4×10^{-5}		Zhang et al. (2010)	Q	288, 291
	4.3×10^{-8}		Zhang et al. (2010)	Q	288, 292
1H,2H-perfluoro-1-iodooct-1-ene	8.4×10^{-4}		Abusallout et al. (2022)	M	
$C_8H_2F_{13}I$					
[150223-14-6]					
WDWNMIBWWPZNJK-OWOJBTEDSA-N					
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-iododecane	1.2×10^{-9}		Zhang et al. (2010)	Q	288, 289
$C_{10}H_4F_{17}I$	7.7×10^{-8}		Zhang et al. (2010)	Q	288, 290
[2043-53-0]	2.0×10^{-5}		Zhang et al. (2010)	Q	288, 291
XVKJSLBVVRCOIT-UHFFFAOYSA-N	2.3×10^{-9}		Zhang et al. (2010)	Q	288, 292

Table A8.1: Iodocarbons (C, H, O, Cl, I) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chloroiodomethane	8.4×10^{-3}	5100	Burkholder et al. (2019)	L	71
CH_2ClI	8.4×10^{-3}	5100	Burkholder et al. (2015)	L	71
[593-71-5]	8.3×10^{-3}	6200	Ooki and Yokouchi (2011)	M	71
PJGJQVRXEUVAFT-UHFFFAOYSA-N	9.1×10^{-3}	4100	Moore et al. (1995)	M	801, 71
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	272, 244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	246
	2.0×10^{-2}		Hilal et al. (2008)	Q	
	5.0×10^{-4}		Modarresi et al. (2007)	Q	68
1-chloro-4-iodobenzene C_6H_4ClI [637-87-6] GWQSENYKCGJTRI-UHFFFAOYSA-N	6.9×10^{-3}		Ebert et al. (2023)	?	317
bromoiodomethane CH_2BrI [557-68-6] TUDWMIUPYRKEFN-UHFFFAOYSA-N	2.0×10^{-2}		Karagodin-Doyennel et al. (2021)	E	802
1-bromo-4-iodobenzene C_6H_4BrI [589-87-7] UCCUXODGPMAHRL-UHFFFAOYSA-N	1.5×10^{-2}		Ebert et al. (2023)	?	317

A9 Organic species with sulfur (S)

A9.1 Sulfur (C, H, O, N, Cl, S)

Table A9.1: Sulfur (C, H, O, N, Cl, S)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methanethiol	3.8×10^{-3}	3400	Burkholder et al. (2019)	L	
CH_3SH	3.8×10^{-3}	3400	Burkholder et al. (2015)	L	
(methyl mercaptan)	3.8×10^{-3}	3400	Sander et al. (2011)	L	
[74-93-1]	3.8×10^{-3}	3400	Sander et al. (2006)	L	
LSDPWZHWYPCBBB-UHFFFAOYSA-N	2.8×10^{-3}	2900	Plyasunova et al. (2004)	L	
	2.8×10^{-3}	3100	Staudinger and Roberts (2001)	L	
	2.0×10^{-3}	2800	De Bruyn et al. (1995b)	M	
	2.3×10^{-3}	2700	Tsuji et al. (1990)	M	63
	3.9×10^{-3}	3400	Przyjazny et al. (1983)	M	
	3.3×10^{-3}		Hine and Weimar (1965)	M	
	3.2×10^{-3}		Duchowicz et al. (2020)	V	187
	3.2×10^{-3}		HSDB (2015)	V	
	3.3×10^{-3}		Hine and Mookerjee (1975)	V	
	2.4×10^{-3}		Yaws (2003)	X	238
	2.6×10^{-3}	1600	Goldstein (1982)	X	299
	1.4×10^{-1}		Duchowicz et al. (2020)	Q	
	2.3×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
	3.5×10^{-3}		Hilal et al. (2008)	Q	
		3300	Kühne et al. (2005)	Q	
	4.1×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.0×10^{-2}		Yao et al. (2002)	Q	230
	2.1×10^{-3}		Katritzky et al. (1998)	Q	
	2.9×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	7.0×10^{-3}		Russell et al. (1992)	Q	280
	4.0×10^{-3}		Suzuki et al. (1992)	Q	233
		3400	Kühne et al. (2005)	?	
	2.4×10^{-3}		Yaws et al. (2003)	?	21
	5.1×10^{-3}		Yaws (1999)	?	21, 81
	4.0×10^{-3}		Abraham et al. (1990)	?	
ethanethiol	2.8×10^{-3}	3700	Burkholder et al. (2019)	L	
C_2H_5SH	2.8×10^{-3}	3700	Burkholder et al. (2015)	L	
(ethyl mercaptan)	2.8×10^{-3}	3700	Sander et al. (2011)	L	
[75-08-1]	2.8×10^{-3}	3700	Sander et al. (2006)	L	
DNJIEGIFACGWOD-UHFFFAOYSA-N	2.3×10^{-3}	3500	Plyasunova et al. (2004)	L	
	2.4×10^{-3}	2800	Jou et al. (2021)	M	
	2.8×10^{-3}	3700	Przyjazny et al. (1983)	M	
	2.2×10^{-3}		Vitenberg et al. (1975)	M	
	3.4×10^{-3}		Mackay et al. (2006d)	V	
	3.4×10^{-3}		Mackay et al. (1995)	V	
	3.4×10^{-3}		Hwang et al. (1992)	V	

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.6×10^{-3}		Hine and Mookerjee (1975)	V	
	3.4×10^{-3}		Yaws (2003)	X	238
	1.8×10^{-3}		Hayer et al. (2022)	Q	20
	1.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
	3.9×10^{-3}		Hilal et al. (2008)	Q	
	5.6×10^{-3}		Modarresi et al. (2007)	Q	68
		3600	Kühne et al. (2005)	Q	
	2.2×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	5.8×10^{-3}		Yao et al. (2002)	Q	230
	3.6×10^{-3}		English and Carroll (2001)	Q	231, 232
	2.9×10^{-3}		Katritzky et al. (1998)	Q	
	1.9×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	1.0×10^{-2}		Russell et al. (1992)	Q	280
	2.9×10^{-3}		Suzuki et al. (1992)	Q	233
		3700	Kühne et al. (2005)	?	
	3.4×10^{-3}		Yaws et al. (2003)	?	21
	3.4×10^{-3}		Yaws (1999)	?	21
	3.4×10^{-3}		Yaws and Yang (1992)	?	21
	2.8×10^{-3}		Abraham et al. (1990)	?	
1,2-ethanedithiol $C_2H_6S_2$ [540-63-6] VYMPLPIFKRHAAC-UHFFFAOYSA-N	8.2×10^{-2}		HSDB (2015)	Q	100
thiirane C_2H_4S (ethylene sulfide) [420-12-2] VOVUARRWDCVURC-UHFFFAOYSA-N	2.8×10^{-2}		HSDB (2015)	Q	100
1-propanethiol C_3H_7SH (propyl mercaptan) [107-03-9] SUVIGLJNEAMWEG-UHFFFAOYSA-N	1.7×10^{-3}	3600	Plyasunova et al. (2004)	L	
	1.8×10^{-3}	4100	Haimi et al. (2006)	M	803
	1.7×10^{-3}	3100	Coquelet and Richon (2005)	M	
	2.4×10^{-3}	3900	Przyjazny et al. (1983)	M	
	9.0×10^{-4}		Mazza (1980)	M	
	2.4×10^{-3}		Yaws et al. (2003)	V	804
	2.4×10^{-3}		Yaws (2003)	X	238
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	4.7×10^{-2}		Duchowicz et al. (2020)	Q	300
	8.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	2.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
	3.4×10^{-3}		Hilal et al. (2008)	Q	
		4000	Kühne et al. (2005)	Q	
	3.9×10^{-3}		Yao et al. (2002)	Q	230, 268
	2.9×10^{-3}		English and Carroll (2001)	Q	231, 261
	1.5×10^{-3}		Nirmalakhandan et al. (1997)	Q	

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.4×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		3800	Kühne et al. (2005)	?	
	2.2×10^{-3}		Yaws (1999)	?	21
	2.4×10^{-3}		Abraham et al. (1990)	?	
2-propanethiol	1.3×10^{-3}	3700	Brockbank (2013)	L	
C_3H_8S	1.6×10^{-3}	4300	Zin et al. (2016)	M	805
(isopropyl mercaptan)	1.3×10^{-3}	3800	Haimi et al. (2006)	M	806
[75-33-2]	2.2×10^{-3}		Yaws et al. (2003)	V	804
KJRCEJOSASVSRA-UHFFFAOYSA-N	2.2×10^{-3}		Yaws (2003)	X	238
	2.1×10^{-3}		HSDB (2015)	Q	100
	1.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.1×10^{-3}		Hilal et al. (2008)	Q	
	2.9×10^{-3}		Yao et al. (2002)	Q	230
	2.4×10^{-3}		Yaws (1999)	?	21
1-butanethiol	1.5×10^{-3}	4300	Brockbank (2013)	L	1
C_4H_9SH	1.4×10^{-3}	4400	Plyasunova et al. (2004)	L	
(butyl mercaptan)	1.5×10^{-3}	4300	Haimi et al. (2006)	M	807
[109-79-5]	1.5×10^{-3}	3600	Coquelet and Richon (2005)	M	
WQAQPCDUOCURKW-UHFFFAOYSA-N	2.2×10^{-3}	4100	Przyjazny et al. (1983)	M	
	1.1×10^{-3}		Mackay et al. (2006d)	V	
	1.1×10^{-3}		Mackay et al. (1995)	V	
	1.4×10^{-3}		Hwang et al. (1992)	V	
	1.1×10^{-3}		Yaws (2003)	X	259
	1.1×10^{-3}		Yaws (2003)	X	238
	1.8×10^{-3}		Dupeux et al. (2022)	Q	260
	2.2×10^{-2}		Keshavarz et al. (2022)	Q	
	4.8×10^{-2}		Duchowicz et al. (2020)	Q	300
	6.1×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.7×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.7×10^{-3}		Hilal et al. (2008)	Q	
	3.4×10^{-3}		Modarresi et al. (2007)	Q	68
		4300	Kühne et al. (2005)	Q	
	2.2×10^{-3}		Yaffe et al. (2003)	Q	249, 273
	3.2×10^{-3}		Yao et al. (2002)	Q	230
	2.3×10^{-3}		English and Carroll (2001)	Q	231, 232
	2.5×10^{-3}		Katritzky et al. (1998)	Q	
	1.2×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	2.2×10^{-3}		Duchowicz et al. (2020)	?	186, 21
	1.1×10^{-3}		Bartelt-Hunt et al. (2008)	?	21
		4200	Kühne et al. (2005)	?	
	1.1×10^{-3}		Yaws et al. (2003)	?	21
	1.1×10^{-3}		Yaws (1999)	?	21
	1.1×10^{-3}		Yaws and Yang (1992)	?	21
	2.2×10^{-3}		Abraham et al. (1990)	?	

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-butanethiol	1.3×10^{-3}		Plyasunova et al. (2004)	L	
$C_4H_{10}S$	1.4×10^{-3}		Duchowicz et al. (2020)	V	187
(*sec*-butyl mercaptan)	1.4×10^{-3}		HSDB (2015)	V	
[513-53-1]	1.9×10^{-3}		Yaws et al. (2003)	V	804
LOCHFZBWPCLPAN-UHFFFAOYSA-N	1.9×10^{-3}		Yaws (2003)	X	238
	1.9×10^{-2}		Duchowicz et al. (2020)	Q	
	9.4×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.8×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.7×10^{-3}		Modarresi et al. (2007)	Q	68
	2.0×10^{-3}		Yao et al. (2002)	Q	230
	1.5×10^{-3}		Yaws (1999)	?	21
2-methyl-1-propanethiol	1.0×10^{-3}	3600	Zin et al. (2016)	M	808
$C_4H_{10}S$	1.9×10^{-3}		Yaws et al. (2003)	V	804
(isobutyl mercaptan)	1.9×10^{-3}		Yaws (2003)	X	238
[513-44-0]	3.3×10^{-4}		Gharagheizi et al. (2012)	Q	
BDFAOUQQXJIZDG-UHFFFAOYSA-N	2.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.4×10^{-3}		Hilal et al. (2008)	Q	
	2.0×10^{-3}		Yao et al. (2002)	Q	230, 268
	1.4×10^{-3}		Yaws (1999)	?	21
2-methyl-2-propanethiol	4.5×10^{-4}		Plyasunova et al. (2004)	L	
$C_4H_{10}S$	1.9×10^{-3}		Yaws et al. (2003)	V	804
(*tert*-butyl mercaptan)	1.9×10^{-3}		Yaws (2003)	X	238
[75-66-1]	1.6×10^{-3}		HSDB (2015)	Q	100
WMXCDAVJEZZYLT-UHFFFAOYSA-N	1.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
	6.1×10^{-4}		Hilal et al. (2008)	Q	
	1.1×10^{-3}		Yao et al. (2002)	Q	230
	1.8×10^{-3}		Yaws (1999)	?	21
1,4-dithiane	2.4×10^{-1}		Duchowicz et al. (2020)	V	187
$C_4H_8S_2$	2.3×10^{-1}		HSDB (2015)	V	
[505-29-3]	6.9		Duchowicz et al. (2020)	Q	
LOZWAPSEEHRYPG-UHFFFAOYSA-N					
1-pentanethiol	8.7×10^{-4}		Plyasunova et al. (2004)	L	
$C_5H_{11}SH$	8.2×10^{-4}		Duchowicz et al. (2020)	V	187
(pentyl mercaptan)	8.2×10^{-4}		HSDB (2015)	V	
[110-66-7]	1.4×10^{-3}		Yaws et al. (2003)	V	804
ZRKMQKLGEQPLNS-UHFFFAOYSA-N	7.3×10^{-4}		Amoore and Buttery (1978)	V	
	1.4×10^{-3}		Yaws (2003)	X	238
	4.8×10^{-2}		Duchowicz et al. (2020)	Q	
	4.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.3×10^{-3}		Hilal et al. (2008)	Q	
	2.5×10^{-3}		Modarresi et al. (2007)	Q	68

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{-3}		Yao et al. (2002)	Q	230, 268
	7.1×10^{-4}		Yaws (1999)	?	21
2,2-dimethyl-1-propanethiol	1.5×10^{-3}		Yaws et al. (2003)	V	804
$C_5H_{12}S$	1.5×10^{-3}		Yaws (2003)	X	238
[1679-08-9]	1.1×10^{-4}		Gharagheizi et al. (2012)	Q	
LSUXMVNABVPWMF-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
2-methyl-1-butanethiol	1.5×10^{-3}		Yaws et al. (2003)	V	804
$C_5H_{12}S$	1.5×10^{-3}		Yaws (2003)	X	238
[1878-18-8]	2.6×10^{-4}		Gharagheizi et al. (2012)	Q	
WGQKBCSACFQGQY-UHFFFAOYSA-N	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
2-methyl-2-butanethiol	1.5×10^{-3}		Yaws et al. (2003)	V	804
$C_5H_{12}S$	1.5×10^{-3}		Yaws (2003)	X	238
[1679-09-0]	8.6×10^{-4}		Gharagheizi et al. (2012)	Q	
IQIBYAHJXQVQGB-UHFFFAOYSA-N	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
	8.9×10^{-4}		Yao et al. (2002)	Q	230, 809
	1.0×10^{-3}		Yaws (1999)	?	21
2-pentanethiol	1.5×10^{-3}		Yaws et al. (2003)	V	804
$C_5H_{12}S$	1.5×10^{-3}		Yaws (2003)	X	259
[2084-19-7]	1.5×10^{-3}		Yaws (2003)	X	238
QUSTYFNPKBDELJ-UHFFFAOYSA-N	1.0×10^{-3}		Dupeux et al. (2022)	Q	260
	6.3×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
3-pentanethiol	1.5×10^{-3}		Yaws et al. (2003)	V	804
$C_5H_{12}S$	1.5×10^{-3}		Yaws (2003)	X	238
[616-31-9]	4.5×10^{-4}		Gharagheizi et al. (2012)	Q	
WICKAMSPKJXSGN-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
3-methyl-1-butanethiol	9.5×10^{-4}		Plyasunova et al. (2004)	L	
$C_5H_{12}S$	1.5×10^{-3}		Yaws et al. (2003)	V	804
[541-31-1]	1.5×10^{-3}		Yaws (2003)	X	238
GIJGXNFNUUFEGH-UHFFFAOYSA-N	3.7×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
3-methyl-2-butanethiol	1.5×10^{-3}		Yaws et al. (2003)	V	804
$C_5H_{12}S$	1.5×10^{-3}		Yaws (2003)	X	238
[2084-18-6]	4.0×10^{-4}		Gharagheizi et al. (2012)	Q	
BFLXFRNPNMTTAA-UHFFFAOYSA-N	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
1-hexanethiol	5.2×10^{-4}		Plyasunova et al. (2004)	L	
$C_6H_{14}S$	1.1×10^{-3}		Yaws et al. (2003)	V	804
(hexyl mercaptan)	1.1×10^{-3}		Yaws (2003)	X	238
[111-31-9]	3.5×10^{-4}		Gharagheizi et al. (2012)	Q	
PMBXCGGQNSVESQ-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.9×10^{-3}		Hilal et al. (2008)	Q	
	1.4×10^{-3}		Yao et al. (2002)	Q	230

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.5×10^{-4}		Yaws (1999)	?	21
2-hexanethiol	1.2×10^{-3}		Yaws et al. (2003)	V	804
$C_6H_{14}S$	1.2×10^{-3}		Yaws (2003)	X	238
[1679-06-7]	4.9×10^{-4}		Gharagheizi et al. (2012)	Q	
ABNPJVOPTXYSQW-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
1-heptanethiol	4.2×10^{-4}		Plyasunova et al. (2004)	L	
$C_7H_{16}S$	4.0×10^{-4}		Duchowicz et al. (2020)	V	187
(heptyl mercaptan)	9.5×10^{-4}		Yaws et al. (2003)	V	804
[1639-09-4]	8.2×10^{-4}		Yaws (2003)	X	238
VPIAKHNXCOTPAY-UHFFFAOYSA-N	4.8×10^{-2}		Duchowicz et al. (2020)	Q	
	2.7×10^{-4}		Gharagheizi et al. (2012)	Q	
	8.4×10^{-4}		Gharagheizi et al. (2010)	Q	247
	2.7×10^{-3}		Hilal et al. (2008)	Q	
	1.2×10^{-3}		Yao et al. (2002)	Q	230, 268
	3.3×10^{-4}		Yaws (1999)	?	21
2-heptanethiol	1.3×10^{-3}		Yaws et al. (2003)	V	804
$C_7H_{16}S$	8.2×10^{-4}		Yaws (2003)	X	238
[628-00-2]	4.1×10^{-4}		Gharagheizi et al. (2012)	Q	
DAZNOIJJVKASGS-UHFFFAOYSA-N	8.3×10^{-4}		Gharagheizi et al. (2010)	Q	247
1-octanethiol	7.1×10^{-4}		Yaws et al. (2003)	V	804
$C_8H_{18}S$	6.9×10^{-4}		Yaws (2003)	X	238
(octyl mercaptan)	4.3×10^{-4}		HSDB (2015)	Q	100
[111-88-6]	2.0×10^{-4}		Gharagheizi et al. (2012)	Q	
KZCOBXFFBQJQHH-UHFFFAOYSA-N	7.4×10^{-4}		Gharagheizi et al. (2010)	Q	247
	1.3×10^{-3}		Hilal et al. (2008)	Q	
	1.1×10^{-3}		Yao et al. (2002)	Q	230
	3.0×10^{-4}		Yaws (1999)	?	21
tert-octanethiol	2.0×10^{-3}		Yaws et al. (2003)	V	804
$C_8H_{18}S$	6.2×10^{-4}		Yaws (2003)	X	238
(*tert*-octyl mercaptan)	5.2×10^{-4}		HSDB (2015)	Q	100
[141-59-3]	2.8×10^{-4}		Gharagheizi et al. (2012)	Q	
QZLAEIZEPJAELS-UHFFFAOYSA-N	6.6×10^{-4}		Gharagheizi et al. (2010)	Q	247
	4.2×10^{-4}		Yao et al. (2002)	Q	230
	2.6×10^{-4}		Yaws (1999)	?	21
2-octanethiol	9.9×10^{-4}		Yaws et al. (2003)	V	804
$C_8H_{18}S$	6.6×10^{-4}		Yaws (2003)	X	238
[3001-66-9]	3.0×10^{-4}		Gharagheizi et al. (2012)	Q	
BZXFEMZFRLXGCY-UHFFFAOYSA-N	6.9×10^{-4}		Gharagheizi et al. (2010)	Q	247

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-nonanethiol	5.7×10^{-4}		Yaws et al. (2003)	V	804
$C_9H_{20}S$	6.7×10^{-4}		Yaws (2003)	X	238
(nonyl mercaptan)	1.5×10^{-4}		Gharagheizi et al. (2012)	Q	
[1455-21-6]	7.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
ZVEZMVFBMOOHAT-UHFFFAOYSA-N	1.2×10^{-3}		Hilal et al. (2008)	Q	
	8.9×10^{-4}		Yao et al. (2002)	Q	230, 268
	3.7×10^{-4}		Yaws (1999)	?	21
2-nonanethiol	7.7×10^{-4}		Yaws et al. (2003)	V	804
$C_9H_{20}S$	5.1×10^{-4}		Yaws (2003)	X	238
[13281-11-3]	2.3×10^{-4}		Gharagheizi et al. (2012)	Q	
UOMSUBPWUZCGQU-UHFFFAOYSA-N	6.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
1-decanethiol	5.0×10^{-4}		Yaws et al. (2003)	V	804
$C_{10}H_{22}S$	8.1×10^{-4}		Yaws (2003)	X	238
(decyl mercaptan)	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[143-10-2]	7.7×10^{-4}		Gharagheizi et al. (2010)	Q	247
VTXVGVNLYGSIAR-UHFFFAOYSA-N	9.9×10^{-4}		Hilal et al. (2008)	Q	
	8.2×10^{-4}		Yao et al. (2002)	Q	230
	6.5×10^{-4}		Yaws (1999)	?	21
2-decanethiol	6.5×10^{-4}		Yaws et al. (2003)	V	804
$C_{10}H_{22}S$	4.4×10^{-4}		Yaws (2003)	X	238
[13402-60-3]	2.5×10^{-4}		Gharagheizi et al. (2012)	Q	
NWKXKAHGQAWFQP-UHFFFAOYSA-N	5.8×10^{-4}		Gharagheizi et al. (2010)	Q	247
1-undecanethiol	4.9×10^{-4}		Yaws et al. (2003)	V	804
$C_{11}H_{24}S$	2.6×10^{-3}		Yaws (2003)	X	238
(undecyl mercaptan)	9.3×10^{-4}		Gharagheizi et al. (2010)	Q	247
[5332-52-5]	6.7×10^{-4}		Yao et al. (2002)	Q	230
CCIDWXHLGNEQSL-UHFFFAOYSA-N	3.4×10^{-3}		Yaws (1999)	?	21
2-undecanethiol	6.1×10^{-4}		Yaws et al. (2003)	V	804
$C_{11}H_{24}S$	6.6×10^{-4}		Yaws (2003)	X	238
[62155-02-6]	2.9×10^{-4}		Gharagheizi et al. (2012)	Q	
KRMLVHZORKTOLI-UHFFFAOYSA-N	6.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
1-dodecanethiol	5.3×10^{-4}		Yaws et al. (2003)	V	804
$C_{12}H_{26}S$	5.8×10^{-4}		Yaws (2003)	X	238
(dodecyl mercaptan)	1.7×10^{-4}		HSDB (2015)	Q	100
[112-55-0]	1.9×10^{-4}		Gharagheizi et al. (2012)	Q	
WNAHIZMDSQCWRP-UHFFFAOYSA-N	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
	5.3×10^{-4}		Yao et al. (2002)	Q	230
	1.4×10^{-3}		Yaws (1999)	?	21
2-dodecanethiol	6.3×10^{-4}		Yaws et al. (2003)	V	804
$C_{12}H_{26}S$	7.2×10^{-4}		Yaws (2003)	X	238
[14402-50-7]	3.0×10^{-4}		Gharagheizi et al. (2012)	Q	
UROXMPKAGAWKPP-UHFFFAOYSA-N	6.9×10^{-4}		Gharagheizi et al. (2010)	Q	247

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5-propyl-5-nonanethiol	1.7×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_{26}S$	5.8×10^{-4}		Zhang et al. (2010)	Q	288, 290
BGQHJKADBZPYGJ-UHFFFAOYSA-N	2.4×10^{-3}		Zhang et al. (2010)	Q	288, 291
	9.7×10^{-5}		Zhang et al. (2010)	Q	288, 292
1-tridecanethiol	6.4×10^{-4}		Yaws et al. (2003)	V	804
$C_{13}H_{28}S$	2.8×10^{-3}		Yaws (2003)	X	238
[19484-26-5]	2.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
IPBROXKVGHZHJV-UHFFFAOYSA-N					
2-tridecanethiol	7.3×10^{-4}		Yaws et al. (2003)	V	804
$C_{13}H_{28}S$	9.6×10^{-4}		Yaws (2003)	X	238
[62155-03-7]	3.2×10^{-4}		Gharagheizi et al. (2012)	Q	
ZAPRCDVCNIREGW-UHFFFAOYSA-N	9.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
1-tetradecanethiol	8.5×10^{-4}		Yaws et al. (2003)	V	804
$C_{14}H_{30}S$	5.1×10^{-3}		Yaws (2003)	X	238
[2079-95-0]	4.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
GEKDEMKPCKTKEC-UHFFFAOYSA-N					
2-tetradecanethiol	9.2×10^{-4}		Yaws et al. (2003)	V	804
$C_{14}H_{30}S$	1.5×10^{-3}		Yaws (2003)	X	238
[62155-04-8]	3.4×10^{-4}		Gharagheizi et al. (2012)	Q	
YESAYZVWGLMPDY-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
dimethyl sulfide	5.3×10^{-3}	3500	Burkholder et al. (2019)	L	
CH_3SCH_3	5.3×10^{-3}	3500	Burkholder et al. (2015)	L	
(DMS)	5.4×10^{-3}	3500	Brockbank (2013)	L	1
[75-18-3]	5.6×10^{-3}	3500	Warneck and Williams (2012)	L	
QMMFVYPAHWMCMS-UHFFFAOYSA-N	5.3×10^{-3}	3500	Sander et al. (2011)	L	
	5.3×10^{-3}	3500	Sander et al. (2006)	L	
	5.3×10^{-3}	3800	Plyasunova et al. (2004)	L	
	5.2×10^{-3}	3600	Fogg and Sangster (2003)	L	
	5.3×10^{-3}	3500	Staudinger and Roberts (2001)	L	
	4.7×10^{-3}	4700	Bruneel et al. (2016)	M	
	4.6×10^{-3}		Schuhfried et al. (2011)	M	
	4.8×10^{-3}	2800	Falabella (2007)	M	11, 340
	5.2×10^{-3}	3600	Coquelet and Richon (2005)	M	
	5.5×10^{-3}	3800	Iliuta and Larachi (2005a)	M	
	4.9×10^{-3}		Straver and de Loos (2005)	M	
	6.4×10^{-3}	4100	Barcellos da Rosa et al. (2003)	M	
	4.9×10^{-3}		Pollien et al. (2003)	M	
	6.4×10^{-3}		van Ruth et al. (2002)	M	14
	7.2×10^{-3}		van Ruth and Villeneuve (2002)	M	14, 363
	4.7×10^{-3}	3700	Gershenzon et al. (2001)	M	
	4.9×10^{-3}		van Ruth et al. (2001)	M	14
	1.6×10^{-2}		Marin et al. (1999)	M	
	4.2×10^{-3}	4300	Wong and Wang (1997)	M	

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.7×10^{-3}	3100	De Bruyn et al. (1995b)	M	
	5.7×10^{-3}	2700	Tsuji et al. (1990)	M	63
	5.5×10^{-3}	3500	Dacey et al. (1984)	M	
	5.6×10^{-3}	4000	Przyjazny et al. (1983)	M	
	6.1×10^{-3}		Vitenberg et al. (1975)	M	12
	1.6×10^{-3}		Lovelock et al. (1972)	M	
			Mackay et al. (2006d)	V	560
	4.2×10^{-3}		Marin et al. (1999)	V	
	1.3×10^{-1}		Mackay et al. (1995)	V	
	5.4×10^{-3}		Hine and Mookerjee (1975)	V	
	5.5×10^{-3}		Hine and Weimar (1965)	V	
	7.0×10^{-3}		Vitenberg et al. (1975)	R	12
	6.0×10^{-3}	3700	Bagno et al. (1991)	T	475
	5.5×10^{-3}		Yaws (2003)	X	238
	6.1×10^{-3}		Gaffney and Senum (1984)	X	391
	4.4×10^{-3}		Cline and Bates (1983)	C	71
	2.3×10^{-3}		Keshavarz et al. (2022)	Q	
	1.7×10^{-1}		Duchowicz et al. (2020)	Q	185
	1.7×10^{-3}		Wang et al. (2017)	Q	81, 239
	1.7×10^{-2}		Wang et al. (2017)	Q	81, 240
	4.9×10^{-3}		Wang et al. (2017)	Q	81, 241
	1.9×10^{-3}		Gharagheizi et al. (2012)	Q	
	8.7×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	3.3×10^{-3}		Modarresi et al. (2007)	Q	68
	7.2×10^{-3}		Hertel et al. (2007)	Q	469
		3100	Kühne et al. (2005)	Q	
	6.2×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	4.8×10^{-3}		English and Carroll (2001)	Q	231, 232
	5.0×10^{-3}		Marin et al. (1999)	Q	
	3.1×10^{-3}		Katritzky et al. (1998)	Q	
	6.5×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	7.9×10^{-4}		Russell et al. (1992)	Q	280
	6.4×10^{-3}		Suzuki et al. (1992)	Q	233
	6.1×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		3500	Kühne et al. (2005)	?	
	5.5×10^{-3}		Yaws et al. (2003)	?	21
	4.9×10^{-3}		Yaws (1999)	?	21
	1.7×10^{-3}		Abraham et al. (1990)	?	

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethyl methyl sulfide	4.2×10^{-3}		Burkholder et al. (2019)	L	
$C_2H_5SCH_3$	4.2×10^{-3}		Burkholder et al. (2015)	L	
[624-89-5]	4.2×10^{-3}		Schuhfried et al. (2011)	M	
WXEHBUMAEPOYKP-UHFFFAOYSA-N	5.4×10^{-3}		Yaws et al. (2003)	V	804
	5.1×10^{-3}		Bagno et al. (1991)	T	475
	5.4×10^{-3}		Yaws (2003)	X	238
	2.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	5.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
	8.6×10^{-3}		Hilal et al. (2008)	Q	
	5.1×10^{-3}		Yao et al. (2002)	Q	230
	3.5×10^{-3}		English and Carroll (2001)	Q	231, 232
	4.4×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	5.0×10^{-3}		Yaws (1999)	?	21
diethyl sulfide	3.5×10^{-3}		Burkholder et al. (2019)	L	
$C_2H_5SC_2H_5$	3.5×10^{-3}		Burkholder et al. (2015)	L	
[352-93-2]	4.7×10^{-3}	4800	Plyasunova et al. (2004)	L	
LJSQFQKUNVCTIA-UHFFFAOYSA-N	3.5×10^{-3}		Schuhfried et al. (2011)	M	
	5.4×10^{-3}	4900	Przyjazny et al. (1983)	M	
	5.1×10^{-1}		Mackay et al. (2006d)	V	
	4.5×10^{-3}		Hine and Mookerjee (1975)	V	
	4.5×10^{-3}		Yaws (2003)	X	238
	4.3×10^{-3}		Keshavarz et al. (2022)	Q	
	2.0×10^{-2}		Duchowicz et al. (2020)	Q	185
	3.4×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.7×10^{-3}		Gharagheizi et al. (2010)	Q	247
	6.0×10^{-3}		Hilal et al. (2008)	Q	
	3.6×10^{-3}		Modarresi et al. (2007)	Q	68
	4.8×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	4.0×10^{-3}		Yao et al. (2002)	Q	230
	4.6×10^{-3}		English and Carroll (2001)	Q	231, 275
	2.6×10^{-3}		Katritzky et al. (1998)	Q	
	2.9×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	1.5×10^{-3}		Russell et al. (1992)	Q	280
	3.9×10^{-3}		Suzuki et al. (1992)	Q	233
	5.9×10^{-3}		Duchowicz et al. (2020)	?	186, 21
	1.1×10^{-2}		Yaws et al. (2003)	?	21
	4.4×10^{-3}		Yaws (1999)	?	21, 12
	5.7×10^{-3}		Yaws and Yang (1992)	?	21, 12
	4.7×10^{-3}		Abraham et al. (1990)	?	

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl isopropyl sulfide	4.5×10^{-3}		Yaws et al. (2003)	V	804
$C_4H_{10}S$	4.5×10^{-3}		Yaws (2003)	X	238
[1551-21-9]	2.7×10^{-3}		Gharagheizi et al. (2012)	Q	
ROSSIHMZZJOVOU-UHFFFAOYSA-N	4.6×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.6×10^{-3}		Yao et al. (2002)	Q	230
	3.5×10^{-3}		Yaws (1999)	?	21
methyl propyl sulfide	4.3×10^{-3}		Plyasunova et al. (2004)	L	
$C_4H_{10}S$	4.3×10^{-3}		Mazza (1980)	M	
[3877-15-4]	4.5×10^{-3}		Yaws et al. (2003)	V	804
ZOASGOXWEHUTKZ-UHFFFAOYSA-N	4.5×10^{-3}		Yaws (2003)	X	238
	1.1×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.2×10^{-3}		Gharagheizi et al. (2010)	Q	247
	4.1×10^{-3}		Yao et al. (2002)	Q	230
	3.1×10^{-3}		Yaws (1999)	?	21
tetrahydrothiophene	2.2×10^{-3}		Yaws et al. (2003)	V	804
C_4H_8S	1.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[110-01-0]					
RAOIDOHSFRTOEL-UHFFFAOYSA-N					
2-methyl-3-thiapentane	3.7×10^{-3}		Yaws et al. (2003)	V	804
$C_5H_{12}S$	3.7×10^{-3}		Yaws (2003)	X	238
[5145-99-3]	3.7×10^{-3}		Gharagheizi et al. (2012)	Q	
NZUQQADVSXWVNW-UHFFFAOYSA-N	3.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
3,3-dimethyl-2-thiabutane	3.6×10^{-3}		Yaws et al. (2003)	V	804
$C_5H_{12}S$	3.6×10^{-3}		Yaws (2003)	X	238
[6163-64-0]	2.9×10^{-3}		Gharagheizi et al. (2012)	Q	
CJFVCTVYZFTORU-UHFFFAOYSA-N	3.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
3-methyl-2-thiapentane	3.6×10^{-3}		Yaws et al. (2003)	V	804
$C_5H_{12}S$	3.5×10^{-3}		Yaws (2003)	X	238
[10359-64-5]	1.3×10^{-3}		Gharagheizi et al. (2012)	Q	
IJRCRFQMYAJPPO-UHFFFAOYSA-N	3.6×10^{-3}		Gharagheizi et al. (2010)	Q	247
4-methyl-2-thiapentane	3.5×10^{-3}		Yaws et al. (2003)	V	804
$C_5H_{12}S$	3.5×10^{-3}		Yaws (2003)	X	238
[5008-69-5]	4.3×10^{-4}		Gharagheizi et al. (2012)	Q	
UYVGFIKOUAFDOZ-UHFFFAOYSA-N	4.2×10^{-3}		Gharagheizi et al. (2010)	Q	247
ethyl propyl sulfide	3.5×10^{-3}		Yaws et al. (2003)	V	804
$C_5H_{12}S$	3.5×10^{-3}		Yaws (2003)	X	238
[4110-50-3]	1.6×10^{-3}		Gharagheizi et al. (2012)	Q	
ZDDDFDQTSXYYSE-UHFFFAOYSA-N	2.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.1×10^{-3}		Yao et al. (2002)	Q	230
	1.9×10^{-3}		Yaws (1999)	?	21

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl butyl sulfide	3.4×10^{-3}		Yaws et al. (2003)	V	804
$C_5H_{12}S$	3.4×10^{-3}		Yaws (2003)	X	238
[628-29-5]	8.6×10^{-4}		Gharagheizi et al. (2012)	Q	
WCXXISMIJBRDQK-UHFFFAOYSA-N	3.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
	2.2×10^{-3}		Yao et al. (2002)	Q	230
	1.8×10^{-3}		Yaws (1999)	?	21
dipropyl sulfide	3.3×10^{-3}	5700	Plyasunova et al. (2004)	L	
$C_3H_7SC_3H_7$	3.3×10^{-3}	4500	Przyjazny et al. (1983)	M	
[111-47-7]	2.7×10^{-3}		Yaws et al. (2003)	V	804
ZERULLAPCVRMCO-UHFFFAOYSA-N	2.7×10^{-3}		Yaws (2003)	X	238
	7.8×10^{-3}		Keshavarz et al. (2022)	Q	
	2.0×10^{-2}		Duchowicz et al. (2020)	Q	300
	8.9×10^{-4}		Gharagheizi et al. (2012)	Q	
	2.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
	3.4×10^{-3}		Hilal et al. (2008)	Q	
		4500	Kühne et al. (2005)	Q	
	4.8×10^{-3}		Yaffe et al. (2003)	Q	249, 273
	1.9×10^{-3}		Yao et al. (2002)	Q	230
	3.1×10^{-3}		English and Carroll (2001)	Q	231, 232
	1.8×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	3.0×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4500	Kühne et al. (2005)	?	
	1.2×10^{-3}		Yaws (1999)	?	21
	3.5×10^{-3}		Abraham et al. (1990)	?	
di-(2-propyl)-sulfide	2.8×10^{-3}	4900	Brockbank (2013)	L	
$(C_3H_7)_2S$	3.0×10^{-3}		Plyasunova et al. (2004)	L	
(diisopropyl sulfide)	3.0×10^{-3}	5000	Przyjazny et al. (1983)	M	
[625-80-9]	2.9×10^{-3}		Yaws et al. (2003)	V	804
XYWDPYKBIRQXQS-UHFFFAOYSA-N	2.9×10^{-3}		Yaws (2003)	X	238
	7.8×10^{-3}		Keshavarz et al. (2022)	Q	
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	4.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.2×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.6×10^{-3}		Hilal et al. (2008)	Q	
		4500	Kühne et al. (2005)	Q	
	3.1×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.1×10^{-3}		Yao et al. (2002)	Q	230
	1.2×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	3.0×10^{-3}		Duchowicz et al. (2020)	?	186, 21
		4200	Kühne et al. (2005)	?	
	1.5×10^{-3}		Yaws (1999)	?	21
	3.1×10^{-3}		Abraham et al. (1990)	?	

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2-dimethyl-3-thiapentane	2.8×10^{-3}		Yaws et al. (2003)	V	804
$C_6H_{14}S$	2.8×10^{-3}		Yaws (2003)	X	238
[14290-92-7]	4.9×10^{-3}		Gharagheizi et al. (2012)	Q	
GZJUDUMQICJSFJ-UHFFFAOYSA-N	2.8×10^{-3}		Gharagheizi et al. (2010)	Q	247
2-methyl-3-thiahexane	2.8×10^{-3}		Yaws et al. (2003)	V	804
$C_6H_{14}S$	2.7×10^{-3}		Yaws (2003)	X	238
[5008-73-1]	2.1×10^{-3}		Gharagheizi et al. (2012)	Q	
BDFDQOJJDDORSR-UHFFFAOYSA-N	2.6×10^{-3}		Gharagheizi et al. (2010)	Q	247
3,3-dimethyl-2-thiapentane	2.7×10^{-3}		Yaws et al. (2003)	V	804
$C_6H_{14}S$	2.7×10^{-3}		Yaws (2003)	X	238
[13286-92-5]	1.9×10^{-3}		Gharagheizi et al. (2012)	Q	
SJOHDSPLOVBXOF-UHFFFAOYSA-N	3.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
3,4-dimethyl-2-thiapentane	2.9×10^{-3}		Yaws et al. (2003)	V	804
$C_6H_{14}S$	2.9×10^{-3}		Yaws (2003)	X	238
[53897-51-1]	6.1×10^{-4}		Gharagheizi et al. (2012)	Q	
AUNQXXJGFDKEMS-UHFFFAOYSA-N	3.2×10^{-3}		Gharagheizi et al. (2010)	Q	247
3-ethyl-2-thiapentane	3.0×10^{-3}		Yaws et al. (2003)	V	804
$C_6H_{14}S$	3.0×10^{-3}		Yaws (2003)	X	238
[57093-84-2]	6.6×10^{-4}		Gharagheizi et al. (2012)	Q	
ZQOHJVSSVAWXQZ-UHFFFAOYSA-N	2.8×10^{-3}		Gharagheizi et al. (2010)	Q	247
3-methyl-2-thiahexane	2.8×10^{-3}		Yaws et al. (2003)	V	804
$C_6H_{14}S$	2.7×10^{-3}		Yaws (2003)	X	238
[13286-91-4]	1.2×10^{-3}		Gharagheizi et al. (2012)	Q	
WGBHWWSSUGCSCP-UHFFFAOYSA-N	2.6×10^{-3}		Gharagheizi et al. (2010)	Q	247
4,4-dimethyl-2-thiapentane	2.7×10^{-3}		Yaws et al. (2003)	V	804
$C_6H_{14}S$	2.7×10^{-3}		Yaws (2003)	X	238
[6079-57-8]	3.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
YUFAJXXIXSYTMS-UHFFFAOYSA-N					
4-methyl-2-thiahexane	2.7×10^{-3}		Yaws et al. (2003)	V	804
$C_6H_{14}S$	2.7×10^{-3}		Yaws (2003)	X	238
[15013-37-3]	3.9×10^{-4}		Gharagheizi et al. (2012)	Q	
XMOUDDXUCXXDTJ-UHFFFAOYSA-N	2.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
4-methyl-3-thiahexane	2.7×10^{-3}		Yaws et al. (2003)	V	804
$C_6H_{14}S$	2.7×10^{-3}		Yaws (2003)	X	238
[5008-72-0]	2.2×10^{-3}		Gharagheizi et al. (2012)	Q	
JFNGZXUPUVUYST-UHFFFAOYSA-N	2.6×10^{-3}		Gharagheizi et al. (2010)	Q	247
5-methyl-2-thiahexane	2.8×10^{-3}		Yaws et al. (2003)	V	804
$C_6H_{14}S$	2.8×10^{-3}		Yaws (2003)	X	238
[13286-90-3]	5.4×10^{-4}		Gharagheizi et al. (2012)	Q	
ABIKQXWLJOURPN-UHFFFAOYSA-N	2.7×10^{-3}		Gharagheizi et al. (2010)	Q	247

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5-methyl-3-thiahexane	2.7×10^{-3}		Yaws et al. (2003)	V	804
$C_6H_{14}S$	2.7×10^{-3}		Yaws (2003)	X	238
[1613-45-2]	7.1×10^{-4}		Gharagheizi et al. (2012)	Q	
OIRKGXWQBSPXLQ-UHFFFAOYSA-N	2.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
ethyl butyl sulfide	2.6×10^{-3}		Yaws et al. (2003)	V	804
$C_6H_{14}S$	2.6×10^{-3}		Yaws (2003)	X	238
[638-46-0]	1.2×10^{-3}		Gharagheizi et al. (2012)	Q	
XJIRSLHMKBUGMR-UHFFFAOYSA-N	2.2×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.9×10^{-3}		Yao et al. (2002)	Q	230
	1.2×10^{-3}		Yaws (1999)	?	21
methyl pentyl sulfide	3.8×10^{-3}		Yaws et al. (2003)	V	804
$C_6H_{14}S$	3.8×10^{-3}		Yaws (2003)	X	238
[1741-83-9]	2.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
FOJGPFUFFHWGFQ-UHFFFAOYSA-N					
ethyl pentyl sulfide	1.0×10^{-3}		Yaws et al. (2003)	V	804
$C_7H_{16}S$	9.6×10^{-4}		Yaws (2003)	X	238
[26158-99-6]	1.1×10^{-3}		Gharagheizi et al. (2012)	Q	
SOGIWVXLDPPMMF-UHFFFAOYSA-N	1.8×10^{-3}		Gharagheizi et al. (2010)	Q	247
methyl hexyl sulfide	1.0×10^{-3}		Yaws et al. (2003)	V	804
$C_7H_{16}S$	9.6×10^{-4}		Yaws (2003)	X	238
[20291-60-5]	5.2×10^{-4}		Gharagheizi et al. (2012)	Q	
LZRXQHHKXDXOIC-UHFFFAOYSA-N	1.8×10^{-3}		Gharagheizi et al. (2010)	Q	247
propyl butyl sulfide	1.0×10^{-3}		Yaws et al. (2003)	V	804
$C_7H_{16}S$	9.6×10^{-4}		Yaws (2003)	X	238
[1613-46-3]	7.6×10^{-4}		Gharagheizi et al. (2012)	Q	
ZBRWJPVULTZZCE-UHFFFAOYSA-N	1.8×10^{-3}		Gharagheizi et al. (2010)	Q	247
dibutyl sulfide	1.3×10^{-3}		Yaws et al. (2003)	V	804
$C_8H_{18}S$	1.3×10^{-3}		Yaws (2003)	X	238
[544-40-1]	3.9×10^{-4}		Gharagheizi et al. (2012)	Q	
HTIRHQRTDBPHNZ-UHFFFAOYSA-N	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
ethyl hexyl sulfide	6.2×10^{-4}		Yaws et al. (2003)	V	804
$C_8H_{18}S$	6.2×10^{-4}		Yaws (2003)	X	238
[7309-44-6]	8.7×10^{-4}		Gharagheizi et al. (2012)	Q	
MGVUJBCOCITTRS-UHFFFAOYSA-N	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
methyl heptyl sulfide	6.2×10^{-4}		Yaws et al. (2003)	V	804
$C_8H_{18}S$	6.2×10^{-4}		Yaws (2003)	X	238
[20291-61-6]	4.0×10^{-4}		Gharagheizi et al. (2012)	Q	
FJDWJOQOEZRIDJ-UHFFFAOYSA-N	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	247

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
propyl pentyl sulfide	6.2×10^{-4}		Yaws et al. (2003)	V	804
$C_8H_{18}S$	6.2×10^{-4}		Yaws (2003)	X	238
[42841-80-5]	5.9×10^{-4}		Gharagheizi et al. (2012)	Q	
MJRCCWJSYFOGBX-UHFFFAOYSA-N	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
butyl pentyl sulfide	9.8×10^{-4}		Yaws et al. (2003)	V	804
$C_9H_{20}S$	9.7×10^{-4}		Yaws (2003)	X	238
[24768-42-1]	7.0×10^{-4}		Gharagheizi et al. (2012)	Q	
RNEUXBDXTNIASG-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
ethyl heptyl sulfide	9.8×10^{-4}		Yaws et al. (2003)	V	804
$C_9H_{20}S$	9.7×10^{-4}		Yaws (2003)	X	238
[24768-44-3]	1.0×10^{-3}		Gharagheizi et al. (2012)	Q	
PYPULUCCVXMPFP-UHFFFAOYSA-N	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
methyl octyl sulfide	9.8×10^{-4}		Yaws et al. (2003)	V	804
$C_9H_{20}S$	9.7×10^{-4}		Yaws (2003)	X	238
[3698-95-1]	4.7×10^{-4}		Gharagheizi et al. (2012)	Q	
AHCJTMBRROLNHV-UHFFFAOYSA-N	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
propyl hexyl sulfide	9.8×10^{-4}		Yaws et al. (2003)	V	804
$C_9H_{20}S$	9.7×10^{-4}		Yaws (2003)	X	238
[24768-43-2]	7.0×10^{-4}		Gharagheizi et al. (2012)	Q	
ABZLKKGJOVPBBL-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
butyl hexyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	804
$C_{10}H_{22}S$	1.6×10^{-3}		Yaws (2003)	X	238
[16967-04-7]	8.1×10^{-4}		Gharagheizi et al. (2012)	Q	
YZUHMAFUXBPUKH-UHFFFAOYSA-N	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
dipentyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	804
$C_{10}H_{22}S$	1.6×10^{-3}		Yaws (2003)	X	238
[872-10-6]	8.1×10^{-4}		Gharagheizi et al. (2012)	Q	
JOZDADPMWLVEJK-UHFFFAOYSA-N	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
ethyl octyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	804
$C_{10}H_{22}S$	1.6×10^{-3}		Yaws (2003)	X	238
[3698-94-0]	1.2×10^{-3}		Gharagheizi et al. (2012)	Q	
WAITXWGCJQLPGH-UHFFFAOYSA-N	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
methyl nonyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	804
$C_{10}H_{22}S$	1.6×10^{-3}		Yaws (2003)	X	238
[59973-07-8]	3.6×10^{-4}		Gharagheizi et al. (2012)	Q	
FCRSULZJMFDBIK-UHFFFAOYSA-N	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	247
propyl heptyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	804
$C_{10}H_{22}S$	1.6×10^{-3}		Yaws (2003)	X	238
[24768-46-5]	8.1×10^{-4}		Gharagheizi et al. (2012)	Q	
PCPVCHFKVPNTBH-UHFFFAOYSA-N	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	247

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
butyl heptyl sulfide	1.7×10^{-3}		Yaws et al. (2003)	V	804
$C_{11}H_{24}S$	1.7×10^{-3}		Yaws (2003)	X	238
[40813-84-1]	9.1×10^{-4}		Gharagheizi et al. (2012)	Q	
HYUPOCGXBZUYFY-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
ethyl nonyl sulfide	1.7×10^{-3}		Yaws et al. (2003)	V	804
$C_{11}H_{24}S$	1.7×10^{-3}		Yaws (2003)	X	238
[59973-08-9]	8.8×10^{-4}		Gharagheizi et al. (2012)	Q	
LUAABLIRQSWMGZ-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
methyl decyl sulfide	1.7×10^{-3}		Yaws et al. (2003)	V	804
$C_{11}H_{24}S$	1.7×10^{-3}		Yaws (2003)	X	238
[22438-39-7]	4.1×10^{-4}		Gharagheizi et al. (2012)	Q	
HKGUUZAACYBIID-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
propyl octyl sulfide	1.7×10^{-3}		Yaws et al. (2003)	V	804
$C_{11}H_{24}S$	1.7×10^{-3}		Yaws (2003)	X	238
[3698-93-9]	9.1×10^{-4}		Gharagheizi et al. (2012)	Q	
GPJXDRJGQAKGLH-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
butyl octyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	804
$C_{12}H_{26}S$	1.5×10^{-3}		Yaws (2003)	X	238
[16900-07-5]	1.0×10^{-3}		Gharagheizi et al. (2012)	Q	
UNIAPWPIAGJFDG-UHFFFAOYSA-N	1.8×10^{-3}		Gharagheizi et al. (2010)	Q	247
dihexyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	804
$C_{12}H_{26}S$	1.5×10^{-3}		Yaws (2003)	X	238
[6294-31-1]	1.0×10^{-3}		Gharagheizi et al. (2012)	Q	
LHNRHYOMDUJLLM-UHFFFAOYSA-N	1.8×10^{-3}		Gharagheizi et al. (2010)	Q	247
ethyl decyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	804
$C_{12}H_{26}S$	1.5×10^{-3}		Yaws (2003)	X	238
[19313-61-2]	9.7×10^{-4}		Gharagheizi et al. (2012)	Q	
VSSRSPLEFYQIEK-UHFFFAOYSA-N	1.8×10^{-3}		Gharagheizi et al. (2010)	Q	247
methyl undecyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	804
$C_{12}H_{26}S$	1.5×10^{-3}		Yaws (2003)	X	238
[7289-44-3]	4.5×10^{-4}		Gharagheizi et al. (2012)	Q	
HDOADYQJIBYVGE-UHFFFAOYSA-N	1.7×10^{-3}		Gharagheizi et al. (2010)	Q	247
propyl nonyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	804
$C_{12}H_{26}S$	1.5×10^{-3}		Yaws (2003)	X	238
[62103-66-6]	6.6×10^{-4}		Gharagheizi et al. (2012)	Q	
AQAOPNMAEGBYHI-UHFFFAOYSA-N	1.8×10^{-3}		Gharagheizi et al. (2010)	Q	247
butyl nonyl sulfide	1.8×10^{-3}		Yaws et al. (2003)	V	804
$C_{13}H_{28}S$	1.8×10^{-3}		Yaws (2003)	X	238
[66577-32-0]	7.1×10^{-4}		Gharagheizi et al. (2012)	Q	
FWRIVMHSSSZAFD-UHFFFAOYSA-N	2.6×10^{-3}		Gharagheizi et al. (2010)	Q	247

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethyl undecyl sulfide	1.8×10^{-3}		Yaws et al. (2003)	V	804
$C_{13}H_{28}S$	1.8×10^{-3}		Yaws (2003)	X	238
[66577-30-8]	1.0×10^{-3}		Gharagheizi et al. (2012)	Q	
OSWITQLVZPPUIR-UHFFFAOYSA-N	2.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
methyl dodecyl sulfide	1.8×10^{-3}		Yaws et al. (2003)	V	804
$C_{13}H_{28}S$	1.8×10^{-3}		Yaws (2003)	X	238
[3698-89-3]	4.8×10^{-4}		Gharagheizi et al. (2012)	Q	
KJWHJDGMOQJLGF-UHFFFAOYSA-N	2.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
propyl decyl sulfide	1.8×10^{-3}		Yaws et al. (2003)	V	804
$C_{13}H_{28}S$	1.8×10^{-3}		Yaws (2003)	X	238
[66577-31-9]	7.1×10^{-4}		Gharagheizi et al. (2012)	Q	
HPJCKXDELORROO-UHFFFAOYSA-N	2.6×10^{-3}		Gharagheizi et al. (2010)	Q	247
butyl decyl sulfide	2.6×10^{-3}		Yaws et al. (2003)	V	804
$C_{14}H_{30}S$	2.6×10^{-3}		Yaws (2003)	X	238
[19313-57-6]	7.5×10^{-4}		Gharagheizi et al. (2012)	Q	
CLBLVLKZMJDLOT-UHFFFAOYSA-N	4.7×10^{-3}		Gharagheizi et al. (2010)	Q	247
diheptyl sulfide	2.6×10^{-3}		Yaws et al. (2003)	V	804
$C_{14}H_{30}S$	2.6×10^{-3}		Yaws (2003)	X	238
[629-65-2]	1.2×10^{-3}		Gharagheizi et al. (2012)	Q	
LEMIDOZYVQXGLI-UHFFFAOYSA-N	4.7×10^{-3}		Gharagheizi et al. (2010)	Q	247
ethyl dodecyl sulfide	2.6×10^{-3}		Yaws et al. (2003)	V	804
$C_{14}H_{30}S$	2.6×10^{-3}		Yaws (2003)	X	238
[2851-83-4]	1.1×10^{-3}		Gharagheizi et al. (2012)	Q	
QECBTJWQRXCSCU-UHFFFAOYSA-N	4.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
methyl tridecyl sulfide	2.6×10^{-3}		Yaws et al. (2003)	V	804
$C_{14}H_{30}S$	2.6×10^{-3}		Yaws (2003)	X	238
[62155-09-3]	5.1×10^{-4}		Gharagheizi et al. (2012)	Q	
QVXOOYOFFITGCV-UHFFFAOYSA-N	4.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
propyl undecyl sulfide	2.6×10^{-3}		Yaws et al. (2003)	V	804
$C_{14}H_{30}S$	2.6×10^{-3}		Yaws (2003)	X	238
[66826-84-4]	7.5×10^{-4}		Gharagheizi et al. (2012)	Q	
ITNOZFAANYXVSG-UHFFFAOYSA-N	4.7×10^{-3}		Gharagheizi et al. (2010)	Q	247
dimethyl disulfide	5.8×10^{-3}		Burkholder et al. (2019)	L	
CH_3SSCH_3	5.8×10^{-3}		Burkholder et al. (2015)	L	
[624-92-0]	8.3×10^{-3}	3700	Brockbank (2013)	L	
WQOXQRCZOLPYPM-UHFFFAOYSA-N	7.4×10^{-3}	4200	Plyasunova et al. (2004)	L	
	6.7×10^{-3}	5200	Bruneel et al. (2016)	M	
	5.8×10^{-3}		Schuhfried et al. (2011)	M	
	6.5×10^{-3}	3200	Falabella (2007)	M	11, 340
	9.1×10^{-3}	4100	Iliuta and Larachi (2005b)	M	
	7.8×10^{-3}		Souchon et al. (2004)	M	
	5.9×10^{-3}		Pollien et al. (2003)	M	

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.6×10^{-3}		McIntosh and Heffron (2000)	M	14
	9.4×10^{-3}	4300	Przyjazny et al. (1983)	M	
	8.6×10^{-3}		Mazza (1980)	M	
	8.3×10^{-3}		Vitenberg et al. (1975)	M	12
	1.7×10^{-2}		Mackay et al. (2006d)	V	
	1.7×10^{-2}		Mackay et al. (1995)	V	
	9.0×10^{-3}		Vitenberg et al. (1975)	R	12
	3.0×10^{-2}		Hilal et al. (2008)	Q	
	8.7×10^{-2}		Modarresi et al. (2007)	Q	68
		1700	Kühne et al. (2005)	Q	
	4.6×10^{-3}		Nirmalakhandan et al. (1997)	Q	
		1600	Kühne et al. (2005)	?	
	9.0×10^{-3}		Abraham et al. (1990)	?	
diethyl disulfide	3.7×10^{-3}		Burkholder et al. (2019)	L	
$C_2H_5SSC_2H_5$	3.7×10^{-3}		Burkholder et al. (2015)	L	
[110-81-6]	4.0×10^{-3}	4900	Plyasunova et al. (2004)	L	
CETBSQOFQKLHHZ-UHFFFAOYSA-N	3.7×10^{-3}		Schuhfried et al. (2011)	M	
	6.3×10^{-3}	4300	Przyjazny et al. (1983)	M	
	4.7×10^{-3}		Vitenberg et al. (1975)	M	12
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	3.7×10^{-2}		Modarresi et al. (2007)	Q	68
	2.3×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	6.4×10^{-3}		Abraham et al. (1990)	?	
dipropyl disulfide	2.2×10^{-3}	5400	Plyasunova et al. (2004)	L	
$C_3H_7SSC_3H_7$	2.4×10^{-3}		Schuhfried et al. (2011)	M	
[629-19-6]	1.8×10^{-2}		Mazza (1980)	M	
ALVPFGSHPUPROW-UHFFFAOYSA-N					
carbon disulfide	6.1×10^{-4}	4300	Burkholder et al. (2019)	L	
CS_2	6.1×10^{-4}	4300	Burkholder et al. (2015)	L	
[75-15-0]	6.1×10^{-4}	3900	Warneck and Williams (2012)	L	
QGJOPFRUJISHPQ-UHFFFAOYSA-N	6.1×10^{-4}	4300	Sander et al. (2011)	L	
	6.1×10^{-4}	4300	Sander et al. (2006)	L	
	5.5×10^{-4}	3700	Plyasunova et al. (2004)	L	
	5.7×10^{-4}	3800	Hiatt (2013)	M	
	5.4×10^{-4}	2800	De Bruyn et al. (1995b)	M	
	6.2×10^{-4}	3800	Elliott (1989)	M	
	5.4×10^{-4}	4300	Rex (1906)	M	
	5.7×10^{-4}		Mackay et al. (2006d)	V	
	5.7×10^{-4}		Mackay et al. (1995)	V	
	8.0×10^{-4}		Hwang et al. (1992)	V	
	4.5×10^{-4}	4100	Winkler (1906)	V	
	5.1×10^{-4}		Yaws (2003)	X	238
	7.5×10^{-4}	1200	Goldstein (1982)	X	299
	5.0×10^{-4}		Hayer et al. (2022)	Q	20

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.3×10^{-2}		Gharagheizi et al. (2012)	Q	
	5.1×10^{-4}		Gharagheizi et al. (2010)	Q	247
	9.4×10^{-5}		Yaws (1999)	?	21
	3.2×10^{-4}		Abraham and Weathersby (1994)	?	21
	5.1×10^{-4}		Yaws and Yang (1992)	?	21
			Schäfer and Lax (1962)	?	810
			Booth and Jolley (1943)	?	811
			Booth and Jolley (1943)	?	812
2,3,4-trithiapentane $C_2H_6S_3$ (dimethyl trisulfide) [3658-80-8] YWHLKYXPLRWGSE-UHFFFAOYSA-N	1.2×10^{-2}		Plyasunova et al. (2004)	L	
	1.4×10^{-2}		Souchon et al. (2004)	M	
	2.1×10^{-2}		Roberts and Pollien (1997)	M	
dicyclohexyldisulfide $C_{12}H_{22}S_2$ [2550-40-5] ODHAQPXNQDBHSH-UHFFFAOYSA-N	2.5×10^{-3}		HSDB (2015)	Q	100
allyl mercaptan C_3H_6S [870-23-5] ULIKDJVNUXNQHS-UHFFFAOYSA-N	1.2×10^{-2}		Hilal et al. (2008)	Q	
3,3'-thiobis-1-propene $(C_3H_5)_2S$ (diallyl sulfide) [592-88-1] UBJVUCKUDDKUJF-UHFFFAOYSA-N	4.1×10^{-3}		Lindinger et al. (1998)	M	813
	7.1×10^{-3}		Mazza (1980)	M	
	7.6×10^{-3}		HSDB (2015)	Q	100
	9.9×10^{-3}		Hilal et al. (2008)	Q	
allyl methyl sulfide $CH_2CHCH_2SCH_3$ (2-propenyl methyl sulfide) [10152-76-8] NVLPQIPTCCLBEU-UHFFFAOYSA-N	4.2×10^{-3}		Burkholder et al. (2019)	L	
	4.2×10^{-3}		Burkholder et al. (2015)	L	
	4.2×10^{-3}		Schuhfried et al. (2011)	M	
	5.0×10^{-3}		Mazza (1980)	M	
thiophene C_4H_4S [110-02-1] YTPLMLYBLZKORZ-UHFFFAOYSA-N	4.1×10^{-3}	4300	Haimi et al. (2006)	M	814
	4.4×10^{-3}	4000	Przyjazny et al. (1983)	M	
	3.4×10^{-3}		HSDB (2015)	V	
			Mackay et al. (2006d)	V	560
	4.5×10^{-3}		Mackay et al. (1995)	V	
	3.4×10^{-3}		Yaws (2003)	X	238
	8.2×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.4×10^{-3}		Hilal et al. (2008)	Q	
	9.8×10^{-3}		Modarresi et al. (2007)	Q	68
		2800	Kühne et al. (2005)	Q	
	3.4×10^{-3}		Yaffe et al. (2003)	Q	249, 250

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.3×10^{-3}		Yao et al. (2002)	Q	230, 268
	8.8×10^{-3}		English and Carroll (2001)	Q	231, 232
	6.9×10^{-4}		Katritzky et al. (1998)	Q	
	4.5×10^{-3}		Mackay et al. (2006d)	?	
		1900	Kühne et al. (2005)	?	
	3.4×10^{-3}		Yaws et al. (2003)	?	21
	3.4×10^{-3}		Yaws (1999)	?	21
	3.4×10^{-3}		Yaws and Yang (1992)	?	21
	4.4×10^{-3}		Abraham et al. (1990)	?	
2-methylthiophene $CH_3C_4H_3S$ [554-14-3] XQQBUAPQHNYYRS-UHFFFAOYSA-N	4.1×10^{-3}	4300	Brockbank (2013)	L	
	4.1×10^{-3}	4300	Przyjazny et al. (1983)	M	
	2.2×10^{-3}		Yaws et al. (2003)	V	804
	1.9×10^{-3}		Yaws (2003)	X	238
	2.9×10^{-2}		Keshavarz et al. (2022)	Q	
	2.7×10^{-2}		Duchowicz et al. (2020)	Q	
	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.4×10^{-3}		Hilal et al. (2008)	Q	
	8.0×10^{-3}		English and Carroll (2001)	Q	231, 232
	4.1×10^{-3}		Duchowicz et al. (2020)	?	186, 21
	4.1×10^{-3}		Abraham et al. (1990)	?	
3-methylthiophene $CH_3C_4H_3S$ [616-44-4] QENGPZGAWFQWCZ-UHFFFAOYSA-N	1.4×10^{-3}		Duchowicz et al. (2020)	V	187
	1.4×10^{-3}		Yaws (2003)	X	238
	2.7×10^{-2}		Duchowicz et al. (2020)	Q	
	4.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.9×10^{-3}		Gharagheizi et al. (2010)	Q	247
	1.7×10^{-3}		Hilal et al. (2008)	Q	
	8.2×10^{-3}		Modarresi et al. (2007)	Q	68
	1.4×10^{-3}		Yaffe et al. (2003)	Q	249, 250
	1.8×10^{-3}		Katritzky et al. (1998)	Q	
	1.4×10^{-3}		Yaws et al. (2003)	?	21
propyl allyl disulfide $C_6H_{12}S_2$ [2179-59-1] FCSSPCOFDUKHPV-UHFFFAOYSA-N	3.5×10^{-3}		HSDB (2015)	Q	100
4,5-dithia-1,7-octadiene $C_6H_{10}S_2$ (diallyl disulfide) [2179-57-9] PFRGXCVKLLPLIP-UHFFFAOYSA-N	7.5×10^{-3}		Mazza (1980)	M	

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-dimethylthiophene	1.5×10^{-3}		Yaws et al. (2003)	V	804
C_6H_8S	1.3×10^{-3}		Yaws (2003)	X	238
[632-16-6]	4.8×10^{-3}		Gharagheizi et al. (2012)	Q	
BZYUMXXOAYSFOW-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
2,4-dimethylthiophene	1.5×10^{-3}		Yaws et al. (2003)	V	804
C_6H_8S	1.3×10^{-3}		Yaws (2003)	X	238
[638-00-6]	4.7×10^{-3}		Gharagheizi et al. (2012)	Q	
CPULIKNSOUFMPL-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
2,5-dimethylthiophene	3.7×10^{-3}		Mazza (1980)	M	
C_6H_8S	1.6×10^{-3}		Yaws et al. (2003)	V	804
[638-02-8]	1.4×10^{-3}		Yaws (2003)	X	238
GWQOOADXMVQEFT-UHFFFAOYSA-N	1.3×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
2-ethylthiophene	1.4×10^{-3}		Yaws (2003)	X	238
C_6H_8S	3.9×10^{-3}		Gharagheizi et al. (2012)	Q	
[872-55-9]	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	247
JCCCMAAJYSNBPR-UHFFFAOYSA-N	1.9×10^{-3}		Yaws et al. (2003)	?	21
3,4-dimethylthiophene	1.5×10^{-3}		Yaws et al. (2003)	V	804
C_6H_8S	1.2×10^{-3}		Yaws (2003)	X	238
[632-15-5]	1.7×10^{-3}		Gharagheizi et al. (2012)	Q	
GPSFYJDZKSRMKZ-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
3-ethylthiophene	1.6×10^{-3}		Yaws et al. (2003)	V	804
C_6H_8S	1.4×10^{-3}		Yaws (2003)	X	238
[1795-01-3]	1.9×10^{-3}		Gharagheizi et al. (2012)	Q	
SLDBAXYJAIRQMX-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	247
2,3,4-trimethylthiophene	1.3×10^{-3}		Yaws et al. (2003)	V	804
$C_7H_{10}S$	1.1×10^{-3}		Yaws (2003)	X	238
[1795-04-6]	2.9×10^{-3}		Gharagheizi et al. (2012)	Q	
MAVVDCDMBKFUES-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
2,3,5-trimethylthiophene	1.1×10^{-3}		Yaws et al. (2003)	V	804
$C_7H_{10}S$	9.3×10^{-4}		Yaws (2003)	X	238
[1795-05-7]	7.2×10^{-3}		Gharagheizi et al. (2012)	Q	
QKZJQIHBRCFDGQ-UHFFFAOYSA-N	9.7×10^{-4}		Gharagheizi et al. (2010)	Q	247
2-isopropylthiophene	1.3×10^{-3}		Yaws et al. (2003)	V	804
$C_7H_{10}S$	1.1×10^{-3}		Yaws (2003)	X	238
[4095-22-1]	1.8×10^{-3}		Gharagheizi et al. (2012)	Q	
LOXBELRNKUFSRD-UHFFFAOYSA-N	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
2-methyl-3-ethylthiophene	1.2×10^{-3}		Yaws et al. (2003)	V	804
$C_7H_{10}S$	1.0×10^{-3}		Yaws (2003)	X	238
[53119-51-0]	2.8×10^{-3}		Gharagheizi et al. (2012)	Q	
RBRAJDCWXUJHIY-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	247

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-4-ethylthiophene	1.1×10^{-3}		Yaws et al. (2003)	V	804
$C_7H_{10}S$	9.6×10^{-4}		Yaws (2003)	X	238
[13678-54-1]	3.3×10^{-3}		Gharagheizi et al. (2012)	Q	
KIWVMUQUYOKTKU-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
2-methyl-5-ethylthiophene	1.2×10^{-3}		Yaws et al. (2003)	V	804
$C_7H_{10}S$	9.9×10^{-4}		Yaws (2003)	X	238
[40323-88-4]	6.6×10^{-3}		Gharagheizi et al. (2012)	Q	
VOIVNYVBGCJFRW-UHFFFAOYSA-N	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
2-propylthiophene	1.2×10^{-3}		Yaws et al. (2003)	V	804
$C_7H_{10}S$	1.0×10^{-3}		Yaws (2003)	X	238
[1551-27-5]	3.1×10^{-3}		Gharagheizi et al. (2012)	Q	
BTXIJTYYMLCUHI-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
3-isopropylthiophene	1.1×10^{-3}		Yaws et al. (2003)	V	804
$C_7H_{10}S$	9.7×10^{-4}		Yaws (2003)	X	238
[29488-27-5]	1.4×10^{-3}		Gharagheizi et al. (2012)	Q	
LJPDBPCGTFTUDE-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
3-methyl-2-ethylthiophene	1.2×10^{-3}		Yaws et al. (2003)	V	804
$C_7H_{10}S$	9.8×10^{-4}		Yaws (2003)	X	238
[31805-48-8]	2.1×10^{-3}		Gharagheizi et al. (2012)	Q	
VVSCPYCHXFEKLF-UHFFFAOYSA-N	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
3-methyl-4-ethylthiophene	1.3×10^{-3}		Yaws et al. (2003)	V	804
$C_7H_{10}S$	1.1×10^{-3}		Yaws (2003)	X	238
[66577-03-5]	8.1×10^{-4}		Gharagheizi et al. (2012)	Q	
QMHNYDJBWOPGHE-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
3-methyl-5-ethylthiophene	1.3×10^{-3}		Yaws et al. (2003)	V	804
$C_7H_{10}S$	1.1×10^{-3}		Yaws (2003)	X	238
(2-ethyl-4-methylthiophene)	1.8×10^{-3}		Gharagheizi et al. (2012)	Q	
[66577-04-6]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	247
NZOYEHPXDWJOCD-UHFFFAOYSA-N					
3-propylthiophene	1.2×10^{-3}		Yaws et al. (2003)	V	804
$C_7H_{10}S$	9.9×10^{-4}		Yaws (2003)	X	238
[1518-75-8]	1.5×10^{-3}		Gharagheizi et al. (2012)	Q	
QZNFRMXKQCIPQY-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	247
benzenethiol	2.9×10^{-2}		Duchowicz et al. (2020)	V	187
C_6H_5SH	2.9×10^{-2}		HSDB (2015)	V	
(thiophenol)	3.0×10^{-2}		Hine and Mookerjee (1975)	V	
[108-98-5]	3.0×10^{-2}		Hine and Weimar (1965)	V	
RMVRSNDYEFQCLF-UHFFFAOYSA-N	3.0×10^{-2}		Schüürmann (2000)	C	21
	3.2×10^{-1}		Duchowicz et al. (2020)	Q	
	4.1×10^{-2}		Hilal et al. (2008)	Q	
	2.6×10^{-2}		Modarresi et al. (2007)	Q	68
	2.9×10^{-2}		Yaffe et al. (2003)	Q	249, 250

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{-2}		English and Carroll (2001)	Q	231, 232
	1.8×10^{-2}		Katritzky et al. (1998)	Q	
	1.0×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	3.0×10^{-2}		Suzuki et al. (1992)	Q	233
	3.0×10^{-2}		Abraham et al. (1990)	?	
methyl phenyl sulfide $C_6H_5SCH_3$ (thioanisole) [100-68-5] HNKJADCVZUBCPG-UHFFFAOYSA-N	4.0×10^{-2}		Hine and Mookerjee (1975)	V	
	4.1×10^{-2}		Hine and Weimar (1965)	V	
	5.8×10^{-2}		Hilal et al. (2008)	Q	
	4.3×10^{-2}		Yaffe et al. (2003)	Q	249, 250
	2.3×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	4.0×10^{-2}		Suzuki et al. (1992)	Q	233
2-methylbenzenethiol C_7H_8S (2-thiocresol) [137-06-4] LXUNZSDDXMPKLP-UHFFFAOYSA-N	2.7×10^{-2}		HSDB (2015)	Q	100
3-methylbenzenethiol C_7H_8S (3-thiocresol) [108-40-7] WRXOZRLZDJAYDR-UHFFFAOYSA-N	2.7×10^{-2}		HSDB (2015)	Q	100
4-methylbenzenethiol C_7H_8S (4-thiocresol) [106-45-6] WLHCBQAPPJAULW-UHFFFAOYSA-N	2.7×10^{-2}		HSDB (2015)	Q	100
benzenemethanethiol C_7H_8S [100-53-8] UENWRTRMUIOCKN-UHFFFAOYSA-N	4.7×10^{-2}		HSDB (2015)	Q	100
benzo[*b*]thiophene C_8H_6S [95-15-8] FCEHBMOGCRZNNI-UHFFFAOYSA-N			Mackay et al. (2006d)	V	560
	4.1×10^{-2}		Mackay et al. (1995)	V	
	3.6×10^{-2}		Smith and Bomberger (1980)	V	24
	3.0×10^{-2}		Yaws (1999)	?	21, 12
dibenzothiophene $C_{12}H_8S$ [132-65-0] IYYZUPMFVPLQIF-UHFFFAOYSA-N	2.9×10^{-1}		Duchowicz et al. (2020)	V	187
	2.9×10^{-1}		HSDB (2015)	V	
	2.3×10^{-2}		Mackay et al. (2006d)	V	
	2.3×10^{-2}		Mackay et al. (1995)	V	
	2.3×10^{-2}		Smith and Bomberger (1980)	V	24
	1.2		Duchowicz et al. (2020)	Q	
	3.3×10^{-1}		Parnis et al. (2015)	Q	371

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
thianthrene $C_{12}H_8S_2$ [92-85-3] GVIJJXMXTUZIOD-UHFFFAOYSA-N	4.0		Abraham et al. (2019)	Q	
2-methyldibenzothiophene $C_{13}H_{10}S$ [20928-02-3] VHUXLBLPAMBOJS-UHFFFAOYSA-N	2.7×10^{-1}		Parnis et al. (2015)	Q	371
2,3-dimethyldibenzothiophene $C_{14}H_{12}S$ [31317-17-6] KEIKATUAMBEIQN-UHFFFAOYSA-N	3.1×10^{-1}		Parnis et al. (2015)	Q	371
2,8-dimethyldibenzothiophene $C_{14}H_{12}S$ [1207-15-4] RRYWCJRYULRSJM-UHFFFAOYSA-N	2.4×10^{-1}		Parnis et al. (2015)	Q	371
benzyl sulfide $C_{14}H_{14}S$ [538-74-9] LUFPJJNWMYZRQE-UHFFFAOYSA-N	1.9		HSDB (2015)	Q	100
2,3,7-trimethyldibenzothiophene $C_{15}H_{14}S$ HJSMFSZKADBZIO-UHFFFAOYSA-N	2.7×10^{-1}		Parnis et al. (2015)	Q	371
2,3,8-trimethyldibenzothiophene $C_{15}H_{14}S$ QSOGKFSFLARZIE-UHFFFAOYSA-N	2.7×10^{-1}		Parnis et al. (2015)	Q	371
2,4,7-trimethyldibenzothiophene $C_{15}H_{14}S$ [216983-03-8] YDWNRDFOOADVGC-UHFFFAOYSA-N	1.9×10^{-1}		Parnis et al. (2015)	Q	371
4,6-diethyldibenzothiophene $C_{16}H_{16}S$ [132034-91-4] UMQGGSYHJPHWFV-UHFFFAOYSA-N	1.3×10^{-1}		Parnis et al. (2015)	Q	371
2-butyldibenzothiophene $C_{16}H_{16}S$ [147792-31-2] BEQMTJNPMZQPKZ-UHFFFAOYSA-N	1.6×10^{-1}		Parnis et al. (2015)	Q	371

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
carbon oxide sulfide	2.0×10^{-4}	3500	Burkholder et al. (2019)	L	
OCS	2.0×10^{-4}	3500	Burkholder et al. (2015)	L	
(carbonyl sulfide)	2.1×10^{-4}	3300	Warneck and Williams (2012)	L	
[463-58-1]	2.0×10^{-4}	3500	Sander et al. (2011)	L	
JJWKPURADFRFRB-UHFFFAOYSA-N	2.0×10^{-4}	3500	Sander et al. (2006)	L	
	2.1×10^{-4}	3000	Wilhelm et al. (1977)	L	
	2.2×10^{-4}	2100	De Bruyn et al. (1995b)	M	
	1.5×10^{-4}	3800	Johnson and Harrison (1986)	M	71
	1.5×10^{-4}	3500	Hoyt (1982)	M	71
	2.4×10^{-4}		Stock and Kuß (1917)	M	
	2.1×10^{-4}	3300	Winkler (1907)	M	
	2.1×10^{-4}	3300	Winkler (1906)	M	
	3.4×10^{-4}		Hempel (1901)	M	621
	1.6×10^{-5}		Duchowicz et al. (2020)	V	187
	1.6×10^{-5}		HSDB (2015)	V	
	1.9×10^{-4}		Yaws (2003)	X	238
	2.0×10^{-4}		Hayer et al. (2022)	Q	20
	5.4		Duchowicz et al. (2020)	Q	
	2.0×10^{-4}		Gharagheizi et al. (2010)	Q	247
		2900	Kühne et al. (2005)	Q	
		3300	Kühne et al. (2005)	?	
	2.0×10^{-4}		Yaws (1999)	?	21
	2.1×10^{-4}	3000	Yaws et al. (1999)	?	21
	1.9×10^{-4}		Yaws and Yang (1992)	?	21
methanesulfonic acid			Brimblecombe and Clegg (1988)	T	815
CH_3SO_3H	7.3×10^{3}		Wang et al. (2017)	Q	81, 239
(MSA)	1.2×10^{6}		Wang et al. (2017)	Q	81, 240
[75-75-2]	5.0×10^{5}		Wang et al. (2017)	Q	81, 241
AFVFQIVMOAPDHO-UHFFFAOYSA-N					
MCM:CH3SO2OOH	1.9×10^{5}		Wang et al. (2017)	Q	81, 239
CH_4O_4S	1.0×10^{7}		Wang et al. (2017)	Q	81, 240
BENVNICSYZXTGE-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	81, 241
MCM:CH3SOOOH	4.3×10^{7}		Wang et al. (2017)	Q	81, 239
CH_4O_3S	5.6×10^{6}		Wang et al. (2017)	Q	81, 240
IZTYBZWDPIUSAG-UHFFFAOYSA-N	2.7×10^{3}		Wang et al. (2017)	Q	81, 241
MCM:MSIA	1.6×10^{6}		Wang et al. (2017)	Q	81, 239
CH_4O_2S	8.0×10^{3}		Wang et al. (2017)	Q	81, 240
XNEFVTBPCXGIRX-UHFFFAOYSA-N	3.6×10^{5}		Wang et al. (2017)	Q	81, 241
sulfuric acid, dimethyl ester	6.9		Hilal et al. (2008)	Q	
$C_2H_6O_4S$	2.5		Yaws (1999)	?	21, 28
(dimethyl sulfate)					
[77-78-1]					
VAYGXNSJCAHWJZ-UHFFFAOYSA-N					

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dimethylsulfoxide	9.8×10^2		Burkholder et al. (2019)	L	
CH_3SOCH_3	9.8×10^2		Burkholder et al. (2015)	L	
(DMSO)	8.0×10^3	7800	Brockbank (2013)	L	
[67-68-5]	9.8×10^2		Sander et al. (2011)	L	
IAZDPXIOMUYVGZ-UHFFFAOYSA-N	9.8×10^2		Sander et al. (2006)	L	
	$>9.9\times10^3$		Lee and Zhou (1994)	M	
	9.4×10^2	1300	Watts and Brimblecombe (1987)	M	
	4.4		Mackay et al. (2006d)	V	
	4.4		Mackay et al. (1995)	V	
	1.0×10^4	8700	Bagno et al. (1991)	T	475
	1.4×10^1		Betterton (1992)	C	
	2.0×10^2		Keshavarz et al. (2022)	Q	
	1.3×10^2		Duchowicz et al. (2020)	Q	
	4.6×10^2		Wang et al. (2017)	Q	81, 239
	3.9×10^4		Wang et al. (2017)	Q	81, 240
	2.0×10^5		Wang et al. (2017)	Q	81, 241
	4.3×10^3		Hilal et al. (2008)	Q	
		3100	Kühne et al. (2005)	Q	
	6.7×10^3		Taft et al. (1985)	Q	
	6.5×10^3		Duchowicz et al. (2020)	?	186, 21
		4100	Kühne et al. (2005)	?	
			Fogg and Sangster (2003)	?	816
dimethylsulfone	5.0×10^{-3}		Mackay et al. (2006d)	V	
$CH_3SO_2CH_3$	5.0×10^{-3}		Mackay et al. (1995)	V	
(DMSO2)	4.0		Wang et al. (2017)	Q	81, 239
[67-71-0]	3.3×10^4		Wang et al. (2017)	Q	81, 240
HHVIBTZHLRERCL-UHFFFAOYSA-N	1.8×10^5		Wang et al. (2017)	Q	81, 241
	$>4.9\times10^2$		De Bruyn et al. (1994)	E	
mercaptoacetic acid $C_2H_4O_2S$ [68-11-1] CWERGRDVMFNCDR-UHFFFAOYSA-N	5.2×10^2		HSDB (2015)	Q	100
2-mercaptoethanol	5.5×10^1		Duchowicz et al. (2020)	V	187
C_2H_6OS	5.5×10^1		HSDB (2015)	V	
[60-24-2]	1.0×10^2		Duchowicz et al. (2020)	Q	
DGVVWUTYPXICAM-UHFFFAOYSA-N					
methanesulfonic acid, methyl ester $C_2H_6O_3S$ [66-27-3] MBABOKRGFJTBAE-UHFFFAOYSA-N	2.5		HSDB (2015)	Q	100
MCM:CH3SCH2OOH	1.1×10^2		Wang et al. (2017)	Q	81, 239
$C_2H_6O_2S$	1.4×10^2		Wang et al. (2017)	Q	81, 240
LDZPECMXMDESRV-UHFFFAOYSA-N	9.8		Wang et al. (2017)	Q	81, 241

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DMSO2OOH $C_2H_6O_4S$ GCLQZLAJAMWHPS-UHFFFAOYSA-N	2.6×10^{5} 6.5×10^{6} 6.8×10^{5}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:CH3SCH2OH C_2H_6OS ZSSFPSNLAUYOFG-UHFFFAOYSA-N	4.2 7.6×10^{1} 1.1×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:DMSO2OH $C_2H_6O_3S$ ICHBUPLXTAHKLA-UHFFFAOYSA-N	1.0×10^{4} 5.6×10^{6} 5.8×10^{6}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:CH3SCHO C_2H_4OS LFJRGYNYRORDDM-UHFFFAOYSA-N	1.3 1.5×10^{-1} 4.8×10^{-2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
MCM:CH3SO2CHO $C_2H_4O_3S$ LUGQISNSRPQOGS-UHFFFAOYSA-N	3.1×10^{3} 3.6×10^{2} 2.2×10^{2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241
mercaptoacetic acid, methyl ester $C_3H_6O_2S$ (methyl thioglycolate) [2365-48-2] MKIJJIMOAABWGF-UHFFFAOYSA-N	1.6		HSDB (2015)	Q	100
1,3-propane sultone $C_3H_6O_3S$ [1120-71-4] FSSPGSAQUIYDCN-UHFFFAOYSA-N	1.6×10^{3}		Ebert et al. (2023)	?	317
methanesulfonic acid, ethyl ester $C_3H_8O_3S$ [62-50-0] PLUBXMRUUVWRLT-UHFFFAOYSA-N	3.8×10^{1} 2.8×10^{-2} 1.8		Duchowicz et al. (2020) Duchowicz et al. (2020) HSDB (2015)	V Q Q	187 100
2,3-dimercapto-1-propanol $C_3H_8OS_2$ [59-52-9] WQABCVAJNWAXTE-UHFFFAOYSA-N	1.1×10^{3} 4.1×10^{3}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
divinyl sulfoxide C_4H_6OS (vinyl sulfoxide) [1115-15-7] HQSMEHLVLOGBCK-UHFFFAOYSA-N	2.5×10^{1}		HSDB (2015)	Q	100
divinyl sulphone $C_4H_6O_2S$ [77-77-0] AFOSIXZFDONLBT-UHFFFAOYSA-N	2.0×10^{-1}		HSDB (2015)	Q	100

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,5-dihydrothiophene sulfone $C_4H_6O_2S$ (2,5-dihydrothiophene 1,1-dioxide) [77-79-2] MBDNRNMVTZADMQ-UHFFFAOYSA-N	2.3		HSDB (2015)	Q	100
thiodiacetic acid $C_4H_6O_4S$ [123-93-3] UVZICZIVKIMRNE-UHFFFAOYSA-N	2.2×10^{8}		HSDB (2015)	Q	100
thiophene, tetrahydro-, 1,1-dioxide $C_4H_8O_2S$ (sulfolane) [126-33-0] HXJUTPCZVOIRIF-UHFFFAOYSA-N	2.1		HSDB (2015)	Q	100
2-(ethylthio)ethanol $C_4H_{10}OS$ [110-77-0] LNRIEBFNWGMXKP-UHFFFAOYSA-N	1.9×10^{2}		HSDB (2015)	Q	100
thiodiglycol $C_4H_{10}O_2S$ [111-48-8] YODZTKMDCQEPHD-UHFFFAOYSA-N	5.2×10^{3}		HSDB (2015)	Q	100
methanesulfonic acid, 1-methylethyl ester $C_4H_{10}O_3S$ [926-06-7] SWWHCQCMVCPLEQ-UHFFFAOYSA-N	1.4		HSDB (2015)	Q	100
diethyl sulfate $C_4H_{10}O_4S$ [64-67-5] DENRZWYUOJLTMF-UHFFFAOYSA-N	1.6		Ebert et al. (2023)	?	317
S-methyl butanethioate $C_5H_{10}OS$ [2432-51-1] GRLJIIJNZJVMGP-UHFFFAOYSA-N	2.6×10^{-2}		Souchon et al. (2004)	M	
4-hydroxybenzenesulfonic acid $C_6H_6O_4S$ [98-67-9] FEPBITJSIHRMRT-UHFFFAOYSA-N	3.8×10^{7}		HSDB (2015)	Q	100

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benzenesulfonic acid $C_6H_6O_3S$ [98-11-3] SRSXLGNVWSONIS-UHFFFAOYSA-N	3.9×10^{3}		HSDB (2015)	Q	100
dimethipin $C_6H_{10}O_4S_2$ [55290-64-7] PHVNLLCAQHGNKU-UHFFFAOYSA-N	4.3×10^{5} 7.0×10^{5} 4.3×10^{5}		Duchowicz et al. (2020) Duchowicz et al. (2020) MacBean (2012a)	V Q ?	187
4-methylbenzenesulfonic acid $C_7H_8O_3S$ [104-15-4] JOXIMZWYDAKGHI-UHFFFAOYSA-N	3.6×10^{3}		HSDB (2015)	Q	100
phenylmethanesulfonic acid $C_7H_8O_3S$ (benzylsulfonic acid) [100-87-8] NIXKBAZVOQAHGC-UHFFFAOYSA-N	9.9×10^{3}		HSDB (2015)	Q	100
isoprothiolane $C_{12}H_{18}O_4S_2$ [50512-35-1] UFHLMYOGRXOCSL-UHFFFAOYSA-N	9.8×10^{-2} 2.8×10^{3}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
4,4'-sulfonyldiphenol $C_{12}H_{10}O_4S$ (bisphenol S) [80-09-1] VPWNQTHUCYMVMZ-UHFFFAOYSA-N	3.7×10^{9}		HSDB (2015)	Q	449
benfuresate $C_{12}H_{16}O_4S$ [68505-69-1] QGQSRQPXXMTJCM-UHFFFAOYSA-N	3.7×10^{2}		Ebert et al. (2023)	?	319
lauryl sulfate $C_{12}H_{26}O_4S$ (dodecyl sulfate) [151-41-7] MOTZDAYCYVMXPC-UHFFFAOYSA-N	5.5×10^{1}		HSDB (2015)	Q	100
ethofumesate $C_{13}H_{18}O_5S$ [26225-79-6] IRCMYGHHKLLGHV-UHFFFAOYSA-N	2.7×10^{2} 2.7×10^{2} 4.5×10^{1} 7.7 1.1×10^{2} 2.7×10^{2}		Duchowicz et al. (2020) HSDB (2015) Barcelo and Hennion (1997) Duchowicz et al. (2020) Goodarzi et al. (2010) Maniere et al. (2011)	V V X Q Q ?	187 569 570, 571 166

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1'-sulfonylbis(4-(1-methylethyl)-benzene	1.0×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_{18}H_{22}O_2S$	2.9×10^{3}		Zhang et al. (2010)	Q	288, 290
[57913-35-6]	6.7×10^{4}		Zhang et al. (2010)	Q	288, 291
PKQWGBLKCJIMDP-UHFFFAOYSA-N	3.1×10^{2}		Zhang et al. (2010)	Q	288, 292
propargite	1.5×10^{1}		Duchowicz et al. (2020)	V	187
$C_{19}H_{26}O_4S$	1.5×10^{1}		HSDB (2015)	V	
[2312-35-8]	1.0×10^{2}		Duchowicz et al. (2020)	Q	
ZYHMJXZULPZUED-UHFFFAOYSA-N					
kadethrin	1.2×10^{4}		HSDB (2015)	Q	100
$C_{23}H_{24}O_4S$					
[58769-20-3]					
UGWALRUNBSBTGI-QJLCOAGJSA-N					
spironolactone	9.0×10^{4}		HSDB (2015)	Q	100
$C_{24}H_{32}O_4S$					
[52-01-7]					
LXMSZDCAJNLERA-PJKOONHHSA-N					
2,2'-thiobis(4-(1,1,3,3-tetramethylbutyl)phenol)	4.5×10^{5}		Zhang et al. (2010)	Q	288, 289
$C_{28}H_{42}O_2S$	1.2×10^{4}		Zhang et al. (2010)	Q	288, 290
[3294-03-9]	2.2×10^{7}		Zhang et al. (2010)	Q	288, 291
WQYFETFRIRDUPJ-UHFFFAOYSA-N	1.8×10^{5}		Zhang et al. (2010)	Q	288, 292
propanoic acid, 3,3'-thiobis-, didodecyl ester	2.5		HSDB (2015)	Q	449
$C_{30}H_{58}O_4S$					
(dilauryl thiodipropionate)					
[123-28-4]					
GHKOFFNLGXMVNJ-UHFFFAOYSA-N					
dioctadecyl 3,3'-thiodipropionate	8.2×10^{-2}		HSDB (2015)	Q	449
$C_{42}H_{82}O_4S$					
[693-36-7]					
PWWSSIYVTQUJQQ-UHFFFAOYSA-N					
methyl isothiocyanate	1.7×10^{-1}		Burkholder et al. (2019)	L	
CH_3NCS	1.7×10^{-1}		Burkholder et al. (2015)	L	
[556-61-6]	1.7×10^{-1}		Sander et al. (2011)	L	
LGDSHSYDSCRFAB-UHFFFAOYSA-N	1.6×10^{-1}		Worthington and Wade (2007)	M	
	2.2×10^{-1}		Duchowicz et al. (2020)	V	187
	2.2×10^{-1}		HSDB (2015)	V	
	2.1		Duchowicz et al. (2020)	Q	
	1.8×10^{-2}		Modarresi et al. (2007)	Q	68

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
thiourea CH_4N_2S [62-56-6] UMGDCJDMYOKAJW-UHFFFAOYSA-N	5.0×10^{3} 4.9×10^{3} 1.7×10^{5}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
hydrazinecarbothioamide CH_5N_3S (1-amino-2-thiourea) [79-19-6] BRWIZMBXBAOCCF-UHFFFAOYSA-N	1.5×10^{4}		HSDB (2015)	Q	100
thiocyanic acid, methyl ester C_2H_3NS [556-64-9] VYHVQEYOFIYNJP-UHFFFAOYSA-N	2.2×10^{-1}		HSDB (2015)	Q	100
ethanethioamide C_2H_5NS (thioacetamide) [62-55-5] YUKQRDCYNOVPGJ-UHFFFAOYSA-N	1.5		HSDB (2015)	Q	100
mercaptamine C_2H_7NS (cysteamine) [60-23-1] UFULAYFCSOUIOV-UHFFFAOYSA-N	2.7×10^{1}		HSDB (2015)	Q	100
thiocyanic acid, ethyl ester C_3H_5NS [542-90-5] WFCLYEAZTHWNEH-UHFFFAOYSA-N	1.7×10^{-1}		HSDB (2015)	Q	100
2-imidazolidinethione $C_3H_6N_2S$ (ethylene thiourea) [96-45-7] PDQAZBWRQCGBEV-UHFFFAOYSA-N	2.9×10^{1}		HSDB (2015)	Q	100
ethylthiourea $C_3H_8N_2S$ [625-53-6] GMEHFXXZSWDEDB-UHFFFAOYSA-N	4.2×10^{2}		HSDB (2015)	Q	100
allyl isothiocyanate C_4H_5NS [57-06-7] ZOJBYZNEUISWFT-UHFFFAOYSA-N	2.1×10^{-2} 4.1×10^{-2} 4.1×10^{-2} 2.7 2.3×10^{-1}		Souchon et al. (2004) Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Modarresi et al. (2007)	M V V Q Q	 187 68

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dazomet $C_5H_{10}N_2S_2$ [533-74-4] QAYICIQNSGETAS-UHFFFAOYSA-N	2.0×10^{4} 4.6×10^{4} 3.7×10^{4} 3.7×10^{5} 2.0×10^{4}		Duchowicz et al. (2020) Mackay et al. (2006d) MacBean (2012b) Duchowicz et al. (2020) Maniere et al. (2011)	V V X Q ?	187 352 12, 166
N,N'-diethylthiourea $C_5H_{12}N_2S$ [105-55-5] FLVIGYVXZHLUHP-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	100
tetramethylthiourea $C_5H_{12}N_2S$ [2782-91-4] MNOILHPDHOHILI-UHFFFAOYSA-N	8.5×10^{2}		HSDB (2015)	Q	100
thiram $C_6H_{12}N_2S_4$ [137-26-8] KUAZQDVKQLNFPE-UHFFFAOYSA-N	9.3×10^{1} 3.0×10^{1}		Mackay et al. (2006d) MacBean (2012b)	V X	 352
bis(dimethylthiocarbamyl) sulfide $C_6H_{12}N_2S_3$ (bis(dimethylthiocarbamoyl) sulfide) [97-74-5] REQPQFUJGGOFQL-UHFFFAOYSA-N	5.8×10^{-1}		HSDB (2015)	Q	100
benzothiazole C_7H_5NS [95-16-9] IOJUPLGTWVMSFF-UHFFFAOYSA-N	2.7×10^{1} 2.7×10^{1} 2.8 1.1×10^{1} 2.0		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	100 288, 289 288, 290 288, 291 288, 292
2-mercaptobenzothiazole $C_7H_5NS_2$ [149-30-4] YXIWHUQXZSMYRE-UHFFFAOYSA-N	2.7×10^{2} 2.7×10^{2} 2.8×10^{3} 2.2×10^{2} 2.1×10^{1}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	100 288, 289 288, 290 288, 291 288, 292
2-benzothiazolamine $C_7H_6N_2S$ [136-95-8] UHGULLIUJBCTEF-UHFFFAOYSA-N	7.6×10^{4}		HSDB (2015)	Q	100
phenylthiourea $C_7H_8N_2S$ [103-85-5] FULZLIGZKMKICU-UHFFFAOYSA-N	9.9×10^{4}		HSDB (2015)	Q	100

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
aziprotryn $C_7H_{11}N_7S$ [4658-28-0] AFIIBUOYKYSPKB-UHFFFAOYSA-N	4.0×10^{2} 9.2×10^{2}		Abraham et al. (2007) MacBean (2012a)	Q ?	
isothiocyanatobenzene C_7H_5NS [103-72-0] QKFJKGMPGYROCL-UHFFFAOYSA-N	3.3×10^{-3} 5.1		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
simetryn $C_8H_{15}N_5S$ [1014-70-6] MGLWZSOBALDPEK-UHFFFAOYSA-N	2.2×10^{4} 2.2×10^{4} 3.8×10^{6} 2.9×10^{4} 1.0×10^{4}		Duchowicz et al. (2020) Mackay et al. (2006d) Duchowicz et al. (2020) Hilal et al. (2008) Abraham et al. (2007)	V V Q Q Q	187
desmetryn $C_8H_{15}N_5S$ [1014-69-3] HCRWJJJUKUVORR-UHFFFAOYSA-N	2.1×10^{4} 5.0×10^{7} 2.2×10^{4} 2.0×10^{4} 1.4×10^{9} 3.9×10^{7} 2.1×10^{4}		HSDB (2015) Delgado and Alderete (2003) Hilal et al. (2008) Abraham et al. (2007) Delgado and Alderete (2003) Delgado and Alderete (2003) MacBean (2012a)	V C Q Q Q Q ?	
thioquinox $C_9H_4N_2S_3$ [93-75-4] ILERPRJWJPJZDN-UHFFFAOYSA-N	1.3×10^{2}		HSDB (2015)	Q	100
thiocyanic acid, (2-benzothiazolylthio)methyl ester $C_9H_6N_2S_3$ [21564-17-0] TUBQDCKAWGHZPF-UHFFFAOYSA-N	1.5×10^{6}		HSDB (2015)	Q	100
ametryn $C_9H_{17}N_5S$ [834-12-8] RQVYBGPQFYCBGX-UHFFFAOYSA-N	2.1×10^{1} 4.1×10^{3} 8.1×10^{3} 8.3×10^{3} 8.2×10^{1} 4.1×10^{3} 1.3×10^{2} 1.2×10^{4} 5.1×10^{3} 8.9×10^{7} 1.1×10^{7}		Chao et al. (2017) HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Delgado and Alderete (2003) Goodarzi et al. (2010) Hilal et al. (2008) Abraham et al. (2007) Delgado and Alderete (2003) Delgado and Alderete (2003)	M V V V X C Q Q Q Q Q	 12 569 570

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cimetidine $C_{10}H_{16}N_6S$ [51481-61-9] AQIXAKUUQRKLND-UHFFFAOYSA-N	1.0×10^{10}		HSDB (2015)	Q	100
prometryn $C_{10}H_{19}N_5S$ [7287-19-6] AAEVYOVXGOFMJO-UHFFFAOYSA-N	8.2×10^{2}		HSDB (2015)	V	
	2.0×10^{3}		Mackay et al. (2006d)	V	
	2.0×10^{3}		Suntio et al. (1988)	V	12
	2.0×10^{1}		Barcelo and Hennion (1997)	X	569
	2.9×10^{6}		Delgado and Alderete (2003)	C	
	7.6×10^{2}		Delgado and Alderete (2003)	C	
	2.5×10^{2}		Goodarzi et al. (2010)	Q	570
	7.5×10^{2}		Hilal et al. (2008)	Q	
	2.5×10^{3}		Abraham et al. (2007)	Q	
	5.1×10^{6}		Delgado and Alderete (2003)	Q	
	1.4×10^{6}		Delgado and Alderete (2003)	Q	
terbutryn $C_{10}H_{19}N_5S$ [886-50-0] IROINLKCQGIITA-UHFFFAOYSA-N	4.7×10^{2}		HSDB (2015)	V	
	7.0×10^{2}		Mackay et al. (2006d)	V	
	7.7×10^{2}		Suntio et al. (1988)	V	12
	7.6		Barcelo and Hennion (1997)	X	569
	1.2×10^{6}		Delgado and Alderete (2003)	C	
	8.7×10^{2}		Delgado and Alderete (2003)	C	
	1.7×10^{2}		Goodarzi et al. (2010)	Q	570
	4.5×10^{3}		Hilal et al. (2008)	Q	
	1.6×10^{3}		Abraham et al. (2007)	Q	
	5.1×10^{6}		Delgado and Alderete (2003)	Q	
	1.4×10^{6}		Delgado and Alderete (2003)	Q	
disulfiram $C_{10}H_{20}N_2S_4$ [97-77-8] AUZONCFQVSMFAP-UHFFFAOYSA-N	1.2×10^{-1}		HSDB (2015)	Q	100
1-naphthalenylthiourea $C_{11}H_{10}N_2S$ [86-88-4] PIVQQUNOTICCSA-UHFFFAOYSA-N	1.2×10^{3}		HSDB (2015)	Q	100
4,4'-thiobisbenzenamine $C_{12}H_{12}N_2S$ (bis(4-aminophenyl) sulfide) [139-65-1] ICNFHJVPAJKPHW-UHFFFAOYSA-N	2.5×10^{6}		HSDB (2015)	Q	100
dipropetryn $C_{11}H_{19}N_5S$ [4147-51-7] NPWMZOGDXOFZIN-UHFFFAOYSA-N	6.0×10^{2}		Hilal et al. (2008)	Q	
	1.6×10^{3}		Abraham et al. (2007)	Q	
	6.5×10^{2}		MacBean (2012a)	?	

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dimethametryn $C_{11}H_{21}N_5S$ [22936-75-0] IKYICRRUVNIHPP-UHFFFAOYSA-N	8.2×10^{3} 1.0×10^{3}		Hilal et al. (2008) Abraham et al. (2007)	Q Q	
phenothiazine $C_{12}H_9NS$ [92-84-2] WJFKNYWRSNBZNX-UHFFFAOYSA-N	1.0×10^{2} 3.5×10^{2} 3.5×10^{2} 6.9×10^{2} 9.7×10^{1} 4.3×10^{2}		Abraham et al. (2019) HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q Q	 100 288, 289 288, 290 288, 291 288, 292
cymiazole $C_{12}H_{14}N_2S$ [61676-87-7] YUAUPYJCVKNAEC-UHFFFAOYSA-N	1.5×10^{2}		Ebert et al. (2023)	?	319
2,2'-dithiobisbenzothiazole $C_{14}H_8N_2S_4$ (2,2'-dibenzothiazyl disulfide) [120-78-5] AFZSMODLJJCVPP-UHFFFAOYSA-N	4.2×10^{7}		HSDB (2015)	Q	100
methapyrilene $C_{14}H_{19}N_3S$ [91-80-5] HNJJXZKZRAWDPF-UHFFFAOYSA-N	3.6×10^{1}		HSDB (2015)	V	
olanzapine $C_{17}H_{20}N_4S$ [132539-06-1] KVWDHTXUZHCGIO-UHFFFAOYSA-N	1.3×10^{9}		HSDB (2015)	Q	100
N-(1,1-dimethylethyl)bis(2-benzothiazolesulfen)amide $C_{18}H_{17}N_3S_4$ [3741-80-8] VILGDADBAQFRJE-UHFFFAOYSA-N	2.4×10^{8} 1.7×10^{3} 2.3×10^{3} 3.9×10^{8}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
buthiobate $C_{21}H_{28}N_2S_2$ [51308-54-4] ZZVVDIVWGXTDRQ-UHFFFAOYSA-N	3.4×10^{1}		Ebert et al. (2023)	?	319
MCM:CH3SO4NO2 CH_3NO_6S IMLJWBRSRKRPAQ-UHFFFAOYSA-N	7.8×10^{3} 1.6×10^{4} 3.2×10^{-2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	81, 239 81, 240 81, 241

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CH3SOO2NO2	1.7×10^{6}		Wang et al. (2017)	Q	81, 239
CH_3NO_5S	3.9×10^{8}		Wang et al. (2017)	Q	81, 240
PGTDFOBGUOOGGZ-UHFFFAOYSA-N	8.3×10^{-2}		Wang et al. (2017)	Q	81, 241
taurine	5.8×10^{6}		HSDB (2015)	Q	449
$C_2H_7NO_3S$					
[107-35-7]					
XOAAWQZATWQOTB-UHFFFAOYSA-N					
2-amino-5-nitrothiazole	1.9×10^{6}		HSDB (2015)	Q	100
$C_3H_3N_3O_2S$					
[121-66-4]					
MIHADVKEHAFNPG-UHFFFAOYSA-N					
N-(aminothioxomethyl)acetamide	3.8×10^{5}		HSDB (2015)	Q	100
$C_3H_6N_2OS$					
(1-acetyl-2-thiourea)					
[591-08-2]					
IPCRBOOJBPETMF-UHFFFAOYSA-N					
acesulfame	1.0×10^{3}		HSDB (2015)	Q	100
$C_4H_5NO_4S$					
[33665-90-6]					
YGCFIWIQZPHFLU-UHFFFAOYSA-N					
methomyl	2.0×10^{2}		Chao et al. (2017)	M	
$C_5H_{10}N_2O_2S$	5.0×10^{5}		Duchowicz et al. (2020)	V	187
[16752-77-5]	5.2×10^{5}		HSDB (2015)	V	
UHXUZOCRWCRNSJ-UHFFFAOYSA-N	5.3×10^{4}		Mackay et al. (2006d)	V	
	1.5×10^{4}		Suntio et al. (1988)	V	12
	1.5×10^{2}		Barcelo and Hennion (1997)	X	569
	1.0×10^{4}		Duchowicz et al. (2020)	Q	
	1.3×10^{2}		Goodarzi et al. (2010)	Q	570, 571
4-aminobenzenesulfonic acid	1.1×10^{7}		HSDB (2015)	Q	449
$C_6H_7NO_3S$					
(sulfanilic acid)					
[121-57-3]					
HVBSAKJJOYLTQU-UHFFFAOYSA-N					
sulfanilamide	6.6×10^{4}		HSDB (2015)	Q	100
$C_6H_8N_2O_2S$					
[63-74-1]					
FDDDEECHVMSUSB-UHFFFAOYSA-N					
nithiazide	6.2×10^{9}		HSDB (2015)	Q	100
$C_6H_8N_4O_3S$					
[139-94-6]					
FQSUTLQHSDLLAN-UHFFFAOYSA-N					

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methylbenzenesulfonamide $C_7H_9NO_2S$ (*o*-toluenesulfonamide) [88-19-7] YCMLQMDWSXFTIF-UHFFFAOYSA-N	2.1×10^{1}		HSDB (2015)	Q	100
4-methylbenzenesulfonamide $C_7H_9NO_2S$ (*p*-toluenesulfonamide) [70-55-3] LMYRWZFENFIFIT-UHFFFAOYSA-N	2.1×10^{1}		HSDB (2015)	Q	100
ethidimuron $C_7H_{12}N_4O_3S_2$ [30043-49-3] KCOCSOWTADCKOL-UHFFFAOYSA-N	1.4×10^{8}		MacBean (2012a)	?	
oxamyl $C_7H_{13}N_3O_3S$ [23135-22-0] KZAUOCCYDRDERY-UITAMQMPSA-N	4.2×10^{4}		Duchowicz et al. (2020)	V	187
	4.2×10^{4}		HSDB (2015)	V	
	4.2×10^{4}		Mackay et al. (2006d)	V	
	3.8×10^{3}		Suntio et al. (1988)	V	12
	3.8×10^{1}		Barcelo and Hennion (1997)	X	569
	3.4×10^{7}		Duchowicz et al. (2020)	Q	
	6.4×10^{1}		Goodarzi et al. (2010)	Q	570
	2.0×10^{7}		Maniere et al. (2011)	?	166
aldicarb $C_7H_{14}N_2O_2S$ [116-06-3] QGLZXHRNAYXIBU-WEVVVXLNSA-N	6.9×10^{3}		Duchowicz et al. (2020)	V	187
	6.6×10^{3}		HSDB (2015)	V	
	7.9×10^{3}		Mackay et al. (2006d)	V	
	3.1×10^{3}		Suntio et al. (1988)	V	12
	3.1×10^{1}		Barcelo and Hennion (1997)	X	569
	1.9		Suntio et al. (1988)	C	12
	8.0×10^{3}		Duchowicz et al. (2020)	Q	
	2.6×10^{1}		Goodarzi et al. (2010)	Q	570, 573
aldicarb sulfoxide $C_7H_{14}N_2O_3S$ [1646-87-3] BXPMAGSOWXBZHS-UHFFFAOYSA-N	1.0×10^{4}		Duchowicz et al. (2020)	V	187
	4.2×10^{6}		Duchowicz et al. (2020)	Q	
aldicarb sulfone $C_7H_{14}N_2O_4S$ [1646-88-4] YRRKLBAKDXSTNC-UHFFFAOYSA-N	2.9×10^{3}		Duchowicz et al. (2020)	V	187
	4.4×10^{6}		Duchowicz et al. (2020)	Q	
	3.7×10^{3}		MacBean (2012a)	?	
butocarboxim $C_7H_{14}N_2O_2S$ [34681-10-2] SFNPDDSJBGRXLW-UHFFFAOYSA-N	1.7×10^{4}		HSDB (2015)	V	
	1.7×10^{4}		MacBean (2012a)	?	

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
butoxycarboxim $C_7H_{14}N_2O_4S$ [34681-23-7] CTJBHIROCMPUKL-UHFFFAOYSA-N	3.5×10^{6}		HSDB (2015)	V	
saccharin $C_7H_5NO_3S$ [81-07-2] CVHZOJJKTDOEJC-UHFFFAOYSA-N	8.2×10^{3}		HSDB (2015)	Q	100
acibenzolar-S-methyl $C_8H_6N_2OS_2$ [135158-54-2] UELITFHSCLAHKR-UHFFFAOYSA-N	8.3×10^{1} 8.2×10^{1} 1.5×10^{6} 7.7×10^{1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Maniere et al. (2011)	V V Q ?	187 242, 166
quinomethionate $C_8H_6N_2OS_2$ [2439-01-2] FBQQHUGEACOBDN-UHFFFAOYSA-N	1.6×10^{2} 1.6×10^{2}		HSDB (2015) MacBean (2012a)	V ?	
nifurthiazole $C_8H_6N_4O_4S$ [3570-75-0] DUWYZHLZDVCZIO-UHFFFAOYSA-N	1.3×10^{12}		HSDB (2015)	Q	100
4-methylbenzenesulfonyl isocyanate $C_8H_7NO_3S$ [4083-64-1] VLJQDHDVZJXNQL-UHFFFAOYSA-N	1.7×10^{-1} 3.2×10^{1} 6.7 4.0×10^{4}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
tinidazole $C_8H_{13}N_3O_4S$ [19387-91-8] HJLSLZFTEKNLFI-UHFFFAOYSA-N	1.9×10^{5}		HSDB (2015)	Q	100
metribuzin $C_8H_{14}N_4OS$ [21087-64-9] FOXFZRUHNHCZPX-UHFFFAOYSA-N	8.2×10^{4} 5.0×10^{4}		HSDB (2015) Maniere et al. (2011)	V ?	 242, 166
tricyclazole $C_9H_7N_3S$ [41814-78-2] DQJCHOQLCLEDLL-UHFFFAOYSA-N	3.2×10^{5} 3.2×10^{5} 5.5×10^{5}		Duchowicz et al. (2020) Mackay et al. (2006d) Duchowicz et al. (2020)	V V Q	187
benzthiazuron $C_9H_9N_3OS$ [1929-88-0] DTCJYIIKPVRVDD-UHFFFAOYSA-N	1.9×10^{6}		Ebert et al. (2023)	?	367

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
thidiazuron $C_9H_8N_4OS$ [51707-55-2] HFCYZXMHUIHAQI-UHFFFAOYSA-N	3.0×10^{7}		HSDB (2015)	V	
sulfathiazole $C_9H_9N_3O_2S_2$ [72-14-0] JNMRHUJNCSQMMB-UHFFFAOYSA-N	1.7×10^{8}		HSDB (2015)	Q	100
sulfamethizole $C_9H_{10}N_4O_2S_2$ [144-82-1] VACCAVUAMIDAGB-UHFFFAOYSA-N	3.8×10^{8}		HSDB (2015)	Q	100
ethiozin $C_9H_{16}N_4OS$ [64529-56-2] ADZSGNDOZREKJK-UHFFFAOYSA-N	2.0×10^{2}		MacBean (2012a)	?	
tebuthiuron $C_9H_{16}N_4OS$ [34014-18-1] HBPDKDSFLXWOAE-UHFFFAOYSA-N	6.9×10^{4} 3.2×10^{4} 8.2×10^{4}		Keshavarz et al. (2022) Duchowicz et al. (2020) Duchowicz et al. (2020)	Q Q ?	 186, 21
molinate $C_9H_{17}NOS$ [2212-67-1] DEDOPGXGGQYYMW-UHFFFAOYSA-N	7.7 2.2 1.7 6.9 1.1×10^{1} 1.0×10^{1} 7.6 7.3 2.3	 7300 	Watanabe (1993) Sagebiel et al. (1992) Sagebiel et al. (1992) Mackay et al. (2006d) Sagebiel et al. (1992) Woodrow et al. (1990) Armbrust (2000) Hilal et al. (2008) Modarresi et al. (2007)	M M M V V V C Q Q	 12 12 68
thiofanox $C_9H_{18}N_2O_2S$ [39196-18-4] FZSVSABTBYGOQH-UHFFFAOYSA-N	1.1×10^{3} 3.4×10^{3}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
amidosulfuron $C_9H_{15}N_5O_7S_2$ [120923-37-7] CTTHWASMBLQOFR-UHFFFAOYSA-N	6.4×10^{5} 1.9×10^{3} 1.5×10^{5}		Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011)	? ? ?	12, 495, 166 12, 579, 166 12, 575, 166

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
S-ethyl dipropylthiocarbamate	5.6×10^{-1}	9100	Reyes-Pérez et al. (2008)	M	
$C_9H_{19}NOS$	3.8×10^{-2}	4800	Breiter et al. (1998)	M	
(eptam; EPTC)	6.2×10^{-1}		HSDB (2015)	V	
[759-94-4]	9.8×10^{-1}		Mackay et al. (2006d)	V	
GUVLYNGULCJVDO-UHFFFAOYSA-N	4.2×10^{-1}		Breiter et al. (1998)	V	
	9.8×10^{-1}		Suntio et al. (1988)	V	12
	7.4×10^{-1}		Burkhard and Guth (1981)	V	
	1.0×10^{-2}		Barcelo and Hennion (1997)	X	569
	1.1×10^{-2}		Goodarzi et al. (2010)	Q	570
	8.2×10^{-1}		Hilal et al. (2008)	Q	
	1.2		Modarresi et al. (2007)	Q	68
		4800	Kühne et al. (2005)	Q	
		4800	Kühne et al. (2005)	?	
thiabendazole	4.7×10^{5}		Duchowicz et al. (2020)	V	187
$C_{10}H_7N_3S$	4.7×10^{5}		HSDB (2015)	V	
[148-79-8]	4.7×10^{5}		Mackay et al. (2006d)	V	
WJCNZQLZVWNLKY-UHFFFAOYSA-N	1.3×10^{5}		Duchowicz et al. (2020)	Q	
	2.7×10^{5}		Maniere et al. (2011)	?	242, 166
benzo[*b*]thiophene-4-ol, methylcarbamate	5.8×10^{3}		HSDB (2015)	Q	100
$C_{10}H_9NO_2S$					
(mobam)					
[1079-33-0]					
BOTUVXISJHKZKJ-UHFFFAOYSA-N					
sulfamethoxazole	1.5×10^{7}		HSDB (2015)	Q	100
$C_{10}H_{11}N_3O_3S$					
[723-46-6]					
JLKIGFTWXXRPMT-UHFFFAOYSA-N					
bentazone	4.5×10^{3}		HSDB (2015)	V	
$C_{10}H_{12}N_2O_3S$	1.3×10^{2}		Barcelo and Hennion (1997)	X	569
[25057-89-0]	3.6×10^{2}		Goodarzi et al. (2010)	Q	570, 571
ZOMSMJKLGFBRBS-UHFFFAOYSA-N	1.4×10^{4}		Maniere et al. (2011)	?	12, 166
	4.7×10^{5}		Maniere et al. (2011)	?	12, 166
buthidazole	4.8×10^{6}		MacBean (2012a)	?	
$C_{10}H_{16}N_4O_2S$					
[55511-98-3]					
SWMGXKSQWDSBKV-UHFFFAOYSA-N					
thiodicarb	1.1×10^{1}		HSDB (2015)	V	
$C_{10}H_{18}N_4O_4S_3$	2.3×10^{1}		Mackay et al. (2006d)	V	
[59669-26-0]					
XDOTVMNBCQVZKG-UHFFFAOYSA-N					

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pebulate	4.1×10^{-2}		HSDB (2015)	V	
$C_{10}H_{21}NOS$	3.8×10^{-1}		Mackay et al. (2006d)	V	
[1114-71-2]	8.6×10^{-2}		Suntio et al. (1988)	V	12
SGEJQUSYQTVSIU-UHFFFAOYSA-N	8.4×10^{-4}		Barcelo and Hennion (1997)	X	569
	6.6×10^{-3}		Goodarzi et al. (2010)	Q	570
	6.4×10^{-1}		Hilal et al. (2008)	Q	
	8.9×10^{-1}		Modarresi et al. (2007)	Q	68
	$>2.3\times10^{10}$		MacBean (2012a)	?	
vernolate	3.2×10^{-1}		HSDB (2015)	V	
$C_{10}H_{21}NOS$	4.9×10^{-1}		Mackay et al. (2006d)	V	
[1929-77-7]	4.9×10^{-1}		Suntio et al. (1988)	V	12
OKUGPJPKMAEJOE-UHFFFAOYSA-N	4.8×10^{-3}		Barcelo and Hennion (1997)	X	569
	2.9×10^{-3}		Goodarzi et al. (2010)	Q	570
	6.5×10^{-1}		Hilal et al. (2008)	Q	
	9.0×10^{-1}		Modarresi et al. (2007)	Q	68
biotin	5.6×10^{2}		Abraham et al. (2019)	Q	
$C_{10}H_{16}N_2O_3S$					
[58-85-5]					
YBJHBAHKTGYVGT-ZKWXMUAHSA-N					
methabenzthiazuron	1.8×10^{4}		Duchowicz et al. (2020)	V	187
$C_{10}H_{11}N_3OS$	6.6×10^{4}		Duchowicz et al. (2020)	Q	
[18691-97-9]					
RRVIAQKBTUQODI-UHFFFAOYSA-N					
sulfisoxazole	6.2×10^{6}		HSDB (2015)	Q	100
$C_{11}H_{13}N_3O_3S$					
[127-69-5]					
NHUHCSRWZMLRLA-UHFFFAOYSA-N					
ethiofencarb	8.6×10^{3}		Duchowicz et al. (2020)	V	187
$C_{11}H_{15}NO_2S$	8.2×10^{3}		HSDB (2015)	V	
[29973-13-5]	7.7×10^{2}		Duchowicz et al. (2020)	Q	
HEZNVIYQEUHLNI-UHFFFAOYSA-N					
methiocarb	8.3		Mackay et al. (2006d)	V	
$C_{11}H_{15}NO_2S$	8.4×10^{3}		MacBean (2012b)	X	352
[2032-65-7]					
YFBPRJGDJKVWAH-UHFFFAOYSA-N					
cycloate	1.9		HSDB (2015)	V	
$C_{11}H_{21}NOS$	3.7		Hilal et al. (2008)	Q	
[1134-23-2]	3.2		Modarresi et al. (2007)	Q	68
DFCAFRGABIXSDS-UHFFFAOYSA-N					

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methoprotryn	3.1×10^{4}		HSDB (2015)	V	
$C_{11}H_{21}N_5OS$	1.5×10^{5}		Hilal et al. (2008)	Q	
[841-06-5]	2.0×10^{5}		Abraham et al. (2007)	Q	
DDUIUBPJPOKOMV-UHFFFAOYSA-N	3.1×10^{4}		MacBean (2012a)	?	
butylate	1.2×10^{-1}		HSDB (2015)	V	
$C_{11}H_{23}NOS$			Mackay et al. (2006d)	V	560
[2008-41-5]	1.8		Suntio et al. (1988)	V	12
BMTAFVWTTFSTOG-UHFFFAOYSA-N	1.8×10^{-2}		Barcelo and Hennion (1997)	X	569
	2.1×10^{-1}		Goodarzi et al. (2010)	Q	570
	5.8×10^{-1}		Hilal et al. (2008)	Q	
	6.0×10^{-1}		Modarresi et al. (2007)	Q	68
2-octyl-3(2H)-isothiazolone	4.8×10^{2}		Duchowicz et al. (2020)	V	187
$C_{11}H_{19}NOS$	1.8		Duchowicz et al. (2020)	Q	
[26530-20-1]					
JPMIIZHYYWMHDT-UHFFFAOYSA-N					
metsulfovax	9.2×10^{5}		Ebert et al. (2023)	?	319
$C_{12}H_{12}N_2OS$					
[21452-18-6]					
UDSJPFPDKCMYBD-UHFFFAOYSA-N					
carboxin	3.1×10^{4}		Duchowicz et al. (2020)	V	187
$C_{12}H_{13}NO_2S$	3.1×10^{4}		HSDB (2015)	V	
[5234-68-4]	6.4×10^{4}		Mackay et al. (2006d)	V	
GYSSRZJIHXQEHQ-UHFFFAOYSA-N	7.6×10^{2}		Duchowicz et al. (2020)	Q	
	3.1×10^{4}		Maniere et al. (2011)	?	242, 166
oxycarboxin	9.3×10^{5}		Duchowicz et al. (2020)	V	187
$C_{12}H_{13}NO_4S$	9.0×10^{5}		HSDB (2015)	V	
[5259-88-1]	2.8×10^{3}		Mackay et al. (2006d)	V	
AMEKQAFGQBKLKX-UHFFFAOYSA-N	5.3×10^{5}		Duchowicz et al. (2020)	Q	
thifensulfuron-methyl	3.4×10^{8}		HSDB (2015)	V	
$C_{12}H_{13}N_5O_6S_2$	1.0×10^{14}		Maniere et al. (2011)	?	242, 495, 166
[79277-27-3]	3.6×10^{12}		Maniere et al. (2011)	?	242, 572, 166
AHTPATJNIAFOLR-UHFFFAOYSA-N					
sulfamethazine	3.2×10^{7}		HSDB (2015)	Q	100
$C_{12}H_{14}N_4O_2S$					
[57-68-1]					
ASWVTGNCAZCNNR-UHFFFAOYSA-N					
thiophanate-methyl	8.2×10^{3}		HSDB (2015)	V	
$C_{12}H_{14}N_4O_4S_2$	7.9×10^{2}		Mackay et al. (2006d)	V	
[23564-05-8]	6.0×10^{3}		Maniere et al. (2011)	?	242, 166
QGHREAKMXXNCOA-UHFFFAOYSA-N					

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,4'-oxydi(benzenesulphonohydrazide) $C_{12}H_{14}N_4O_5S_2$ [80-51-3] NBOCQTNZUPTTEI-UHFFFAOYSA-N	7.8×10^{11}		HSDB (2015)	Q	100
albendazole $C_{12}H_{15}N_3O_2S$ [54965-21-8] HXHWSAZORRCQMX-UHFFFAOYSA-N	1.3×10^{8}		HSDB (2015)	Q	100
oryzalin	5.2×10^{3}		HSDB (2015)	V	
$C_{12}H_{18}N_4O_6S$	5.3×10^{3}		Mackay et al. (2006d)	V	
[19044-88-3]	3.6×10^{7}		Maniere et al. (2011)	?	12, 572, 166
UNAHYJYOSSSJHH-UHFFFAOYSA-N	2.5×10^{8}		Maniere et al. (2011)	?	12, 574, 166
	3.0×10^{7}		Maniere et al. (2011)	?	12, 495, 166
STK366145 $C_{12}H_{19}N_3O_3S$ (N-(2-ethyl(3-methyl-4-nitrosophenyl)amino)ethyl)-methanesulfonamide) [56046-62-9] XWQURWIJAIIPQP-UHFFFAOYSA-N	9.9×10^{4}		HSDB (2015)	V	
isomethiozin $C_{12}H_{20}N_4OS$ [57052-04-7] MZTLOILRKLUURT-UHFFFAOYSA-N	7.9×10^{2}		MacBean (2012a)	?	
thiencarbazone-methyl	2.1×10^{12}		Maniere et al. (2011)	?	242, 817, 166
$C_{12}H_{14}N_4O_7S_2$	5.0×10^{12}		Maniere et al. (2011)	?	242, 579, 166
[317815-83-1]	1.3×10^{13}		Maniere et al. (2011)	?	242, 495, 166
XSKZXGDFSCCXQX-UHFFFAOYSA-N	1.2×10^{13}		Maniere et al. (2011)	?	242, 575, 166
2,8-dinitrodibenzothiophene $C_{12}H_6N_2O_4S$ [109041-38-5] VMQHOWOVMXIROE-UHFFFAOYSA-N	4.0×10^{4}		Parnis et al. (2015)	Q	371

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-nitrodibenzothiophene $C_{12}H_7NO_2S$ [6639-36-7] GXLYVLHWXVRVKI-UHFFFAOYSA-N	1.2×10^{2}		Parnis et al. (2015)	Q	371
azimsulfuron	2.0×10^{9}		Maniere et al. (2011)	?	242, 495, 166
$C_{13}H_{16}N_{10}O_5S$	1.2×10^{8}		Maniere et al. (2011)	?	242, 572, 166
[120162-55-2]	1.1×10^{10}		Maniere et al. (2011)	?	242, 575, 166
MAHPNPYYQAIOJN-UHFFFAOYSA-N					
fenothiocarb $C_{13}H_{19}NO_2S$ [62850-32-2] HMIBKHHNXANVHR-UHFFFAOYSA-N	5.3×10^{2}		Ebert et al. (2023)	?	317
isobornyl thiocyanoacetate $C_{13}H_{19}NO_2S$ [115-31-1] IXEVGHXRXDBAOB-RUETXSTFSA-N	3.8×10^{1}		HSDB (2015)	Q	100
nitralin	1.4×10^{3}		HSDB (2015)	V	
$C_{13}H_{19}N_3O_6S$	7.2×10^{-3}		Mackay et al. (2006d)	V	
[4726-14-1]	7.2×10^{-3}		Suntio et al. (1988)	V	12
UMKANAFDOQQUKE-UHFFFAOYSA-N					
bupirimate	6.9×10^{2}		Duchowicz et al. (2020)	V	187
$C_{13}H_{24}N_4O_3S$	1.0×10^{2}		Mackay et al. (2006d)	V	
[41483-43-6]	1.5×10^{3}		Duchowicz et al. (2020)	Q	
DSKJPMWIHSOYEA-UHFFFAOYSA-N	7.4×10^{-1}		Maniere et al. (2011)	?	12, 166
timolol $C_{13}H_{24}N_4O_3S$ [26839-75-8] BLJRIMJGRPQVNF-JTQLQIEISA-N	2.3×10^{11}		HSDB (2015)	Q	100
triazamate	8.6×10^{4}		Duchowicz et al. (2020)	V	187
$C_{13}H_{22}N_4O_3S$	1.2×10^{5}		Duchowicz et al. (2020)	Q	
[112143-82-5] NKNFWVNSBIXGLL-UHFFFAOYSA-N					
dithianone	1.7×10^{5}		HSDB (2015)	V	
$C_{14}H_4N_2O_2S_2$			Mackay et al. (2006d)	V	560
[3347-22-6]	7.4×10^{6}		Maniere et al. (2011)	?	12, 166
PYZSVQVRHDXQSL-UHFFFAOYSA-N					

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-(cyclohexylthio)phthalimide $C_{14}H_{15}NO_2S$ [17796-82-6] UEZWYKZHXASYJN-UHFFFAOYSA-N	1.5×10^{2}		HSDB (2015)	Q	100
metsulfuron-methyl $C_{14}H_{15}N_5O_6S$ [74223-64-6] RSMUVYRMZCOLBH-UHFFFAOYSA-N	7.5×10^{10} 2.1×10^{8}		HSDB (2015) Maniere et al. (2011)	V ?	 242, 166
rimsulfuron $C_{14}H_{17}N_5O_7S_2$ [122931-48-0] MEFOUWRMVYJCQC-UHFFFAOYSA-N	1.5×10^{4} 9.1×10^{6} 2.2×10^{5} 1.2×10^{7}		HSDB (2015) Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011)	V ? ? ?	 575, 166 572, 166 495, 166
thiophanate $C_{14}H_{18}N_4O_4S_2$ [23564-06-9] YFNCATAIYKQPOO-UHFFFAOYSA-N	1.9×10^{7}		HSDB (2015)	Q	100
sumatriptan $C_{14}H_{21}N_3O_2S$ [103628-46-2] KQKPFRSPSRPDEB-UHFFFAOYSA-N	2.2×10^{8}		HSDB (2015)	Q	100
mesotrione $C_{14}H_{13}NO_7S$ [104206-82-8] KPUREKXXPHOJQT-UHFFFAOYSA-N	$>2.0\times10^{6}$		Maniere et al. (2011)	?	12, 166
prosulfocarb $C_{14}H_{21}NOS$ [52888-80-9] NQLVQOSNDJXLKG-UHFFFAOYSA-N	7.6×10^{2} 9.5×10^{1} 6.6×10^{1}		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	187 12, 166
pyriftalid $C_{15}H_{14}N_2O_4S$ [135186-78-6] RRKHIAYNPVQKEF-UHFFFAOYSA-N	2.5×10^{5}		Ebert et al. (2023)	?	319
nicosulfuron $C_{15}H_{18}N_6O_6S$ [111991-09-4] RTCOGUMHFFWOJV-UHFFFAOYSA-N	6.8×10^{10}		Maniere et al. (2011)	?	12, 166
sulfometuron methyl $C_{15}H_{16}N_4O_5S$ [74222-97-2] ZDXMLEQEMNLCQG-UHFFFAOYSA-N	8.2×10^{12} 1.9×10^{8}		Armbrust (2000) HSDB (2015)	C Q	 100

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tribenuron-methyl	9.7×10^{7}		MacBean (2012b)	X	352
$C_{15}H_{17}N_5O_6S$	6.1×10^{7}		Keshavarz et al. (2022)	Q	
[101200-48-0]	8.4×10^{8}		Duchowicz et al. (2020)	Q	
VLCQZHSMCYCDJL-UHFFFAOYSA-N	9.7×10^{7}		Duchowicz et al. (2020)	?	186, 21
	1.1×10^{9}		Maniere et al. (2011)	?	242, 572, 166
	$>7.5\times10^{9}$		Maniere et al. (2011)	?	242, 575, 166
ethametsulfuron-methyl	2.1×10^{9}		Ebert et al. (2023)	?	319
$C_{15}H_{18}N_6O_6S$					
[97780-06-8]					
ZINJLDJMHCUBIP-UHFFFAOYSA-N					
propoxycarbazone	7.0×10^{11}		HSDB (2015)	Q	100
$C_{15}H_{18}N_4O_7S$					
[145026-81-9]					
JTHMVYBOQLDDIY-UHFFFAOYSA-N					
dimepiperate	2.8×10^{2}		Ebert et al. (2023)	?	319
$C_{15}H_{21}NOS$					
[61432-55-1]					
BWUPSGJXXPATLU-UHFFFAOYSA-N					
esprocarb	1.8×10^{1}		Duchowicz et al. (2020)	V	187
$C_{15}H_{23}NOS$	1.5×10^{1}		Duchowicz et al. (2020)	Q	
[85785-20-2]					
BXEHUCNTIZGSOJ-UHFFFAOYSA-N					
valdecoxib	4.5×10^{5}		HSDB (2015)	Q	100
$C_{16}H_{14}N_2O_3S$					
[181695-72-7]					
LNPDTQAFDNKSHK-UHFFFAOYSA-N					
topramezone	1.0×10^{12}		HSDB (2015)	Q	100
$C_{16}H_{17}N_3O_5S$					
[210631-68-8]					
BPPVUXSMLBXYGG-UHFFFAOYSA-N					
sulfosulfuron	4.3×10^{5}		HSDB (2015)	V	
$C_{16}H_{18}N_6O_7S_2$	3.4×10^{7}		Maniere et al. (2011)	?	12, 575, 166
[141776-32-1]	1.2×10^{6}		Maniere et al. (2011)	?	12, 572, 166
RBSXHDIPCIWOMG-UHFFFAOYSA-N	1.1×10^{8}		Maniere et al. (2011)	?	12, 495, 166

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
orthosulfamuron $C_{16}H_{20}N_6O_6S$ [213464-77-8] UCDPMNSCCRBWIC-UHFFFAOYSA-N	1.3×10^{4}		HSDB (2015)	V	
cafenstrole $C_{16}H_{22}N_4O_3S$ [125306-83-4] HFEJHAAIJZXXRE-UHFFFAOYSA-N	8.0×10^{5}		Ebert et al. (2023)	?	319
buprofezin $C_{16}H_{23}N_3OS$ [69327-76-0] PRLVTUNWOQKEAI-UHFFFAOYSA-N	2.4 2.3 2.5×10^{2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
bensulfuron methyl $C_{16}H_{18}N_4O_7S$ [83055-99-6] XMQFTWRPUQYINF-UHFFFAOYSA-N	7.0×10^{10} 2.5×10^{12} 5.0×10^{10} 1.7×10^{9}		Armbrust (2000) Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011)	C ? ? ?	 575, 166 495, 166 572, 166
mefenacet $C_{16}H_{14}N_2O_2S$ [73250-68-7] XIGAUIHYSDTJHW-UHFFFAOYSA-N	2.1×10^{4} 3.4×10^{4}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
alanycarb $C_{17}H_{25}N_3O_4S_2$ [83130-01-2] GMAUQNJOSOMMHI-JXAWBTAJSA-N	1.1×10^{4} 1.8×10^{5}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
fenamidone $C_{17}H_{17}N_3OS$ [161326-34-7] LMVPQMGRYSRMIW-KRWDZBQOSA-N	8.6×10^{4}		Ebert et al. (2023)	?	367
esomeprazole $C_{17}H_{19}N_3O_3S$ [119141-88-7] SUBDBMMJDZJVOS-UHFFFAOYSA-N	3.3×10^{13}		HSDB (2015)	Q	100
foramsulfuron $C_{17}H_{20}N_6O_7S$ [173159-57-4] PXDNXJSDGQBLKS-UHFFFAOYSA-N	1.7×10^{11} 1.7×10^{11}		HSDB (2015) Maniere et al. (2011)	V ?	 12, 166
sethoxydim $C_{17}H_{29}NO_3S$ [74051-80-2] NMHGOXYVOKDNHF-UHFFFAOYSA-N	4.5×10^{5}		HSDB (2015)	Q	100

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
mesosulfuron-methyl	9.0×10^{10}		HSDB (2015)	V	
$C_{17}H_{21}N_5O_9S_2$	8.7×10^{12}		Maniere et al. (2011)	?	12, 575, 166
[208465-21-8]	2.7×10^{11}		Maniere et al. (2011)	?	12, 495, 166
NIFKBBMCXCMCAO-UHFFFAOYSA-N	4.1×10^{9}		Maniere et al. (2011)	?	12, 572, 166
cycloxydim $C_{17}H_{27}NO_3S$ [101205-02-1] HAHCNFVGRVWFIP-VKAVYKQESA-N	1.6×10^{4}		Maniere et al. (2011)	?	12, 166
fenpyrazamine $C_{17}H_{21}N_3O_2S$ [473798-59-3] UTOHZQYBSYOOGC-UHFFFAOYSA-N	6.2×10^{3}		Maniere et al. (2011)	?	12, 166
cyprosulfamide	7.0×10^{6}		Maniere et al. (2011)	?	242, 575, 166
$C_{18}H_{18}N_2O_5S$	9.1×10^{2}		Maniere et al. (2011)	?	242, 579, 166
[221667-31-8]	2.9×10^{5}		Maniere et al. (2011)	?	242, 495, 166
OAWUUPVZMNKZRY-UHFFFAOYSA-N					
rosiglitazone $C_{18}H_{19}N_3O_3S$ [122320-73-4] YASAKCUCGLMORW-UHFFFAOYSA-N	5.8×10^{8}		HSDB (2015)	Q	100
rabeprazole $C_{18}H_{21}N_3O_3S$ [117976-89-3] YREYEVIYCVEVJK-UHFFFAOYSA-N	8.2×10^{11}		HSDB (2015)	Q	100
pyributicarb $C_{18}H_{22}N_2O_2S$ [88678-67-5] VTRWMTJQBQJKQH-UHFFFAOYSA-N	4.3×10^{1}		Ebert et al. (2023)	?	319
furathiocarb $C_{18}H_{26}N_2O_5S$ [65907-30-4] HAWJXYBZNNRMNO-UHFFFAOYSA-N	7.6×10^{3}		HSDB (2015)	V	
lincomycin $C_{18}H_{34}N_2O_6S$ [154-21-2] OJMMVQQUTAEWLP-UHFFFAOYSA-N	3.3×10^{17}		HSDB (2015)	Q	100

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pioglitazone $C_{19}H_{20}N_2O_3S$ [111025-46-8] HYAFETHFCAUJAY-UHFFFAOYSA-N	5.8×10^{6}		HSDB (2015)	Q	100
isofetamid $C_{20}H_{25}NO_3S$ [875915-78-9] WMKZDPFZIZQROT-UHFFFAOYSA-N	3.5×10^{4}		Ebert et al. (2023)	?	319
tamsulosin $C_{20}H_{28}N_2O_5S$ [106133-20-4] DRHKJLXJIQTDTD-OAHLLOKOSA-N	2.0×10^{9}		HSDB (2015)	Q	100
carbosulfan $C_{20}H_{32}N_2O_3S$ [55285-14-8] JLQUFIHWVLZVTJ-UHFFFAOYSA-N	1.9×10^{1} 1.7		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
sufentanil $C_{22}H_{30}N_2O_2S$ [56030-54-7] GGCSSNBKKAUURC-UHFFFAOYSA-N	2.4×10^{9}		HSDB (2015)	Q	100
sildenafil $C_{22}H_{30}N_6O_4S$ [139755-83-2] BNRNXUUZRGQAQC-UHFFFAOYSA-N	1.4×10^{15}		HSDB (2015)	Q	100
benfuracarb $C_{20}H_{30}N_2O_5S$ [82560-54-1] FYZBOYWSHKHDMT-UHFFFAOYSA-N	4.9×10^{2}		Ebert et al. (2023)	?	319
tirofiban $C_{22}H_{36}N_2O_5S$ [144494-65-5] COKMIXFXJJXBQG-NRFANRHFSA-N	1.3×10^{9}		HSDB (2015)	Q	100
vardenafil $C_{23}H_{32}N_6O_4S$ [224785-90-4] SECKRCOLJRRGGV-UHFFFAOYSA-N	5.2×10^{15}		HSDB (2015)	Q	100
taurocholic acid $C_{26}H_{45}NO_7S$ [81-24-3] WBWWGRHZICKQGZ-HZAMXZRMSA-N	1.9×10^{15}		HSDB (2015)	Q	449

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dalfopristin $C_{34}H_{50}N_4O_9S$ [112362-50-2] SUYRLXYYZQTJHF-FUODUHIRSA-N	2.2×10^{24}		HSDB (2015)	Q	100
C.I. acid green 3 $C_{37}H_{37}N_2O_6S_2$ [4680-78-8] SRRJCDUOSQWHGS-UHFFFAOYSA-O	2.0×10^{23}		HSDB (2015)	Q	449
tinopal $C_{40}H_{40}N_{12}O_8S_2$ [24231-46-7] YGUMVDWOQQJBGA-VAWYXSNFSA-N	1.2×10^{38} 1.4×10^{40} 4.2×10^{26} 2.2×10^{37}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
quinupristin $C_{53}H_{67}N_9O_{10}S$ [120138-50-3] WTHRRGMBUAHGNI-UHFFFAOYSA-N	4.9×10^{22}		HSDB (2015)	Q	100
3,3,4,4,4-pentafluorobutane-1-thiol $C_4H_5F_5S$ [68140-18-1] WEILNYJKAUGBAU-UHFFFAOYSA-N	5.2×10^{-5} 1.4×10^{-3} 1.5×10^{-3} 1.2×10^{-5}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
3,3,4,4,5,5,6,6,6-nonafluoro-1-hexanethiol $C_6H_5F_9S$ [68140-20-5] GQJXVHYUQPXZOL-UHFFFAOYSA-N	1.9×10^{-6} 4.7×10^{-4} 3.1×10^{-4} 1.9×10^{-6}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
3,3,4,4,5,5,7,7,8,8,9,9,10,10,10-pentadecafluoro-1-decanethiol $C_{10}H_7F_{15}S$ [68140-21-6] ROKKEEDUUQVHFZ-UHFFFAOYSA-N	9.7×10^{-9} 6.5×10^{-6} 8.6×10^{-4} 1.3×10^{-8}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
3,3,4,4,5,5-hexafluoro-1-(3,3,4,4,5,5-hexafluorohexyldisulfanyl)hexane $C_{12}H_{14}F_{12}S_2$ [118400-71-8] CIZUOSOWGOENRE-UHFFFAOYSA-N	1.2×10^{-7} 9.0×10^{-6} 1.9×10^{-2} 3.5×10^{-7}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
methanesulfonyl fluoride CH_3FO_2S [558-25-8] KNWQLFOXPQZGPX-UHFFFAOYSA-N	1.6×10^{-1}		Ebert et al. (2023)	?	319

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
perfluorobutane sulfonic acid $C_4HF_9O_3S$ (PFBS) [375-73-5] JGTNAGYHADQMCM-UHFFFAOYSA-N	2.0		Plassmann et al. (2011)	E	
4-(pentafluorosulfanyl)phenol $C_6H_5F_5OS$ [774-94-7] XHJLGVIUMCBMHL-UHFFFAOYSA-N	4.0×10^{1}		Ebert et al. (2023)	?	373
1H,1H,2H,2H-perfluorohexane sulfonic acid $C_6H_5F_9O_3S$ (4:2 FTS) [757124-72-4] TXGIGTRUEITPSC-UHFFFAOYSA-N	4.5×10^{-3}		Abusallout et al. (2022)	M	
perfluorohexane sulfonic acid $C_6HF_{13}O_3S$ (PFHxS) [355-46-4] QZHDEAJFRJCDMF-UHFFFAOYSA-N	5.1×10^{-1}		Plassmann et al. (2011)	E	
1H,1H,2H,2H-perfluorooctane sulfonic acid $C_8H_5F_{13}O_3S$ (6:2 FTS) [27619-97-2] VIONGDJUYAYOPU-UHFFFAOYSA-N	2.1×10^{-3}	11000	Abusallout et al. (2022)	M	
perfluorooctane sulfonic acid $C_8HF_{17}O_3S$ (PFOS) [1763-23-1] YFSUTJLHUFNCNZ-UHFFFAOYSA-N	9.0×10^{-4} 8.6×10^{-3} 1.6×10^{-1} 9.9×10^{-3} 1.0×10^{-1} 4.6×10^{-3}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Arp et al. (2006) Arp et al. (2006)	Q Q Q Q Q Q	288, 289 288, 290 288, 291 288, 292 635 636
heptadecafluorooctanesulphonyl fluoride $C_8F_{18}O_2S$ (perfluorooctylsulfonyl fluoride) [307-35-7] BHFJBHMTEDLICO-UHFFFAOYSA-N	1.5×10^{-7}		HSDB (2015)	Q	100

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1H,1H,2H,2H-perfluorodecane sulfonic acid $C_{10}H_5F_{17}O_3S$ (8:2 FTS) [39108-34-4] ALVYVCQIFHTIRD-UHFFFAOYSA-N	2.2×10^{-3}		Abusallout et al. (2022)	M	
fluticasone $C_{22}H_{27}F_3O_4S$ [90566-53-3] MGNNYOODZCAHBA-GQKYHHCASA-N	4.3×10^{3}		HSDB (2015)	Q	100
3-aminophenylsulfur pentafluoride $C_6H_6F_5NS$ [2993-22-8] NUFLICUHOXHWER-UHFFFAOYSA-N	6.4		Ebert et al. (2023)	?	373
4-aminophenylsulfur pentafluoride $C_6H_6F_5NS$ [2993-24-0] MZGZUHNSMNNSRJ-UHFFFAOYSA-N	4.0		Ebert et al. (2023)	?	373
flubenzimine $C_{17}H_{10}F_6N_4S$ [37893-02-0] IZFZCMFMJKDHJZ-UHFFFAOYSA-N	$>2.3\times10^{10}$		MacBean (2012a)	?	
thiazafluron $C_6H_7F_3N_4OS$ [25366-23-8] BBJPZPLAZVZTGR-UHFFFAOYSA-N	3.2×10^{4}		MacBean (2012a)	?	
4-nitrophenylsulfur pentafluoride $C_6H_4F_5NO_2S$ [2613-27-6] AGNCKMHGYZKMLN-UHFFFAOYSA-N	1.6×10^{-1}		Ebert et al. (2023)	?	373
undecafluoro-N-methyl-1-pentanesulfonamide	3.5×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_6H_4F_{11}NO_2S$	4.4×10^{-2}		Zhang et al. (2010)	Q	288, 290
[68298-13-5]	5.6×10^{-4}		Zhang et al. (2010)	Q	288, 291
BKKNDZBSSSAGIB-UHFFFAOYSA-N	6.2×10^{-1}		Zhang et al. (2010)	Q	288, 292
1,1,2,2,3,3,4,4,4-nonafluoro-N-(2-hydroxyethyl)-N-methylbutane-1-sulfonamide	1.8×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_7H_8F_9NO_3S$	1.1×10^{1}		Zhang et al. (2010)	Q	288, 290
[34454-97-2]	4.6×10^{-1}		Zhang et al. (2010)	Q	288, 291
DSRUAYIFDCHEEV-UHFFFAOYSA-N	2.7×10^{2}		Zhang et al. (2010)	Q	288, 292

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tridecafluoro-N-methyl-1-hexanesulfonamide	6.7×10^{-5}		Zhang et al. (2010)	Q	288, 289
$C_7H_4F_{13}NO_2S$	9.2×10^{-3}		Zhang et al. (2010)	Q	288, 290
[68259-15-4]	2.5×10^{-4}		Zhang et al. (2010)	Q	288, 291
HPPDPHZGXWMRHN-UHFFFAOYSA-N	1.2×10^{-1}		Zhang et al. (2010)	Q	288, 292
perfluorooctane sulfonamide	5.5×10^{-6}		HSDB (2015)	Q	100
$C_8H_2F_{17}NO_2S$	3.4		Arp et al. (2006)	Q	635
(PFOSA)	7.9×10^{-6}		Arp et al. (2006)	Q	636
[754-91-6]					
RRRXPPIDPYTNJG-UHFFFAOYSA-N					
emtricitabine	9.0×10^{11}		HSDB (2015)	Q	100
$C_8H_{10}FN_3O_3S$					
[143491-57-0]					
XQSPYNMVSIKCOC-NTSWFWBYSA-N					
N-ethyl-1,1,2,2,3,3,4,4,4-nonafluoro-N-(2-hydroxyethyl)butane-1-sulfonamide	1.3×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_8H_{10}F_9NO_3S$	8.8		Zhang et al. (2010)	Q	288, 290
[34449-89-3]	1.4×10^{-1}		Zhang et al. (2010)	Q	288, 291
ZSBOIPHQFKYRMG-UHFFFAOYSA-N	2.1×10^{2}		Zhang et al. (2010)	Q	288, 292
1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-N-methylheptane-1-sulphonamide	1.3×10^{-5}		Zhang et al. (2010)	Q	288, 289
$C_8H_4NO_2F_{15}S$	1.6×10^{-3}		Zhang et al. (2010)	Q	288, 290
[68259-14-3]	1.2×10^{-4}		Zhang et al. (2010)	Q	288, 291
KDHCALLFPWZTPN-UHFFFAOYSA-N	2.4×10^{-2}		Zhang et al. (2010)	Q	288, 292
1,1,2,2,3,3,4,4,5,5,5-undecafluoro-N-(2-hydroxyethyl)-N-methylpentane-1-sulphonamide	3.4		Zhang et al. (2010)	Q	288, 289
$C_8H_8NO_3F_{11}S$	2.9		Zhang et al. (2010)	Q	288, 290
[68555-74-8]	2.1×10^{-1}		Zhang et al. (2010)	Q	288, 291
BRBCKWCOTRPYGH-UHFFFAOYSA-N	5.6×10^{1}		Zhang et al. (2010)	Q	288, 292
N-(3-(dimethylamino)propyl)-nonafluoro-1-butanesulfonamide	2.1		Zhang et al. (2010)	Q	288, 289
$C_9H_{13}F_9N_2O_2S$	3.1×10^{1}		Zhang et al. (2010)	Q	288, 290
[68555-77-1]	1.1		Zhang et al. (2010)	Q	288, 291
XMRMVBVJGSKMEN-UHFFFAOYSA-N	6.0×10^{2}		Zhang et al. (2010)	Q	288, 292

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N- methylperfluorooctanesulphonamide	4.4×10^{-4}		Abusallout et al. (2022)	M	
$C_9H_4F_{17}NO_2S$	2.4×10^{-6}		Zhang et al. (2010)	Q	288, 289
(N-MeFOSA)	2.1×10^{-4}		Zhang et al. (2010)	Q	288, 290
[31506-32-8]	5.2×10^{-5}		Zhang et al. (2010)	Q	288, 291
SRMWNTGHXHOWBT-UHFFFAOYSA-N	5.0×10^{-3}		Zhang et al. (2010)	Q	288, 292
N-ethyl-1,1,2,2,3,3,4,4,5,5,5- undecafluoro-N-(2-hydroxyethyl)- 1-pentanesulfonamide	2.5		Zhang et al. (2010)	Q	288, 289
$C_9H_{10}NO_3F_{11}S$	2.3		Zhang et al. (2010)	Q	288, 290
[68555-72-6]	6.0×10^{-2}		Zhang et al. (2010)	Q	288, 291
GBPAQIZWHVCENQ-UHFFFAOYSA-N	4.1×10^{1}		Zhang et al. (2010)	Q	288, 292
1,1,2,2,3,3,4,4,5,5,6,6,6- tridecafluoro-N-(2-hydroxyethyl)- N-methyl-1-hexanesulfonamide	6.4×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_9H_8NO_3F_{13}S$	6.0×10^{-1}		Zhang et al. (2010)	Q	288, 290
[68555-75-9]	9.2×10^{-2}		Zhang et al. (2010)	Q	288, 291
UYIBZOUSVFOPJK-UHFFFAOYSA-N	9.9		Zhang et al. (2010)	Q	288, 292
N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,6- tridecafluoro-N-(2- hydroxyethyl)hexane-1- sulfonamide	4.7×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{10}H_{10}F_{13}NO_3S$	4.6×10^{-1}		Zhang et al. (2010)	Q	288, 290
[34455-03-3]	3.1×10^{-2}		Zhang et al. (2010)	Q	288, 291
SSGYCIQAXNQIBC-UHFFFAOYSA-N	8.8		Zhang et al. (2010)	Q	288, 292
2- methyl[(nonafluorobutyl)sulfonyl] aminoethyl acrylate	5.1×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{10}H_{10}F_9NO_4S$	5.3×10^{-1}		Zhang et al. (2010)	Q	288, 290
[67584-55-8]	8.2×10^{1}		Zhang et al. (2010)	Q	288, 291
KEMCLRGAIUJRAN-UHFFFAOYSA-N	4.8×10^{1}		Zhang et al. (2010)	Q	288, 292
N- ethylperfluorooctanesulfonamide	9.4×10^{-4}		Abusallout et al. (2022)	M	
$C_{10}H_6F_{17}NO_2S$	1.8×10^{-6}		HSDB (2015)	Q	100
(N-EtFOSA)	1.8×10^{-6}		Zhang et al. (2010)	Q	288, 289
[4151-50-2]	1.4×10^{-4}		Zhang et al. (2010)	Q	288, 290
CCEKAJIANROZEO-UHFFFAOYSA-N	9.5×10^{-6}		Zhang et al. (2010)	Q	288, 291
	3.8×10^{-3}		Zhang et al. (2010)	Q	288, 292
	6.4×10^{-3}		Arp et al. (2006)	Q	635
	7.5×10^{-3}		Arp et al. (2006)	Q	636

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-N-(2-hydroxyethyl)-N-methylheptane-1-sulphonamide	1.2×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{10}H_8NO_3F_{15}S$	9.5×10^{-2}		Zhang et al. (2010)	Q	288, 290
[68555-76-0]	4.5×10^{-2}		Zhang et al. (2010)	Q	288, 291
UIZUTEDYGNRNSW-UHFFFAOYSA-N	2.1		Zhang et al. (2010)	Q	288, 292
N-methyl perfluorooctane sulfonamidoethanol	2.3×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{11}H_8F_{17}NO_3S$	1.2×10^{-2}		Zhang et al. (2010)	Q	288, 290
(MeFOSE)	1.9×10^{-2}		Zhang et al. (2010)	Q	288, 291
[24448-09-7]	4.3×10^{-1}		Zhang et al. (2010)	Q	288, 292
PLGACQRCZCVKGK-UHFFFAOYSA-N	4.8×10^{-1}		Arp et al. (2006)	Q	635
	2.1×10^{-3}		Arp et al. (2006)	Q	636
N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-N-(2-hydroxyethyl)-1-heptanesulfonamide	9.0×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{11}H_{10}NO_3F_{15}S$	7.2×10^{-2}		Zhang et al. (2010)	Q	288, 290
[68555-73-7]	1.5×10^{-2}		Zhang et al. (2010)	Q	288, 291
HINASMOVWHGCAK-UHFFFAOYSA-N	1.8		Zhang et al. (2010)	Q	288, 292
mefluidide $C_{11}H_{13}F_3N_2O_3S$ [53780-34-0] OKIBNKKYNPBDRS-UHFFFAOYSA-N	7.6×10^{5}		HSDB (2015)	Q	100
N-(3-(dimethylamino)propyl)-1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonamide	7.7×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{11}H_{13}N_2O_2F_{13}S$	1.5		Zhang et al. (2010)	Q	288, 290
[50598-28-2]	2.2×10^{-1}		Zhang et al. (2010)	Q	288, 291
INDOGKYZYLAGEM-UHFFFAOYSA-N	2.5×10^{1}		Zhang et al. (2010)	Q	288, 292
2-(methyl((undecafluoropentyl) sulfonyl)amino)ethyl prop-2-enoate	9.7×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{11}H_{10}F_{11}NO_4S$	2.0×10^{-1}		Zhang et al. (2010)	Q	288, 290
[67584-56-9]	7.5×10^{1}		Zhang et al. (2010)	Q	288, 291
FZWFDJBZTLTRGH-UHFFFAOYSA-N	9.7		Zhang et al. (2010)	Q	288, 292

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-(methyl((nonafluorobutyl) sulphonyl)amino)ethyl methacrylate	3.3×10^{-1}		Zhang et al. (2010)	Q	288, 289
$C_{11}H_{12}F_9NO_4S$	5.0×10^{-1}		Zhang et al. (2010)	Q	288, 290
[67584-59-2]	1.9×10^{-1}		Zhang et al. (2010)	Q	288, 291
BEIWUHUHJDEMQO-UHFFFAOYSA-N	2.9×10^{1}		Zhang et al. (2010)	Q	288, 292
N-(3-(dimethylamino)propyl) pentadecafluoro-1-heptanesulfonamide	1.5×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_{13}F_{15}N_2O_2S$	2.3×10^{-1}		Zhang et al. (2010)	Q	288, 290
[67584-54-7]	1.8×10^{-2}		Zhang et al. (2010)	Q	288, 291
RFJQYRXZGNILIY-UHFFFAOYSA-N	5.2		Zhang et al. (2010)	Q	288, 292
acrylic acid 2-[methyl[(tridecafluorohexyl)sulfonyl] amino]ethyl ester	1.8×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_{10}F_{13}NO_4S$	6.0×10^{-2}		Zhang et al. (2010)	Q	288, 290
[67584-57-0]	3.4×10^{1}		Zhang et al. (2010)	Q	288, 291
HLKZFXXWGVPYAY-UHFFFAOYSA-N	2.0		Zhang et al. (2010)	Q	288, 292
N-ethyl perfluorooctane sulfonamidoethanol	1.7×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_{10}F_{17}NO_3S$	8.6×10^{-3}		Zhang et al. (2010)	Q	288, 290
(EtFOSE)	6.2×10^{-3}		Zhang et al. (2010)	Q	288, 291
[1691-99-2]	3.3×10^{-1}		Zhang et al. (2010)	Q	288, 292
HUFHNYZNTFSKCT-UHFFFAOYSA-N	5.7×10^{-2}		Arp et al. (2006)	Q	635
	1.2×10^{-3}		Arp et al. (2006)	Q	636
flumetsulam $C_{12}H_9F_2N_5O_2S$ [98967-40-9] RXCPQSJAVKGONC-UHFFFAOYSA-N	1.5×10^{11}		Ebert et al. (2023)	?	317
florasulam	1.7×10^{6}		HSDB (2015)	V	
$C_{12}H_8F_3N_5O_3S$	2.3×10^{6}		Maniere et al. (2011)	?	12, 495, 166
[145701-23-1]	3.4×10^{7}		Maniere et al. (2011)	?	12, 575, 166
QZXATCCPQKOEIH-UHFFFAOYSA-N	3.0×10^{4}		Maniere et al. (2011)	?	12, 572, 166
2-(methyl((pentadecafluoroheptyl) sulphonyl)amino)ethyl acrylate	3.5×10^{-3}		Zhang et al. (2010)	Q	288, 289
$C_{13}H_{10}F_{15}NO_4S$	1.5×10^{-2}		Zhang et al. (2010)	Q	288, 290
[68084-62-8]	9.9		Zhang et al. (2010)	Q	288, 291
BEYGZFVOTUDDJK-UHFFFAOYSA-N	4.2×10^{-1}		Zhang et al. (2010)	Q	288, 292

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
flazasulfuron $C_{13}H_{12}F_3N_5O_5S$ [104040-78-0] HWATZEJQIXKWQS-UHFFFAOYSA-N	1.6×10^{6} $>3.9\times10^{5}$		HSDB (2015) Maniere et al. (2011)	Q ?	100 166
tritosulfuron $C_{13}H_9F_6N_5O_4S$ [142469-14-5] KVEQCVKVIFQSGC-UHFFFAOYSA-N	$>1.0\times10^{4}$		Maniere et al. (2011)	?	12, 166
pyroxsulam $C_{14}H_{13}F_3N_6O_5S$ [422556-08-9] GLBLPMUBLHYFCW-UHFFFAOYSA-N	1.4×10^{6}		Maniere et al. (2011)	?	242, 166
N-methyl perfluorooctane sulfonamidoethylacrylate $C_{14}H_{10}F_{17}NO_4S$ (MeFOSEA) [25268-77-3] RTJZWOGSCLVJLD-UHFFFAOYSA-N	4.4×10^{-2} 2.2×10^{-3}		Arp et al. (2006) Arp et al. (2006)	Q Q	635 636
pyrasulfotole $C_{14}H_{13}F_3N_2O_4S$ [365400-11-9] CZRVDACSCJKRFL-UHFFFAOYSA-N	7.0×10^{8}		HSDB (2015)	V	
triafamone $C_{14}H_{13}F_3N_4O_5S$ [874195-61-6] GBHVIWKSEHWFDD-UHFFFAOYSA-N	8.2×10^{3}		Ebert et al. (2023)	?	319
flufenacet $C_{14}H_{13}F_4N_3O_2S$ [142459-58-3] IANUJLZYFUDJIH-UHFFFAOYSA-N	1.7×10^{3} 1.1×10^{3}		HSDB (2015) Maniere et al. (2011)	V ?	 12, 166
N-butyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-N-(2-hydroxyethyl)-1-octanesulfonamide $C_{14}H_{14}F_{17}NO_3S$ [2263-09-4] AQWROZBAYZBWIH-UHFFFAOYSA-N	9.7×10^{-3} 4.1×10^{-3} 3.8×10^{-2} 2.2×10^{-1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethyl N-ethyl-N-[(heptadecafluorooctyl) sulphonyl]glycinate	1.3×10^{-5}		Zhang et al. (2010)	Q	288, 289
$C_{14}H_{12}NO_4F_{17}S$	1.8×10^{-3}		Zhang et al. (2010)	Q	288, 290
[1869-77-8]	4.3		Zhang et al. (2010)	Q	288, 291
LMUUXHHNCDERBQ-UHFFFAOYSA-N	3.0×10^{-2}		Zhang et al. (2010)	Q	288, 292
perfluidone	1.3×10^{2}		Duchowicz et al. (2020)	V	187
$C_{14}H_{12}F_3NO_4S_2$	1.6×10^{8}		Duchowicz et al. (2020)	Q	
[37924-13-3]					
WHTBVLXUSXVMEV-UHFFFAOYSA-N					
2-(((heptadecafluorooctyl)sulfonyl) methylamino)ethyl methacrylate	4.2×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_{15}H_{12}F_{17}NO_4S$	3.3×10^{-3}		Zhang et al. (2010)	Q	288, 290
[14650-24-9]	2.5		Zhang et al. (2010)	Q	288, 291
UZMOXNBUTMPDCX-UHFFFAOYSA-N	5.4×10^{-2}		Zhang et al. (2010)	Q	288, 292
2-(N-ethylperfluorooctane- sulfonamido)ethyl acrylate	1.1		Ebert et al. (2023)	?	373
$C_{15}H_{12}F_{17}NO_4S$					
[423-82-5]					
ZAZJGBCGMUKZEL-UHFFFAOYSA-N					
isoxaflutole	5.3×10^{4}		MacBean (2012b)	X	352
$C_{15}H_{12}F_3NO_4S$	5.3×10^{4}		Maniere et al. (2011)	?	12, 166
[141112-29-0]					
OYIKARCXOQLFHF-UHFFFAOYSA-N					
primisulfuron-methyl	7.0×10^{6}		HSDB (2015)	Q	100
$C_{15}H_{12}F_4N_4O_7S$					
[86209-51-0]					
ZTYVMAQSHCZXLF-UHFFFAOYSA-N					
dithiopyr	6.5		Ebert et al. (2023)	?	741
$C_{15}H_{16}F_5NO_2S_2$					
[97886-45-8]					
YUBJPYNSGLJZPQ-UHFFFAOYSA-N					
penoxsulam	9.0×10^{12}		HSDB (2015)	V	
$C_{16}H_{14}F_5N_5O_5S$	1.2×10^{14}		Maniere et al. (2011)	?	242, 575, 166
[219714-96-2]	4.7×10^{11}		Maniere et al. (2011)	?	242, 572, 166
SYJGKVOENHZYMQ-UHFFFAOYSA-N	3.4×10^{13}		Maniere et al. (2011)	?	242, 495, 166

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pantoprazole $C_{16}H_{15}F_2N_3O_4S$ [102625-70-7] IQPSEEYGBUAQFF-UHFFFAOYSA-N	1.7×10^{14}		HSDB (2015)	Q	100
2-(N-ethylperfluorooctanesulfamido)ethyl methacrylate	3.2×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_{16}H_{14}F_{17}NO_4S$	3.9×10^{-3}		Zhang et al. (2010)	Q	288, 290
[376-14-7]	1.5		Zhang et al. (2010)	Q	288, 291
DBCGADAHIXJHCE-UHFFFAOYSA-N	4.1×10^{-2}		Zhang et al. (2010)	Q	288, 292
thiazopyr	2.1×10^{1}		Duchowicz et al. (2020)	V	187
$C_{16}H_{17}F_5N_2O_2S$	2.1×10^{1}		HSDB (2015)	V	
[117718-60-2]	8.7×10^{3}		Duchowicz et al. (2020)	Q	
YIJZJEYQBAAWRJ-UHFFFAOYSA-N					
penthiopyrad	7.1×10^{3}		Maniere et al. (2011)	?	12, 572, 166
$C_{16}H_{20}F_3N_3OS$	1.3×10^{2}		Maniere et al. (2011)	?	12, 495, 166
[183675-82-3]	2.4×10^{3}		Maniere et al. (2011)	?	12, 579, 166
PFFIDZXUXFLSSR-UHFFFAOYSA-N	1.6×10^{2}		Maniere et al. (2011)	?	12, 574, 166
triflusulfuron-methyl	$>4.2\times10^{2}$		Maniere et al. (2011)	?	242, 579, 166
$C_{17}H_{19}F_3N_6O_6S$ [126535-15-7] IMEVJVISCHQJRM-UHFFFAOYSA-N					
celecoxib $C_{17}H_{14}F_3N_3O_2S$ [169590-42-5] RZEKVGVHFLEQIL-UHFFFAOYSA-N	1.3×10^{7}		HSDB (2015)	Q	100
2-(butyl((heptadecafluorooctyl) sulfonyl)amino)ethyl acrylate	2.9×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_{17}H_{16}F_{17}NO_4S$	4.1×10^{-3}		Zhang et al. (2010)	Q	288, 290
[383-07-3]	1.8		Zhang et al. (2010)	Q	288, 291
AQQNNAXBGPWALO-UHFFFAOYSA-N	4.3×10^{-2}		Zhang et al. (2010)	Q	288, 292
thidiazimin $C_{18}H_{17}N_4O_2FS$ [123249-43-4] HZKBYBNLTLVSPX-JZJYNLBNSA-N	3.5×10^{8}		MacBean (2012a)	?	

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benthiavalicarb isopropyl $C_{18}H_{24}FN_3O_3S$ [177406-68-7] USRKFGIXLGKMKU-IAQYHMDHSA-N	1.1×10^{2} $>1.1\times10^{2}$		MacBean (2012b) Maniere et al. (2011)	X ?	352 12, 166
flutianil $C_{19}H_{14}F_4N_2OS_2$ [958647-10-4] KGXUEPOHGFWQKF-ZCXUNETKSA-N	7.2×10^{1}		Ebert et al. (2023)	?	319
rosuvastatin $C_{22}H_{28}N_3O_6FS$ [287714-41-4] BPRHUIZQVSMCRT-YXWZHEERSA-N	2.9×10^{14}		HSDB (2015)	Q	100
oxathiapiprolin $C_{24}H_{22}F_5N_5O_2S$ [1003318-67-9] IAQLCKZJGNTRDO-UHFFFAOYSA-N	2.8×10^{2}		Maniere et al. (2011)	?	12, 166
trichloromethanesulfenyl chloride CCl_4S [594-42-3] RYFZYYUIAZYQLC-UHFFFAOYSA-N	4.1×10^{-2} 6.9×10^{-4} 9.5×10^{-4} 5.3×10^{-3}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
1,1,2,2-tetrachloroethanesulfenyl chloride C_2HCl_5S [1185-09-7] LCVOCDOSGJHZFH-UHFFFAOYSA-N	8.8×10^{-2} 3.7×10^{-3} 1.9×10^{-2} 6.7×10^{-2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
2-chloroethyl methyl sulfide C_3H_7ClS [542-81-4] MYFKLQFBFSHBPA-UHFFFAOYSA-N	5.3×10^{-2}		Bartelt-Hunt et al. (2008)	?	21
2-chloroethyl ethyl sulfide C_4H_9ClS [693-07-2] GBNVXYXIRHSYEG-UHFFFAOYSA-N	2.0×10^{-2} 2.7×10^{-2}		HSDB (2015) Bartelt-Hunt et al. (2008)	Q ?	100 21
2,2'-dichlorodiethylsulfide $(ClCH_2CH_2)_2S$ (mustard gas) [505-60-2] QKSKPIVNLNLAAV-UHFFFAOYSA-N	3.0×10^{-1} 2.2×10^{-2} 1.5×10^{-1} 1.6×10^{-1} 4.0×10^{-1} 4.1×10^{-1} 4.1×10^{-1}		Hine and Mookerjee (1975) Keshavarz et al. (2022) Duchowicz et al. (2020) Modarresi et al. (2007) Duchowicz et al. (2020) Bartelt-Hunt et al. (2008) Opresko et al. (1998)	V Q Q Q ? ? ?	 300 68 186, 21 21

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-bis(2-chloroethylthio)ethane $C_6H_{12}Cl_2S_2$ (sesquimustard) [3563-36-8] AMGNHZVUZWILSB-UHFFFAOYSA-N	8.8×10^{1}		Ebert et al. (2023)	?	319
pentachlorobenzenethiol	6.6×10^{-2}		HSDB (2015)	Q	100
C_6HCl_5S	8.4×10^{-2}		Zhang et al. (2010)	Q	288, 289
[133-49-3]	2.7×10^{-2}		Zhang et al. (2010)	Q	288, 290
LLMLGZUZTFMXSA-UHFFFAOYSA-N	1.3		Zhang et al. (2010)	Q	288, 291
	2.2×10^{-2}		Zhang et al. (2010)	Q	288, 292
chloroethyl phenyl sulfide C_8H_9ClS [5535-49-9] QDXIHHOPZFCEAP-UHFFFAOYSA-N	1.3×10^{-1}		Bartelt-Hunt et al. (2008)	?	21
tetrasul $C_{12}H_6Cl_4S$ [2227-13-6] QUWSDLYBOVGOCW-UHFFFAOYSA-N	9.3×10^{-1}		MacBean (2012a)	?	
methanesulfonyl chloride CH_3ClO_2S [124-63-0] QARBMVPHQWIHKH-UHFFFAOYSA-N	2.2×10^{-1}		HSDB (2015)	Q	100
bis(trichloromethyl)sulfone	8.2×10^{2}		HSDB (2015)	Q	100
$C_2Cl_6O_2S$	8.2×10^{2}		Zhang et al. (2010)	Q	288, 289
[3064-70-8]	1.2×10^{-2}		Zhang et al. (2010)	Q	288, 290
YBNLWIZAWPBUKQ-UHFFFAOYSA-N	3.1×10^{3}		Zhang et al. (2010)	Q	288, 291
	1.0×10^{1}		Zhang et al. (2010)	Q	288, 292
benzenesulfonyl chloride	1.1		Zhang et al. (2010)	Q	288, 289
$C_6H_5ClO_2S$	1.7×10^{1}		Zhang et al. (2010)	Q	288, 290
[98-09-9]	6.7		Zhang et al. (2010)	Q	288, 291
CSKNSYBAZOQPLR-UHFFFAOYSA-N	1.6×10^{2}		Zhang et al. (2010)	Q	288, 292
4-methylbenzenesulfonyl chloride	1.0		Zhang et al. (2010)	Q	288, 289
$C_7H_7ClO_2S$	1.8×10^{1}		Zhang et al. (2010)	Q	288, 290
[98-59-9]	1.2×10^{1}		Zhang et al. (2010)	Q	288, 291
YYROPELSRYBVMQ-UHFFFAOYSA-N	9.2×10^{1}		Zhang et al. (2010)	Q	288, 292
endosulfan	9.4×10^{-1}		Mackay et al. (2006d)	V	
$C_9H_6Cl_6O_3S$	1.1×10^{2}		Zhang et al. (2010)	Q	288, 289
[115-29-7]	2.4×10^{1}		Zhang et al. (2010)	Q	288, 290
RDYMFSUJUZBWLH-UHFFFAOYSA-N	1.1×10^{2}		Zhang et al. (2010)	Q	288, 291
	2.3×10^{8}		Zhang et al. (2010)	Q	288, 292
	3.1×10^{1}		Hilal et al. (2008)	Q	
	7.8×10^{-1}		Modarresi et al. (2007)	Q	68

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
α-endosulfan	1.4		Shen and Wania (2005)	L	368
$C_9H_6Cl_6O_3S$	1.4		Shen and Wania (2005)	L	369
(endosulfan I)	1.4		Muir et al. (2004)	L	369
[959-98-8]	1.4		Muir et al. (2004)	L	368
RDYMFSUJUZBWLH-AMHWMVONSA-N	1.2		Chao et al. (2017)	M	
	1.3	4200	Cetin et al. (2006)	M	
	1.4		Altschuh et al. (1999)	M	
	1.5×10^{-1}		Rice et al. (1997b)	M	12
	1.3×10^{-1}	2300	Rice et al. (1997a)	M	
	1.5		Cotham and Bidleman (1989)	V	
	3.4×10^{-1}		Suntio et al. (1988)	V	12
	9.2×10^{-1}		Suntio et al. (1988)	C	
	9.6×10^{-2}		Keshavarz et al. (2022)	Q	
	5.2×10^{1}		Duchowicz et al. (2020)	Q	
	8.0×10^{-1}		Modarresi et al. (2007)	Q	68
		3200	Kühne et al. (2005)	Q	
	1.4		Duchowicz et al. (2020)	?	186, 21
		2300	Kühne et al. (2005)	?	
β-endosulfan	2.5×10^{1}		Shen and Wania (2005)	L	368
$C_9H_6Cl_6O_3S$	2.2×10^{1}		Shen and Wania (2005)	L	369
(endosulfan II)	6.4		Chao et al. (2017)	M	
[33213-65-9]	1.9×10^{1}	3700	Cetin et al. (2006)	M	
RDYMFSUJUZBWLH-MDBBVBRHSA-N	2.5		Altschuh et al. (1999)	M	
	1.1		Rice et al. (1997b)	M	12
	1.1		Rice et al. (1997a)	M	12
	1.6×10^{1}		Cotham and Bidleman (1989)	V	
	1.6×10^{3}		Keshavarz et al. (2022)	Q	
	5.2×10^{1}		Duchowicz et al. (2020)	Q	185
	3.1×10^{1}		Hilal et al. (2008)	Q	
	8.0×10^{-1}		Modarresi et al. (2007)	Q	68
	2.5×10^{1}		Duchowicz et al. (2020)	?	186, 21
endosulfan sulfate	8.2×10^{5}		HSDB (2015)	V	
$C_9H_6Cl_6O_4S$					
[1031-07-8]					
AAPVQEMYVNZIOO-UHFFFAOYSA-N					
mcpa-thioethyl	4.5×10^{-1}		Mackay et al. (2006d)	V	
$C_{11}H_{13}ClO_2S$					
[25319-90-8]					
AZFKQCNGMSSWDS-UHFFFAOYSA-N					
1,1'-sulfonylbis(4-chlorobenzene)	7.0×10^{1}		HSDB (2015)	Q	100
$C_{12}H_8Cl_2O_2S$	7.2×10^{1}		Zhang et al. (2010)	Q	288, 289
[80-07-9]	6.5×10^{3}		Zhang et al. (2010)	Q	288, 290
GPAPPPVRLPGFEQ-UHFFFAOYSA-N	5.0×10^{4}		Zhang et al. (2010)	Q	288, 291
	3.1×10^{3}		Zhang et al. (2010)	Q	288, 292

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2'-thiobis-4,6-dichlorophenol $C_{12}H_6Cl_4O_2S$ (bithionol) [97-18-7] JFIOVJDNOJYLKP-UHFFFAOYSA-N	1.1×10^{5}		Ebert et al. (2023)	?	319
1,2,4-trichloro-5-[(4-chlorophenyl)sulfonyl]benzene	6.9×10^{3}		Duchowicz et al. (2020)	V	187
$C_{12}H_6Cl_4O_2S$	6.9×10^{3}		HSDB (2015)	V	
(tetradifon)	1.0×10^{3}		Duchowicz et al. (2020)	Q	
[116-29-0] MLGCXEBRWGEOQX-UHFFFAOYSA-N					
ovex $C_{12}H_8Cl_2O_3S$ (chlorfenson) [80-33-1] RZXLPPRPEOUENN-UHFFFAOYSA-N	6.2×10^{1}		HSDB (2015)	Q	100
sulphenone $C_{12}H_9ClO_2S$ [80-00-2] OFCFYWOKHPOXKF-UHFFFAOYSA-N	5.2×10^{1}		HSDB (2015)	Q	100
sulcotrione $C_{14}H_{13}ClO_5S$ [99105-77-8] PQTBTIFWAXVEPB-UHFFFAOYSA-N	1.7×10^{6}		Maniere et al. (2011)	?	12, 818, 166
aramite $C_{15}H_{23}ClO_4S$ [140-57-8] YKFRAOGHWKADFJ-UHFFFAOYSA-N	5.2×10^{1}		HSDB (2015)	Q	100
6-chloro-2-(6-chloro-4-methyl-3-oxobenzo[*b*]thien-2(3H)-ylidene)-4-methylbenzo[*b*]thiophene-3(2H)-one	3.2×10^{7}		Zhang et al. (2010)	Q	288, 289
$C_{18}H_{10}Cl_2O_2S_2$	1.2×10^{7}		Zhang et al. (2010)	Q	288, 290
[2379-74-0]	5.4×10^{4}		Zhang et al. (2010)	Q	288, 291
NDDLLTAIKYHPOD-ISLYRVAYSA-N	2.4×10^{6}		Zhang et al. (2010)	Q	288, 292
5-chloro-3-(trichloromethyl)-1,2,4-thiadiazole	1.6×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_3Cl_4N_2S$	1.9×10^{1}		Zhang et al. (2010)	Q	288, 290
[5848-93-1]	7.3×10^{-1}		Zhang et al. (2010)	Q	288, 291
MARKPJMFLDWCID-UHFFFAOYSA-N	4.2×10^{-1}		Zhang et al. (2010)	Q	288, 292

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4-dichloro-6-(methylthio)-1,3,5-triazine	1.3×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_4H_3Cl_2N_3S$	1.3×10^{1}		Zhang et al. (2010)	Q	288, 290
[13705-05-0]	9.7×10^{-1}		Zhang et al. (2010)	Q	288, 291
MWPZLWRHHPWTFS-UHFFFAOYSA-N	1.7×10^{1}		Zhang et al. (2010)	Q	288, 292
chlorthiamid $C_7H_5Cl_2NS$ [1918-13-4] KGKGSIUWJCAFPX-UHFFFAOYSA-N	3.5×10^{4}		MacBean (2012a)	?	
(2-chlorophenyl)thiourea $C_7H_7ClN_2S$ [5344-82-1] YZUKKTCDYSIWKJ-UHFFFAOYSA-N	$>9.9\times10^{1}$		HSDB (2015)	Q	547
2-chloroallyl-N,N-diethyldithiocarbamate	1.5		Duchowicz et al. (2020)	V	187
$C_8H_{14}ClNS_2$	1.5		HSDB (2015)	V	
[95-06-7]	2.1×10^{2}		Duchowicz et al. (2020)	Q	
XJCLWVXTCRQIDI-UHFFFAOYSA-N	2.1×10^{1}		Hilal et al. (2008)	Q	
	4.1		Modarresi et al. (2007)	Q	68
thiacloprid	9.0×10^{8}		HSDB (2015)	V	
$C_{10}H_9ClN_4S$	2.1×10^{9}		Maniere et al. (2011)	?	242, 166
[111988-49-9] HOKKPVIRMVDYPB-UHFFFAOYSA-N					
chloromethiuron $C_{10}H_{13}N_2ClS$ [28217-97-2] IBZZDPVVVSNQOY-UHFFFAOYSA-N	2.0×10^{5}		MacBean (2012a)	?	
imibenconazole	4.9×10^{4}		Duchowicz et al. (2020)	V	187
$C_{17}H_{13}Cl_3N_4S$	6.8×10^{3}		Duchowicz et al. (2020)	Q	
[86598-92-7] AGKSTYPVMZODRV-UHFFFAOYSA-N					
etridiazole	3.6×10^{1}		Duchowicz et al. (2020)	V	187
$C_5H_5Cl_3N_2OS$	3.3×10^{-1}		HSDB (2015)	V	
[2593-15-9]	1.6×10^{1}		Mackay et al. (2006d)	V	
KQTVWCSONPJJPE-UHFFFAOYSA-N	5.3×10^{1}		Duchowicz et al. (2020)	Q	
4-chloro-3-nitrobenzenesulfonamide	8.2×10^{3}		HSDB (2015)	Q	100
$C_6H_5ClN_2O_4S$					
[97-09-6] SPZGXONNVLTQDE-UHFFFAOYSA-N					

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
clothianidin $C_6H_8ClN_5O_2S$ [210880-92-5] PGOOBECODWQEAB-UHFFFAOYSA-N	3.4×10^{10} 3.4×10^{10}		MacBean (2012b) Maniere et al. (2011)	X ?	352 12, 166
chlobenthiazone C_8H_6NOClS [63755-05-5] QCPASDYEQAVIJF-UHFFFAOYSA-N	1.3		MacBean (2012a)	?	
prothiocarb hydrochloride $C_8H_{19}ClN_2OS$ [19622-19-6] NMFAMPYSJHIYMR-UHFFFAOYSA-N	2.5×10^{9}		MacBean (2012a)	?	
thicyofen $C_8H_5N_2OClS_2$ [116170-30-0] GNOOAFGERMHQJE-UHFFFAOYSA-N	$>2.3\times10^{10}$		MacBean (2012a)	?	
thiamethoxam $C_8H_{10}ClN_5O_3S$ [153719-23-4] NWWZPOKUUAIXIW-DHZHZOJOSA-N	2.1×10^{9} 2.1×10^{9}		HSDB (2015) Maniere et al. (2011)	V ?	 166
4-amino-3,5-dichloro-N-ethyl-2-methylbenzenesulfonamide $C_9H_{12}Cl_2N_2O_2S$ [151574-12-8] SBBHTEMLRJJIGK-UHFFFAOYSA-N	3.8×10^{4} 1.1×10^{4} 1.2×10^{6} 1.5×10^{7}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
dichlofluanid $C_9H_{11}Cl_2FN_2O_2S_2$ [1085-98-9] WURGXGVFSMYFCG-UHFFFAOYSA-N	2.6×10^{2} 1.9×10^{2} 2.5×10^{4} 5.7×10^{2} 1.5×10^{1}		Duchowicz et al. (2020) Mackay et al. (2006d) Siebers and Mattusch (1996) Duchowicz et al. (2020) HSDB (2015)	V V V Q Q	187 12 100
captan $C_9H_8Cl_3NO_2S$ [133-06-2] LDVVMCZRFWMZSG-UHFFFAOYSA-N	1.4×10^{3} 1.5×10^{3} 1.7 1.6×10^{-2} 2.1×10^{-3} 3.3×10^{3} 5.0×10^{3}		HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Goodarzi et al. (2010) Maniere et al. (2011) Maniere et al. (2011)	V V V X Q ? ?	 12 569 570, 573 12, 572, 166 12, 495, 166

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benazolin $C_9H_6ClNO_3S$ [3813-05-6] HYJSGOXICXYZGS-UHFFFAOYSA-N	4.2×10^{6}		Ebert et al. (2023)	?	317
folpet	1.3×10^{2}		Duchowicz et al. (2020)	V	187
$C_9H_4Cl_3NO_2S$	1.3×10^{2}		HSDB (2015)	V	
[133-07-3]	2.6		Mackay et al. (2006d)	V	
HKIOYBQGHSTUDB-UHFFFAOYSA-N	2.6×10^{-2}		Barcelo and Hennion (1997)	X	569
	1.9×10^{1}		Duchowicz et al. (2020)	Q	
	1.2×10^{-1}		Goodarzi et al. (2010)	Q	570
	1.2×10^{2}		Maniere et al. (2011)	?	166
captafol	2.0×10^{3}		Duchowicz et al. (2020)	V	187
$C_{10}H_9Cl_4NO_2S$	3.7×10^{3}		HSDB (2015)	V	
(difolatan)	3.7×10^{1}		Duchowicz et al. (2020)	Q	
[2425-06-1]					
JHRWWRDRBPCWTF-UHFFFAOYSA-N					
diallate	2.6		HSDB (2015)	V	
$C_{10}H_{17}Cl_2NOS$	9.3		Mackay et al. (2006d)	V	
(avadex)	4.0		Suntio et al. (1988)	V	12
[2303-16-4]	2.6		MacBean (2012a)	?	
SPANOECCGNXGNR-UITAMQMPSA-N					
triallate	8.2×10^{-1}		HSDB (2015)	V	
$C_{10}H_{16}Cl_3NOS$	8.8×10^{-1}		Mackay et al. (2006d)	V	
[2303-17-5]	9.8×10^{-1}		Suntio et al. (1988)	V	12
MWBPRDONLNQCFV-UHFFFAOYSA-N	1.0×10^{-2}		Barcelo and Hennion (1997)	X	569
	1.6×10^{-2}		Goodarzi et al. (2010)	Q	570
	1.1		Maniere et al. (2011)	?	12, 166
tolylfluanid	1.3×10^{1}		Duchowicz et al. (2020)	V	187
$C_{10}H_{13}Cl_2FN_2O_2S_2$	1.3×10^{1}		HSDB (2015)	V	
[731-27-1]	1.6×10^{2}		Mackay et al. (2006d)	V	
HYVWIQDYBVKITD-UHFFFAOYSA-N	3.7×10^{2}		Duchowicz et al. (2020)	Q	
tiadinil $C_{11}H_{10}ClN_3OS$ [223580-51-6] VJQYLJSMBWXGDV-UHFFFAOYSA-N	5.3×10^{4}		Ebert et al. (2023)	?	319
benazolin-ethyl	4.7×10^{2}		Duchowicz et al. (2020)	V	187
$C_{11}H_{10}NO_3ClS$	5.2×10^{3}		Duchowicz et al. (2020)	Q	
[25059-80-7]					
WQRCEBAZAUAUQC-UHFFFAOYSA-N					

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
orbencarb $C_{12}H_{16}ClNOS$ [34622-58-7] LLLFASISUZUJEQ-UHFFFAOYSA-N	2.0×10^{1}		Ebert et al. (2023)	?	319
S-(4-chlorobenzyl) diethylthiocarbamate $C_{12}H_{16}ClNOS$ (thiobencarb) [28249-77-6] QHTQREMOGMZHJV-UHFFFAOYSA-N	1.9×10^{1} 4.9 3.7×10^{1} 5.8×10^{1} 3.7×10^{1}		Watanabe (1993) Kawamoto and Urano (1989) HSDB (2015) Woodrow et al. (1990) Armbrust (2000) Mackay et al. (2006d)	M M V V C W	 12 819
furosemide $C_{12}H_{11}ClN_2O_5S$ [54-31-9] ZZUFCTLCJUWOSV-UHFFFAOYSA-N	2.5×10^{10}		HSDB (2015)	Q	100
chlorsulfuron $C_{12}H_{12}ClN_5O_4S$ [64902-72-3] VJYIFXVZLXQVHO-UHFFFAOYSA-N	3.2×10^{4} 1.5×10^{5} 2.9×10^{10}		Mackay et al. (2006d) Armbrust (2000) Maniere et al. (2011)	V C ?	 242, 166
phosalone $C_{12}H_{15}ClNO_4S_2$ [2310-17-0] IOUNQDKNJZEDEP-UHFFFAOYSA-N	2.5×10^{1}		HSDB (2015)	Q	100
dimethenamid $C_{12}H_{18}ClNO_2S$ [87674-68-8] JLYFCTQDENRSOL-UHFFFAOYSA-N	8.9×10^{2} 4.7 4.5×10^{2} 2.3×10^{2} 1.2×10^{2}		Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Duchowicz et al. (2020)	Q Q Q Q ?	 68 186, 21
dimethenamid-p $C_{12}H_{18}ClNO_2S$ [163515-14-8] JLYFCTQDENRSOL-VIFPVBQESA-N	2.1×10^{3} 2.1×10^{3}		MacBean (2012b) Maniere et al. (2011)	X ?	352 166
cyazofamid $C_{13}H_{13}ClN_4O_2S$ [120116-88-3] YXKMMRDKEKCERS-UHFFFAOYSA-N	2.5×10^{1} $>2.5\times10^{1}$		HSDB (2015) Maniere et al. (2011)	V ?	 242, 166
metosulam $C_{14}H_{13}Cl_2N_5O_4S$ [139528-85-1] VGHPMIFEKOFHHQ-UHFFFAOYSA-N	1.2×10^{12}		Maniere et al. (2011)	?	12, 166

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
prothioconazole $C_{14}H_{15}Cl_2N_3OS$ [178928-70-6] MNHVNIJQQRJYDH-UHFFFAOYSA-N	2.2×10^4 $>3.3\times10^4$		HSDB (2015) Maniere et al. (2011)	V ?	 12, 166
triasulfuron $C_{14}H_{16}ClN_5O_5S$ [82097-50-5] XOPFESVZMSQIKC-UHFFFAOYSA-N	8.0×10^8		Ebert et al. (2023)	?	317
chlorimuron-ethyl $C_{15}H_{15}ClN_4O_6S$ [90982-32-4] NSWAMPCUPHPTTC-UHFFFAOYSA-N	5.5×10^9		HSDB (2015)	V	
clopidogrel $C_{16}H_{16}ClNO_2S$ [113665-84-2] GKTWGGQPFAXNFI-HNNXBMFYSA-N	4.5×10^3		HSDB (2015)	Q	100
thenylchlor $C_{16}H_{18}ClNO_2S$ [96491-05-3] KDWQYMVPYJGPHS-UHFFFAOYSA-N	1.2×10^3 6.3×10^1		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
chlorpromazine $C_{17}H_{19}ClN_2S$ [50-53-3] ZPEIMTDSQAKGNT-UHFFFAOYSA-N	6.5×10^4		Ebert et al. (2023)	?	317
hexythiazox $C_{17}H_{21}N_2O_2ClS$ [78587-05-0] XGWIJUOSCAQSSV-XHDPSFHLSA-N	4.2×10^2 8.4×10^1		HSDB (2015) Maniere et al. (2011)	V ?	 12, 166
clethodim $C_{17}H_{26}ClNO_3S$ [99129-21-2] INNPZTGYZSAJFN-ZTVUPKSFSA-N	8.2×10^5 7.1×10^6		HSDB (2015) Maniere et al. (2011)	Q ?	100 12, 166
clindamycin $C_{18}H_{33}N_2O_5ClS$ [18323-44-9] KDLRVYVGXIQJDK-AWPVFWJPSA-N	3.4×10^{16}		HSDB (2015)	Q	100
pyridate $C_{19}H_{23}ClN_2O_2S$ [55512-33-9] JTZCTMAVMHRNTR-UHFFFAOYSA-N	3.0×10^2 4.9 8.3×10^3		Barcelo and Hennion (1997) Goodarzi et al. (2010) Maniere et al. (2011)	X Q ?	569 570 12, 166

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
vismodegib $C_{19}H_{14}Cl_2N_2O_3S$ [879085-55-9] BPQMGSKTAYIVFO-UHFFFAOYSA-N	6.2×10^{11}		HSDB (2015)	Q	100
pyridaben $C_{19}H_{25}ClN_2OS$ [96489-71-3] DWFZBUWUXWZWKD-UHFFFAOYSA-N	2.1×10^{-1}		HSDB (2015)	V	
tembotrione $C_{17}H_{16}ClF_3O_6S$ [335104-84-2] IUQAXCIUEPFPSF-UHFFFAOYSA-N	5.8×10^{9} 5.8×10^{9}		HSDB (2015) Maniere et al. (2011)	V ?	 12, 166
fluensulfone $C_7H_5ClF_3NO_2S_2$ [318290-98-1] XSNMWAPKHUGZGQ-UHFFFAOYSA-N	6.1×10^{1}		Ebert et al. (2023)	?	319
fluothiuron $C_{10}H_{10}Cl_2F_2N_2OS$ [33439-45-1] YFEUKKUPOVGUIW-UHFFFAOYSA-N	$>2.3\times10^{10}$		MacBean (2012a)	?	
sulfentrazone $C_{11}H_{10}Cl_2F_2N_4O_3S$ [122836-35-5] OORLZFUTLGXMEF-UHFFFAOYSA-N	1.5×10^{7} 1.5×10^{7} 3.7×10^{8}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
flurazole $C_{12}H_7NO_2ClF_3S$ [72850-64-7] MKQSWTQPLLCSOB-UHFFFAOYSA-N	4.0×10^{1} 1.2×10^{2} 4.0×10^{1}		Duchowicz et al. (2020) Duchowicz et al. (2020) MacBean (2012a)	V Q ?	187
fipronil $C_{12}H_4Cl_2F_6N_4OS$ [120068-37-3] ZOCSXAVNDGMNBV-UHFFFAOYSA-N	1.2×10^{4} 1.2×10^{4} 4.4×10^{7}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
flusulfamide $C_{13}H_7Cl_2F_3N_2O_4S$ [106917-52-6] GNVDAZSPJWCIQZ-UHFFFAOYSA-N	4.0×10^{3}		Ebert et al. (2023)	?	319
ethiprole $C_{13}H_9Cl_2F_3N_4OS$ [181587-01-9] FNELVJVBIYMIMC-UHFFFAOYSA-N	2.5×10^{5}		Ebert et al. (2023)	?	319

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
diclosulam $C_{13}H_{10}Cl_2FN_5O_3S$ [145701-21-9] QNXAVFXEJCPCJO-UHFFFAOYSA-N	2.5×10^{10}		Ebert et al. (2023)	?	319
cloransulam-methyl $C_{15}H_{13}ClFN_5O_5S$ [147150-35-4] BIKACRYIQSLICJ-UHFFFAOYSA-N	1.6×10^{11}		Ebert et al. (2023)	?	319
fluthiacet-methyl	4.8×10^{3}		Duchowicz et al. (2020)	V	187
$C_{15}H_{15}ClFN_3O_3S_2$	4.7×10^{3}		HSDB (2015)	V	
[117337-19-6]	4.2×10^{5}		Duchowicz et al. (2020)	Q	
ZCNQYNHDVRPZIH-UHFFFAOYSA-N	6.6×10^{5}		Modarresi et al. (2007)	Q	68
vemurafenib $C_{23}H_{18}ClF_2N_3O_3S$ [918504-65-1] GPXBXXGIAQBQNI-UHFFFAOYSA-N	8.2×10^{11}		HSDB (2015)	Q	100
tetrabromobisphenol S	1.5×10^{11}		Zhang et al. (2010)	Q	288, 289
$C_{12}H_6Br_4O_4S$	9.7×10^{5}		Zhang et al. (2010)	Q	288, 290
[39635-79-5]	5.8×10^{6}		Zhang et al. (2010)	Q	288, 291
JHJUYGMZIWDHMO-UHFFFAOYSA-N	1.2×10^{7}		Zhang et al. (2010)	Q	288, 292
1,3-dibromo-5-[3,5-dibromo-4-(2,3-dibromopropoxy)benzenesulfonyl]-2-(2,3-dibromopropoxy)benzene	8.2×10^{8}		Zhang et al. (2010)	Q	288, 289
$C_{18}H_{14}Br_8O_4S$	5.2×10^{8}		Zhang et al. (2010)	Q	288, 290
[42757-55-1]	1.8×10^{11}		Zhang et al. (2010)	Q	288, 291
CWZVMVIHYSYLSI-UHFFFAOYSA-N	6.4×10^{8}		Zhang et al. (2010)	Q	288, 292
bromphenol blue	1.9×10^{13}		Zhang et al. (2010)	Q	288, 289
$C_{19}H_{10}Br_4O_5S$	5.1×10^{5}		Zhang et al. (2010)	Q	288, 290
[115-39-9]	9.2×10^{9}		Zhang et al. (2010)	Q	288, 291
UDSAIICHUKSCKT-UHFFFAOYSA-N	5.3×10^{10}		Zhang et al. (2010)	Q	288, 292
bromcresol green	1.5×10^{13}		Zhang et al. (2010)	Q	288, 289
$C_{21}H_{14}Br_4O_5S$	1.0×10^{6}		Zhang et al. (2010)	Q	288, 290
[76-60-8]	1.8×10^{9}		Zhang et al. (2010)	Q	288, 291
FRPHFZCDPYBUAU-UHFFFAOYSA-N	1.6×10^{10}		Zhang et al. (2010)	Q	288, 292
bromocresol purple $C_{21}H_{16}Br_2O_5S$ [115-40-2] ABIUHPWEYMSGSR-UHFFFAOYSA-N	9.9×10^{12}		HSDB (2015)	Q	100

Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
difethialone $C_{31}H_{23}BrO_2S$ [104653-34-1] VSVAQRUUFVBBFS-UHFFFAOYSA-N	9.9 9.9 5.4×10^{6}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187
amisulbrom $C_{13}H_{13}BrFN_5O_4S_2$ [348635-87-0] BREATYVWRHIPIY-UHFFFAOYSA-N	4.7×10^{1} 3.6×10^{4}		MacBean (2012b) Maniere et al. (2011)	X ?	352 242, 166
thifluzamide $C_{13}H_6Br_2F_6N_2O_2S$ [130000-40-7] WOSNCVAPUOFXEH-UHFFFAOYSA-N	1.2×10^{6}		Ebert et al. (2023)	?	319
amical 48 $C_8H_8I_2O_2S$ (diiodomethyl *p*-tolyl sulfone) [20018-09-1] XOILGBPDXMVFIP-UHFFFAOYSA-N	1.3×10^{3}		HSDB (2015)	Q	100
flubendiamide $C_{23}H_{22}F_7IN_2O_4S$ [272451-65-7] ZGNITFSDLCMLGI-UHFFFAOYSA-N	4.5×10^{-2}		HSDB (2015)	V	

A10 Organic species with phosphorus (P)

A10.1 Phosphorus (C, H, O, N, Cl, Br, S, P)

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
9-icosyl-9-phosphabicyclo[4.2.1]nonane	3.1×10^{-5}		Zhang et al. (2010)	Q	288, 289
$C_{28}H_{55}P$	3.1×10^{-3}		Zhang et al. (2010)	Q	288, 290
[13886-99-2]	2.2×10^{-2}		Zhang et al. (2010)	Q	288, 291
UNOOEFGBOLKBFW-UHFFFAOYSA-N	8.0×10^{-6}		Zhang et al. (2010)	Q	288, 292
triphenylphosphine	4.3×10^{2}		Zhang et al. (2010)	Q	288, 289
$C_{18}H_{15}P$	9.5×10^{-3}		Zhang et al. (2010)	Q	288, 290
[603-35-0]	1.3×10^{1}		Zhang et al. (2010)	Q	288, 291
RIOQSEWOXXDEQQ-UHFFFAOYSA-N	4.8		Zhang et al. (2010)	Q	288, 292
phosphoric acid, trimethyl ester	1.4×10^{3}		Wolfenden and Williams (1983)	M	12
$C_3H_9O_4P$	6.3×10^{1}		Yaws (2003)	X	238
(trimethyl phosphate)	6.1×10^{1}		Gharagheizi et al. (2010)	Q	247
[512-56-1]	1.4×10^{3}		Bartelt-Hunt et al. (2008)	?	21
WVLBCYQITXONBZ-UHFFFAOYSA-N	5.2×10^{1}		Yaws (1999)	?	21
trimethyl phosphite	9.0×10^{-1}		HSDB (2015)	Q	100
$C_3H_9O_3P$					
[121-45-9]					
CYTQBVOFDCPGCX-UHFFFAOYSA-N					
dimethyl methylphosphonate	7.6		HSDB (2015)	Q	100
$C_3H_9O_3P$	7.6		Bartelt-Hunt et al. (2008)	?	21
[756-79-6]					
VONWDASPFIQPDY-UHFFFAOYSA-N					
diethyl hydrogen phosphite	1.7		HSDB (2015)	Q	100
$C_4H_{11}O_3P$	5.5×10^{-3}		Bartelt-Hunt et al. (2008)	?	21
[762-04-9]					
MJUJXFBTEFXVKU-UHFFFAOYSA-N					
triethylphosphate	2.7×10^{2}		Wolfenden and Williams (1983)	M	12
$C_6H_{15}O_4P$	1.4×10^{2}		Abraham et al. (1994a)	R	
[78-40-0]	6.7×10^{1}		Yaws (2003)	X	259
DQWPFSLDHJDLRL-UHFFFAOYSA-N	6.6×10^{1}		Yaws (2003)	X	238
	5.2×10^{1}		Dupeux et al. (2022)	Q	260
	6.7×10^{1}		Gharagheizi et al. (2010)	Q	247
	6.6		Bartelt-Hunt et al. (2008)	?	21
	9.6×10^{1}		Yaws (1999)	?	21
diethyl ethyl phosphonate	3.4		Bartelt-Hunt et al. (2008)	?	21
$C_6H_{15}O_3P$					
[78-38-6]					
AATNZNJRDOVKDD-UHFFFAOYSA-N					

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
mevinphos			Mackay et al. (2006d)	V	560
$C_7H_{13}O_6P$	2.4×10^5		Sanders and Seiber (1983)	V	88
[7786-34-7]	2.5×10^3		HSDB (2015)	Q	100
GEPDYQSQVLXLEU-AATRIKPKSA-N					
diisopropyl methanephosphonate	2.2×10^{-1}		HSDB (2015)	V	
$C_7H_{17}O_3P$	2.2×10^{-1}		Bartelt-Hunt et al. (2008)	?	21
[1445-75-6]					
WOAFDHWYKSOANX-UHFFFAOYSA-N					
dibutyl hydrogen phosphite	5.5×10^{-1}		HSDB (2015)	Q	100
$C_8H_{19}O_3P$					
[1809-19-4]					
NFJPGAKRJKLOJK-UHFFFAOYSA-N					
dibutyl phosphate	2.3×10^3		HSDB (2015)	Q	100
$C_8H_{19}O_4P$					
[107-66-4]					
JYFHYPJRHGVZDY-UHFFFAOYSA-N					
tetraethyl pyrophosphate	4.5×10^4		HSDB (2015)	V	
$C_8H_{20}O_7P_2$					
[107-49-3]					
IDCBOTIENDVCBQ-UHFFFAOYSA-N					
tripropyl phosphate	1.5×10^1		Wolfenden and Williams (1983)	M	12
$C_9H_{21}O_4P$					
[513-08-6]					
RXPQRKFMDQNODS-UHFFFAOYSA-N					
triallyl phosphate	1.8×10^1		HSDB (2015)	Q	100
$C_9H_{15}O_4P$					
[1623-19-4]					
XHGIFBQQEGRTPB-UHFFFAOYSA-N					
tributylphosphate	7.0		HSDB (2015)	V	
$C_{12}H_{27}O_4P$	1.6×10^1		Glotfelty et al. (1987)	V	
[126-73-8]	4.8		Yoshida et al. (1983)	V	
STCOOQWBFONSKY-UHFFFAOYSA-N					
hexaethyl tetraphosphate	3.0×10^{11}		HSDB (2015)	Q	100
$C_{12}H_{30}O_{13}P_4$					
[757-58-4]					
DAJYZXUXDOSMCG-UHFFFAOYSA-N					
crotoxyphos	1.7×10^3		HSDB (2015)	V	
$C_{14}H_{19}O_6P$	1.7×10^3		Mackay et al. (2006d)	V	
[7700-17-6]	1.7×10^3		MacBean (2012a)	?	
XXXSILNSXNPGKG-ZHACJKMWSA-N					

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
phosphoric acid, dibutyl phenyl ester $C_{14}H_{23}O_4P$ [2528-36-1] YICSVBJRVMLQNS-UHFFFAOYSA-N	2.0×10^{1}		HSDB (2015)	Q	100
bis(2-ethylhexyl) hydrogen phosphite $C_{16}H_{35}O_3P$ [3658-48-8] HZIUHEQKVCPTAJ-UHFFFAOYSA-N	5.8×10^{-2} 6.6×10^{-4}		HSDB (2015) Bartelt-Hunt et al. (2008)	Q ?	100 21
bis(2-ethylhexyl)hydrogen phosphate $C_{16}H_{35}O_4P$ (bis(2-ethylhexyl) phosphate) [298-07-7] SEGLCEQVOFDUPX-UHFFFAOYSA-N	2.4×10^{2}		HSDB (2015)	Q	100
triphenyl phosphate $C_{18}H_{15}O_4P$ [115-86-6] XZZNDPSIHUTMOC-UHFFFAOYSA-N	3.0		HSDB (2015)	V	
tris(2-butoxyethyl) phosphate $C_{18}H_{39}O_7P$ [78-51-3] WTLBZVNBAKMVDP-UHFFFAOYSA-N	8.2×10^{5}		HSDB (2015)	Q	100
p-cresyl diphenyl phosphate $C_{19}H_{17}O_4P$ [78-31-9] OJUZRFGUKHQNJX-UHFFFAOYSA-N	9.9×10^{1}		HSDB (2015)	Q	449
triphenylphosphine oxide $C_{18}H_{15}OP$ [791-28-6] FIQMHBFVRAXMOP-UHFFFAOYSA-N	1.9×10^{4} 4.6×10^{4} 1.1×10^{7} 2.5×10^{-1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
phosphorous acid, triphenyl ester $C_{18}H_{15}O_3P$ [101-02-0] HVLLSGMXQDNUAL-UHFFFAOYSA-N	1.8×10^{1} 4.4×10^{-2} 1.5×10^{2} 7.0×10^{4}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
trihexylphosphine oxide $C_{18}H_{39}OP$ [3084-48-8] PPDZLUVUQQGIOJ-UHFFFAOYSA-N	4.5×10^{-3} 2.9×10^{-3} 5.8×10^{4} 3.5×10^{-7}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
phosphoric acid, octyl diphenyl ester $C_{20}H_{27}O_4P$ [115-88-8] YAFOVCNAQTZDQB-UHFFFAOYSA-N	3.9×10^{1}		HSDB (2015)	Q	100
octyldihexylphosphine oxide $C_{20}H_{43}OP$ [31160-64-2] XHRRUIJGMKIISX-UHFFFAOYSA-N	2.5×10^{-3} 3.1×10^{-3} 5.3×10^{4} 2.3×10^{-7}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	288, 289 288, 290 288, 291 288, 292
octicizer $C_{20}H_{27}O_4P$ [1241-94-7] CGSLYBDCEGBZCG-UHFFFAOYSA-N	1.0×10^{-1} 2.7 1.8×10^{-1}		Keshavarz et al. (2022) Duchowicz et al. (2020) Duchowicz et al. (2020)	Q Q ?	 186, 21
tris(methylphenyl) phosphate $C_{21}H_{21}O_4P$ (tricresyl phosphate) [1330-78-5] IUJIYUAKFBGBCG-UHFFFAOYSA-N	1.2×10^{1}		HSDB (2015)	V	
phosphoric acid, (1-methylethyl)phenyl diphenyl ester $C_{21}H_{21}O_4P$ [28108-99-8] JJXNVYMIYBNZQX-UHFFFAOYSA-N	1.3×10^{2}		HSDB (2015)	Q	100
phosphoric acid, tris(2-methylphenyl) ester $C_{21}H_{21}O_4P$ (tri-*o*-cresyl phosphate) [78-30-8] YSMRWXYRXBRSND-UHFFFAOYSA-N	5.2		HSDB (2015)	Q	449
phosphoric acid, tris(3-methylphenyl) ester $C_{21}H_{21}O_4P$ (tri-*m*-cresyl phosphate) [563-04-2] RMLPZKRPSQVRAB-UHFFFAOYSA-N	1.4×10^{-1} 5.1 9.9 1.2×10^{-1}		Keshavarz et al. (2022) Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	Q Q Q ?	 449 186, 21
phosphoric acid, tris(4-methylphenyl) ester $C_{21}H_{21}O_4P$ (tri-*p*-cresyl phosphate) [78-32-0] BOSMZFBHAYFUBJ-UHFFFAOYSA-N	1.8×10^{2}		HSDB (2015)	Q	449

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(3-*tert*-butylphenyl) diphenyl phosphate $C_{22}H_{23}O_4P$ NIAVXHWAURFNOW-UHFFFAOYSA-N	1.1×10^{1}		Ebert et al. (2023)	?	367
(4-*tert*-butylphenyl) diphenyl phosphate	4.5×10^{1}		HSDB (2015)	V	
$C_{22}H_{23}O_4P$	1.8×10^{2}		Keshavarz et al. (2022)	Q	
[981-40-8]	3.6		Duchowicz et al. (2020)	Q	
ULGAVXUJJBOWOD-UHFFFAOYSA-N	1.1×10^{1}		Duchowicz et al. (2020)	?	186, 21
isodecyl diphenyl phosphate $C_{22}H_{31}O_4P$ [29761-21-5] RYUJRXVZSJCHDZ-UHFFFAOYSA-N	2.3×10^{1}		HSDB (2015)	Q	100
dioctylhexylphosphine oxide	1.4×10^{-3}		Zhang et al. (2010)	Q	288, 289
$C_{22}H_{47}OP$	3.4×10^{-3}		Zhang et al. (2010)	Q	288, 290
[31160-66-4]	4.0×10^{4}		Zhang et al. (2010)	Q	288, 291
MKEFGIKZZDCMQC-UHFFFAOYSA-N	1.4×10^{-7}		Zhang et al. (2010)	Q	288, 292
tris(2,4-dimethylphenyl)phosphate $C_{24}H_{27}O_4P$ [3862-12-2] KOWVWXQNQNCRRS-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	100
tris(2,5-dimethylphenyl)phosphate $C_{24}H_{27}O_4P$ [19074-59-0] MDHAARLWBHZGIP-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	100
tris(2,6-dimethylphenyl)phosphate $C_{24}H_{27}O_4P$ [121-06-2] QLORRTLBSJTMSN-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	100
tris(3,4-dimethylphenyl)phosphate $C_{24}H_{27}O_4P$ [3862-11-1] BCTKCHOESSAGCN-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	100
tris(3,5-dimethylphenyl)phosphate $C_{24}H_{27}O_4P$ [25653-16-1] LLPMAOBOEQFPRE-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	100
tris(4-isopropylphenyl) phosphate $C_{27}H_{33}O_4P$ [26967-76-0] ANVREEJNGJMLOV-UHFFFAOYSA-N	3.4×10^{1}		HSDB (2015)	Q	100

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
trioctylphosphine oxide	8.2×10^{-4}		Zhang et al. (2010)	Q	288, 289
$C_{24}H_{51}OP$	3.7×10^{-3}		Zhang et al. (2010)	Q	288, 290
[78-50-2]	3.4×10^{4}		Zhang et al. (2010)	Q	288, 291
ZMBHCYHQLYEYDV-UHFFFAOYSA-N	9.2×10^{-8}		Zhang et al. (2010)	Q	288, 292
bis(2-ethylhexyl)-2-ethylhexyl phosphonate	2.1×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{24}H_{51}O_3P$	6.2×10^{-6}		Zhang et al. (2010)	Q	288, 290
[126-63-6]	5.4×10^{4}		Zhang et al. (2010)	Q	288, 291
GOCVCBDBQYEFQD-UHFFFAOYSA-N	7.7×10^{-5}		Zhang et al. (2010)	Q	288, 292
	1.3×10^{-3}		Bartelt-Hunt et al. (2008)	?	21
didodecyl hydrogen phosphate $C_{24}H_{51}O_4P$ [7057-92-3] JTXUVYOABGUBMX-UHFFFAOYSA-N	2.5×10^{1}		HSDB (2015)	Q	100
phosphoric acid, tris(2-ethylhexyl) ester $C_{24}H_{51}O_4P$ (trioctyl phosphate) [78-42-2] GTVWRXDRKAHEAD-UHFFFAOYSA-N	1.2×10^{2}		HSDB (2015)	V	
diisodecylphenyl phosphite	1.9		Zhang et al. (2010)	Q	288, 289
$C_{26}H_{47}O_3P$	2.5		Zhang et al. (2010)	Q	288, 290
[25550-98-5]	1.6×10^{3}		Zhang et al. (2010)	Q	288, 291
SXXILWLQSQDLDL-UHFFFAOYSA-N	3.9×10^{-3}		Zhang et al. (2010)	Q	288, 292
4-nonylphenyl diphenyl phosphate	8.1×10^{2}		Keshavarz et al. (2022)	Q	
$C_{27}H_{33}O_4P$	2.5×10^{1}		Duchowicz et al. (2020)	Q	185
[64532-97-4]	7.0×10^{2}		Duchowicz et al. (2020)	?	186, 21
LMCLPMXCYFSRNG-UHFFFAOYSA-N					
resorcinol bis(diphenyl phosphate)	3.4×10^{7}		Zhang et al. (2010)	Q	288, 289
$C_{30}H_{24}O_8P_2$	1.4×10^{-2}		Zhang et al. (2010)	Q	288, 290
[57583-54-7]	2.6×10^{8}		Zhang et al. (2010)	Q	288, 291
OWICEWMBIBPFAH-UHFFFAOYSA-N	3.9×10^{16}		Zhang et al. (2010)	Q	288, 292
hydroquinone bis(diphenyl phosphate) $C_{30}H_{24}O_8P_2$ [51732-57-1] RECLNCPBBUHRDY-UHFFFAOYSA-N	3.4×10^{12}		Abraham et al. (2019)	Q	
tris(4-*tert*-butylphenyl) phosphate	1.4×10^{1}		Zhang et al. (2010)	Q	288, 289
$C_{30}H_{39}O_4P$	8.4×10^{-4}		Zhang et al. (2010)	Q	288, 290
[78-33-1]	1.6×10^{3}		Zhang et al. (2010)	Q	288, 291
LORSVOJSXMHDHF-UHFFFAOYSA-N	3.5×10^{1}		Zhang et al. (2010)	Q	288, 292

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tris-(2,4-di-*tert*-butylphenyl) phosphite	6.1×10^{-2}		Zhang et al. (2010)	Q	288, 289
$C_{42}H_{63}O_3P$	6.5×10^{-5}		Zhang et al. (2010)	Q	288, 290
[31570-04-4]	1.5×10^{2}		Zhang et al. (2010)	Q	288, 291
JKIJEFPNVSHHEI-UHFFFAOYSA-N	5.8		Zhang et al. (2010)	Q	288, 292
glyphosate	1.8×10^{6}		Mackay et al. (2006d)	V	
$C_3H_8NO_5P$	4.8×10^{6}		Maniere et al. (2011)	?	166
[1071-83-6]					
XDDAORKBJWWYJS-UHFFFAOYSA-N					
krenite	2.0×10^{7}		HSDB (2015)	V	
$C_3H_{11}N_2O_4P$					
(fosamine-ammonium)					
[25954-13-6]					
OTSAMNSACVKIOJ-UHFFFAOYSA-N					
tabun	6.6×10^{1}		HSDB (2015)	V	
$C_5H_{11}N_2O_2P$	6.2×10^{2}		Bartelt-Hunt et al. (2008)	?	21
[77-81-6]	6.5×10^{1}		Opresko et al. (1998)	?	
PJVJTCIRVMBVIA-UHFFFAOYSA-N					
glufosinate-ammonium	2.2×10^{8}		MacBean (2012b)	X	352
$C_5H_{15}N_2O_4P$					
[77182-82-2]					
ZBMRKNMTMPPMMK-UHFFFAOYSA-N					
hexamethylphosphoramide	4.9×10^{2}		Duchowicz et al. (2020)	V	187
$C_6H_{18}N_3OP$	5.3×10^{-4}		Duchowicz et al. (2020)	Q	
[680-31-9]					
GNOIPBMMFNIUFM-UHFFFAOYSA-N					
monocrotophos	1.5×10^{7}		HSDB (2015)	V	
$C_7H_{14}NO_5P$			Mackay et al. (2006d)	V	560
[6923-22-4]					
KRTSDMXIXPKRQR-AATRIKPKSA-N					
dicrotophos	2.0×10^{5}		Mackay et al. (2006d)	V	
$C_8H_{16}NO_5P$	7.8×10^{4}		Keshavarz et al. (2022)	Q	
[141-66-2]	1.0×10^{3}		Duchowicz et al. (2020)	Q	
VEENJGZXVHKXNB-VOTSOKGWSA-N	2.0×10^{5}		Duchowicz et al. (2020)	?	186, 21
octamethyldiphosphoramide	1.6×10^{11}		HSDB (2015)	Q	100
$C_8H_{24}N_4O_3P_2$					
(schradan)					
[152-16-9]					
SZKKRCSOSQAJDE-UHFFFAOYSA-N					

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
fyrol 6 $C_9H_{22}NO_5P$ (diethyl ((diethanolamino)methyl) phosphonate) [2781-11-5] CCJKFLLIJCGHMO-UHFFFAOYSA-N	6.2×10^{1}		HSDB (2015)	V	
diethyl 4-nitrophenyl phosphate $C_{10}H_{14}NO_6P$ (paraoxon) [311-45-5] WYMSBXTXOHUIGT-UHFFFAOYSA-N	9.1×10^{4} 1.6×10^{3} 9.0×10^{1} 1.5×10^{4} 2.7×10^{-1}		Duchowicz et al. (2020) Glotfelty et al. (1987) Duchowicz et al. (2020) HSDB (2015) Bartelt-Hunt et al. (2008)	V V Q Q ?	187 100 21
dimethyl 4-nitrophenyl phosphate $C_8H_{10}NO_6P$ (methyl paraoxon) [950-35-6] BAFQDKPJKOLXFZ-UHFFFAOYSA-N	$>1.1\times10^{4}$		Woodrow et al. (1990)	V	
buminafos $C_{18}H_{38}NO_3P$ [51249-05-9] NMBXMBCZBXUXAM-UHFFFAOYSA-N	5.0		MacBean (2012a)	?	12
methylphosphonyldifluoride CH_3F_2OP [676-99-3] PQIOSYKVBBWRRI-UHFFFAOYSA-N	4.5×10^{-1}		HSDB (2015)	Q	100
sarin $C_4H_{10}FO_2P$ [107-44-8] DYAHQFWOVKZOOW-UHFFFAOYSA-N	1.7×10^{1} 1.1 1.8×10^{1}		HSDB (2015) Bartelt-Hunt et al. (2008) Opresko et al. (1998)	V ? ?	 21
dimefox $C_4H_{12}FN_2OP$ [115-26-4] PGJBQBDNXAZHBP-UHFFFAOYSA-N	4.5×10^{2}		HSDB (2015)	V	
isoflurophate $C_6H_{14}FO_3P$ (diisopropyl fluorophosphate) [55-91-4] MUCZHBLJLSDCSD-UHFFFAOYSA-N	3.1 7.6×10^{-5}		HSDB (2015) Bartelt-Hunt et al. (2008)	Q ?	100 21

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyclohexyl methylphosphonofluoridate $C_7H_{14}FO_2P$ (cyclosarin) [329-99-7] SNTRKUOVAPUGAY-UHFFFAOYSA-N	3.5		Duchowicz et al. (2020)	V	187
	3.5		HSDB (2015)	V	
	4.3×10^{3}		Duchowicz et al. (2020)	Q	
soman $C_7H_{16}FO_2P$ [96-64-0] GRXKLBBBQUKJJZ-UHFFFAOYSA-N	2.1		HSDB (2015)	V	
	2.1		Bartelt-Hunt et al. (2008)	?	21
	2.2		Opresko et al. (1998)	?	
mipafox $C_6H_{16}FN_2OP$ [371-86-8] UOSHUBFBCPGQAY-UHFFFAOYSA-N	3.3×10^{3}		HSDB (2015)	V	
phenylphosphonous dichloride $C_6H_5Cl_2P$ [644-97-3] IMDXZWRLUZPMDH-UHFFFAOYSA-N	6.5×10^{-1}		Zhang et al. (2010)	Q	288, 289
	2.5×10^{-3}		Zhang et al. (2010)	Q	288, 290
	6.2×10^{-2}		Zhang et al. (2010)	Q	288, 291
	3.3×10^{-2}		Zhang et al. (2010)	Q	288, 292
chlorphonium chloride $C_{19}H_{32}Cl_3P$ [115-78-6] IVHVNMLJNASKHW-UHFFFAOYSA-M	2.8×10^{7}		MacBean (2012a)	?	12
triclofos $C_2H_4Cl_3O_4P$ [306-52-5] YYQRGCZGSFRBAM-UHFFFAOYSA-N	7.0×10^{7}		HSDB (2015)	Q	100
(2-chloroethyl)-phosphonic acid $C_2H_6ClO_3P$ (ethephon) [16672-87-0] UDPGUMQDCGORJQ-UHFFFAOYSA-N	6.9×10^{7}		HSDB (2015)	V	
	$>6.9\times10^{6}$		Maniere et al. (2011)	?	242, 166
1-hydroxy-2,2,2- trichloroethylphosphonic acid, dimethyl ester $C_4H_8Cl_3O_4P$ (trichlorfon) [52-68-6] NFACJZMKEDPNKN-UHFFFAOYSA-N	5.5×10^{1}		Chao et al. (2017)	M	
	$>8.1\times10^{2}$		Kawamoto and Urano (1989)	M	
	5.8×10^{5}		HSDB (2015)	V	
	6.0×10^{5}		Mackay et al. (2006d)	V	
	5.9×10^{5}		Suntio et al. (1988)	V	12
	5.8×10^{3}		Barcelo and Hennion (1997)	X	569
	3.8×10^{1}		Goodarzi et al. (2010)	Q	570

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dimethyl-2,2-dichlorovinyl phosphate	3.9×10^{1}	11000	Gautier et al. (2003)	M	
$C_4H_7Cl_2O_4P$	8.1×10^{-2}		Kawamoto and Urano (1989)	M	
(dichlorvos)	1.7×10^{1}		HSDB (2015)	V	
[62-73-7]	5.2		Mackay et al. (2006d)	V	
OEBRKCOSUFCWJD-UHFFFAOYSA-N	5.3		Suntio et al. (1988)	V	12
	5.2×10^{-2}		Barcelo and Hennion (1997)	X	569
	9.7×10^{-1}		Goodarzi et al. (2010)	Q	570, 573
tris(2-chloroethyl) phosphate $C_6H_{12}Cl_3O_4P$ [115-96-8] HQUQLFOMPYWACS-UHFFFAOYSA-N	3.0		HSDB (2015)	V	
cyclophosphamide $C_7H_{15}Cl_2N_2O_2P$ [50-18-0] CMSMOCZEIVJLDB-UHFFFAOYSA-N	7.0×10^{5}		HSDB (2015)	Q	100
ifosfamide $C_7H_{15}Cl_2N_2O_2P$ [3778-73-2] HOMGKSMUEGBAAB-UHFFFAOYSA-N	7.0×10^{5}		HSDB (2015)	Q	100
butonate $C_8H_{14}Cl_3O_5P$ [126-22-7] BKAQXYNWONVOAX-UHFFFAOYSA-N	3.3×10^{4}		HSDB (2015)	Q	100
phosphoric acid, 7-chlorobicyclo[3.2.0]hepta-2,6-dien-6-yl dimethyl ester	5.8×10^{1}		HSDB (2015)	V	
$C_9H_{12}ClO_4P$	4.3×10^{3}		MacBean (2012a)	?	
(heptenophos) [23560-59-0] GBAWQJNHVWMTLU-UHFFFAOYSA-N					
tris(2,3-dichloropropyl) phosphate $C_9H_{15}Cl_6O_4P$ [78-43-3] JZZBTMVTLBHJHL-UHFFFAOYSA-N	3.8×10^{3}		HSDB (2015)	Q	100
tris(1,3-dichloroisopropyl)phosphate	3.8×10^{3}		HSDB (2015)	Q	100
$C_9H_{15}Cl_6O_4P$	3.8×10^{3}		Zhang et al. (2010)	Q	288, 289
[13674-87-8]	4.1×10^{-2}		Zhang et al. (2010)	Q	288, 290
ASLWPAWFJZFCKF-UHFFFAOYSA-N	1.3×10^{7}		Zhang et al. (2010)	Q	288, 291
	3.0		Zhang et al. (2010)	Q	288, 292

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tris(2-chloropropyl) phosphate	1.6×10^{2}		Zhang et al. (2010)	Q	288, 289
$C_9H_{18}Cl_3O_4P$	1.4×10^{-3}		Zhang et al. (2010)	Q	288, 290
[6145-73-9]	6.7×10^{2}		Zhang et al. (2010)	Q	288, 291
GTRSAMFYSUBAGN-UHFFFAOYSA-N	3.8×10^{-1}		Zhang et al. (2010)	Q	288, 292
tri-(2-chloroisopropyl)phosphate	1.6×10^{2}		HSDB (2015)	Q	100
$C_9H_{18}Cl_3O_4P$	1.6×10^{2}		Zhang et al. (2010)	Q	288, 289
[13674-84-5]	1.9×10^{-4}		Zhang et al. (2010)	Q	288, 290
KVMPUXDNESXNOH-UHFFFAOYSA-N	3.6×10^{4}		Zhang et al. (2010)	Q	288, 291
	3.8×10^{-1}		Zhang et al. (2010)	Q	288, 292
bis(2-chloropropyl) 2-chloro-1-methylethyl phosphate	1.6×10^{2}		Zhang et al. (2010)	Q	288, 289
$C_9H_{18}Cl_3O_4P$	7.2×10^{-4}		Zhang et al. (2010)	Q	288, 290
[76649-15-5]	5.6×10^{3}		Zhang et al. (2010)	Q	288, 291
WDLBXPUJJVVRGX-UHFFFAOYSA-N	3.8×10^{-1}		Zhang et al. (2010)	Q	288, 292
tetrachlorvinphos	5.5×10^{3}		HSDB (2015)	V	
$C_{10}H_9Cl_4O_4P$	2.4×10^{3}		Ebert et al. (2023)	?	317
[22248-79-9]	5.4×10^{3}		MacBean (2012a)	?	
UBCKGWBNUIFUST-YHYXMXQVSA-N					
dimethylvinphos	3.0×10^{2}		Ebert et al. (2023)	?	319
$C_{10}H_{10}Cl_3O_4P$					
[2274-67-1]					
QSGNQELHULIMSJ-UHFFFAOYSA-N					
diphenyl chlorophosphate	3.7×10^{-2}		Bartelt-Hunt et al. (2008)	?	21
$C_{12}H_{10}ClO_3P$					
[2524-64-3]					
BHIIGRBMZRSDRI-UHFFFAOYSA-N					
chlorfenvinphos	3.4×10^{2}		HSDB (2015)	V	
$C_{12}H_{14}Cl_3O_4P$	3.4×10^{3}		Mackay et al. (2006d)	V	
(clofenvinfos)	3.6×10^{3}		Suntio et al. (1988)	V	12
[470-90-6]	3.5×10^{1}		Barcelo and Hennion (1997)	X	569
FSAVDKDHPDSCTO-XYOKQWHBSA-N	4.1		Goodarzi et al. (2010)	Q	570
crufomate	3.9×10^{3}		HSDB (2015)	Q	100
$C_{12}H_{19}ClNO_3P$					
(ruelene)					
[299-86-5]					
BOFHKBLZOYVHSI-UHFFFAOYSA-N					
phosdiphen	2.6×10^{-2}		MacBean (2012a)	?	
$C_{14}H_{11}O_4Cl_4P$					
[36519-00-3]					
HEMINMLPKZELPP-UHFFFAOYSA-N					

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
phosphamidon	2.8		Mackay et al. (2006d)	V	
$C_{10}H_{19}ClNO_5P$	2.8		Suntio et al. (1988)	V	12
[13171-21-6]	6.6×10^{6}		HSDB (2015)	Q	100
RGCLLPNLLBQHPF-HJWRWDBZSA-N					
tris(2,3-dibromo-1-propyl) phosphate	3.8×10^{-1}		HSDB (2015)	V	
$C_9H_{15}Br_6O_4P$					
[126-72-7]					
PQYJRMFWJJONBO-UHFFFAOYSA-N					
naled	1.5×10^{-1}		HSDB (2015)	V	
$C_4H_7Br_2Cl_2O_4P$					
[300-76-5]					
BUYMVQAILCEWRR-UHFFFAOYSA-N					
2-bromo-1,1-dimethylethyl 2-bromoethyl 2-chloroethyl phosphate	1.5×10^{3}		Zhang et al. (2010)	Q	288, 289
$C_9H_{18}Br_2ClO_4P$	1.3×10^{-2}		Zhang et al. (2010)	Q	288, 290
[125997-20-8]	4.4×10^{3}		Zhang et al. (2010)	Q	288, 291
GZSKSYDWLZIPOX-UHFFFAOYSA-N	8.2×10^{-1}		Zhang et al. (2010)	Q	288, 292
leptophos	3.7		Mackay and Shiu (1981)	L	
$C_{13}H_{10}O_3BrCl_2P$	3.7		HSDB (2015)	V	
[21609-90-5]	4.0		Mackay et al. (2006d)	V	
CVRALZAYCYJELZ-UHFFFAOYSA-N	4.0		Suntio et al. (1988)	V	12
	2.6×10^{1}		Hilal et al. (2008)	Q	
tributyl phosphorotrithioite	4.3×10^{-1}		HSDB (2015)	Q	100
$C_{12}H_{27}PS_3$	4.3×10^{-1}		Zhang et al. (2010)	Q	288, 289
[150-50-5]	6.0×10^{-4}		Zhang et al. (2010)	Q	288, 290
KLAPGAOQRZTCBI-UHFFFAOYSA-N	1.5×10^{-1}		Zhang et al. (2010)	Q	288, 291
	5.1×10^{-2}		Zhang et al. (2010)	Q	288, 292
bis(2,6,6-trimethylbicyclo[3.1.1]hept-2-enyl) bis(2,6,6-trimethylbicyclo[3.1.1]hept-2-enyl)thiodiphosphonate	8.2×10^{-5}		Zhang et al. (2010)	Q	288, 289
$C_{40}H_{60}P_2S_5$	5.8×10^{4}		Zhang et al. (2010)	Q	288, 290
[68400-79-3]	1.9×10^{5}		Zhang et al. (2010)	Q	288, 291
ZZMOHCWFHCHISQ-UHFFFAOYSA-N	1.6×10^{2}		Zhang et al. (2010)	Q	288, 292
thiometon	3.5×10^{-1}		HSDB (2015)	V	
$C_6H_{15}O_2PS_3$					
[640-15-3]					
OPASCBHCTNRLRM-UHFFFAOYSA-N					

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
demeton-S-methyl sulfone $C_6H_{15}O_5PS_2$ [17040-19-6] PZIRJMYRYORVIT-UHFFFAOYSA-N	$<2.3\times10^{10}$		MacBean (2012a)	?	
oxydemeton-methyl $C_6H_{15}O_4PS_2$ [301-12-2] PMCVMORKVPSKHZ-UHFFFAOYSA-N	6.2×10^{7}		HSDB (2015)	Q	100
demeton-O-methyl $C_6H_{15}O_3PS_2$ [867-27-6] ZVZQKNVMDKSGGF-UHFFFAOYSA-N	3.2		Ebert et al. (2023)	?	317
demeton-S-methyl $C_6H_{15}O_3PS_2$ [919-86-8] WEBQKRLKWNIYKK-UHFFFAOYSA-N	3.7×10^{2} 3.6×10^{2}		HSDB (2015) Mackay et al. (2006d)	V V	
methacrifos $C_7H_{13}O_5PS$ [62610-77-9] NTAHCMPOMKHKEU-AATRIKPKSA-N	1.0×10^{1}		MacBean (2012a)	?	
phorate $C_7H_{17}O_2PS_3$ [298-02-2] BULVZWIRKLYCBC-UHFFFAOYSA-N	2.1 9.9×10^{-1} 1.5 1.5×10^{-2} 4.5×10^{-2}		HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V V X Q	 12 569 570
salithion $C_8H_9O_3PS$ [3811-49-2] OUNSASXJZHBGAI-UHFFFAOYSA-N	4.7×10^{-1}		MacBean (2012a)	?	
acetoxon $C_8H_{17}O_5PS$ [2425-25-4] ZRCQYAQOWIQUBA-UHFFFAOYSA-N	1.3×10^{4}		HSDB (2015)	Q	100
demeton-O $C_8H_{19}O_3PS_2$ [298-03-3] DGLIBALSRMUQDD-UHFFFAOYSA-N	6.1		MacBean (2012a)	?	12
demeton-S $C_8H_{19}O_3PS_2$ (isosystox) [126-75-0] GRPRVIYRYGLIJU-UHFFFAOYSA-N	2.0×10^{2}		HSDB (2015)	V	

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
sulfotep	2.2		HSDB (2015)	V	
$C_8H_{20}O_5P_2S_2$	3.4		Mackay et al. (2006d)	V	
[3689-24-5]	9.9×10^{-3}		Barcelo and Hennion (1997)	X	569
XIUROWKZWPIAIB-UHFFFAOYSA-N	4.4×10^{-3}		Goodarzi et al. (2010)	Q	570, 573
tetrakis(hydroxymethyl) phosphonium sulfate	5.8×10^{17}		HSDB (2015)	Q	100
$C_8H_{24}O_{12}P_2S$					
[55566-30-8]					
YIEDHPBKGZGLIK-UHFFFAOYSA-L					
ethoprophos	6.1×10^{1}		HSDB (2015)	V	
$C_8H_{19}O_2PS_2$	6.1×10^{1}		Mackay et al. (2006d)	V	
[13194-48-4]					
VJYFKVYYMZPMAB-UHFFFAOYSA-N					
disulfoton	1.1×10^{1}		Muir et al. (2004)	L	369
$C_8H_{19}O_2PS_3$	4.5		HSDB (2015)	V	
[298-04-4]	4.5		Mackay et al. (2006d)	V	
DOFZAZXDOSGAJZ-UHFFFAOYSA-N	4.5		Suntio et al. (1988)	V	12
	4.5×10^{-2}		Barcelo and Hennion (1997)	X	569
	6.4×10^{-1}		Goodarzi et al. (2010)	Q	570, 573
endothion	1.5×10^{6}		HSDB (2015)	Q	100
$C_9H_{13}O_6PS$					
[2778-04-3]					
YCAGGFXSFQFVQL-UHFFFAOYSA-N					
terbufos	4.1×10^{-1}		HSDB (2015)	V	
$C_9H_{21}O_2PS_3$	4.1×10^{-1}		Mackay et al. (2006d)	V	
[13071-79-9]	9.9×10^{-3}		Barcelo and Hennion (1997)	X	569
XLNZEKHULJKQBA-UHFFFAOYSA-N	3.0×10^{-1}		Goodarzi et al. (2010)	Q	570
ethion	2.6×10^{1}		HSDB (2015)	V	
$C_9H_{22}O_4P_2S_4$	3.1×10^{1}		Mackay et al. (2006d)	V	
[563-12-2]	3.1×10^{1}		Suntio et al. (1988)	V	12
RIZMRRKBZQXFOY-UHFFFAOYSA-N	3.1×10^{-1}		Barcelo and Hennion (1997)	X	569
	6.8×10^{-1}		Goodarzi et al. (2010)	Q	570
fonofos	1.4		Duchowicz et al. (2020)	V	187
$C_{10}H_{15}OPS_2$	1.4		HSDB (2015)	V	
[944-22-9]	1.4		Mackay et al. (2006d)	V	
KVGLBTYUCJYMND-UHFFFAOYSA-N	1.9×10^{5}		Duchowicz et al. (2020)	Q	
fenthion	6.8		HSDB (2015)	V	
$C_{10}H_{15}O_3PS_2$	4.5×10^{1}		Mackay et al. (2006d)	V	
[55-38-9]	4.5×10^{1}		Suntio et al. (1988)	V	12
PNVJTZOFSHSLTO-UHFFFAOYSA-N	4.5×10^{-1}		Barcelo and Hennion (1997)	X	569
	1.9		Goodarzi et al. (2010)	Q	570

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
malathion $C_{10}H_{19}O_6PS_2$ [121-75-5] JXSJBGJIGXNWCI-UHFFFAOYSA-N	2.0×10^{1}	8300	Brockbank (2013)	L	
	1.5×10^{1}		Chao et al. (2017)	M	
	6.7×10^{2}		Watanabe (1993)	M	
	2.0×10^{3}		Fendinger and Glotfelty (1990)	M	
	4.4×10^{2}		Mackay et al. (2006d)	V	
	2.5×10^{2}		Cotham and Bidleman (1989)	V	
	4.3×10^{2}		Suntio et al. (1988)	V	12
	1.7×10^{2}		Glotfelty et al. (1987)	V	
	7.3×10^{3}		Sanders and Seiber (1983)	V	88
	2.6×10^{1}		Mackay and Shiu (1981)	V	
	4.3		Barcelo and Hennion (1997)	X	569
	1.8		Goodarzi et al. (2010)	Q	570
	1.5×10^{2}		Hilal et al. (2008)	Q	
	2.0×10^{3}		Bartelt-Hunt et al. (2008)	?	21
malaoxon $C_{10}H_{19}O_7PS$ [1634-78-2] WSORODGWGUUOBO-UHFFFAOYSA-N	5.5×10^{6}		HSDB (2015)	Q	100
cadusafos $C_{10}H_{23}O_2PS_2$ [95465-99-9] KXRPCFINVWWFHQ-UHFFFAOYSA-N	7.6		HSDB (2015)	V	
fensulfothion $C_{11}H_{17}O_4PS_2$ [115-90-2] XDNBJTQLKCIJBV-UHFFFAOYSA-N	7.0×10^{4}		HSDB (2015)	Q	100
phenthoate $C_{12}H_{17}O_4PS_2$ [2597-03-7] XAMUDJHXFNRLCY-UHFFFAOYSA-N	1.8×10^{3}		HSDB (2015)	V	
	9.8×10^{1}		Mackay et al. (2006d)	V	
sulprofos $C_{12}H_{19}O_2PS_3$ [35400-43-2] JXHJNEJVUNHLKO-UHFFFAOYSA-N	1.1×10^{1}		HSDB (2015)	V	
	1.1×10^{1}		MacBean (2012a)	?	12
S,S,S-tributyl phosphorotrithioate $C_{12}H_{27}OPS_3$ (DEF) [78-48-8] ZOKXUAHZSKEQSS-UHFFFAOYSA-N	3.4×10^{1}		Fendinger and Glotfelty (1990)	M	
	1.3		Glotfelty et al. (1987)	V	

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
aspon $C_{12}H_{28}O_5P_2S_2$ (tetrapropyl dithiopyrophosphate) [3244-90-4] IIDFEIDMIKSJSV-UHFFFAOYSA-N	6.1		Ebert et al. (2023)	?	319
iprobenphos $C_{13}H_{21}O_3PS$ [26087-47-8] FCOAHACKGGIURQ-UHFFFAOYSA-N	2.6×10^{2}		Watanabe (1993)	M	
propaphos $C_{13}H_{21}O_4PS$ [7292-16-2] PWYIUEFFPNVCMW-UHFFFAOYSA-N	3.4×10^{3} 3.4×10^{3} 3.6×10^{1} 3.4×10^{3}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) MacBean (2012a)	V V Q ?	187
edifenphos $C_{14}H_{15}O_2PS_2$ [17109-49-8] AWZOLILCOUMRDG-UHFFFAOYSA-N	5.0×10^{3} 1.3×10^{4} 1.4×10^{1}		Watanabe (1993) HSDB (2015) Mackay et al. (2006d)	M V V	
systox $C_{16}H_{38}O_6P_2S_4$ [8065-48-3] FAXIJTUDSBIMHY-UHFFFAOYSA-N	5.5×10^{1}		HSDB (2015)	V	
temefos $C_{16}H_{20}O_6P_2S_3$ (temephos) [3383-96-8] WWJZWCUNLNYYAU-UHFFFAOYSA-N	1.7 4.9×10^{3} 4.4		Barcelo and Hennion (1997) HSDB (2015) Goodarzi et al. (2010)	X Q Q	569 100 570
methamidophos $C_2H_8NOPS_2$ [10265-92-6] NNKVPIKMPCQWCG-UHFFFAOYSA-N	1.1×10^{4}		HSDB (2015)	Q	100
acephate $C_4H_{10}NO_3PS$ [30560-19-1] YASYVMFAVPKPKE-UHFFFAOYSA-N	2.0×10^{7} 2.0×10^{7} 1.9×10^{5} 4.4×10^{2}		HSDB (2015) Mackay et al. (2006d) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V X Q	 569 570
dimethoate $C_5H_{12}NO_3PS_2$ [60-51-5] MCWXGJITAZMZEV-UHFFFAOYSA-N	4.1×10^{4} 8.7×10^{3} 9.1×10^{3} 9.0×10^{1} 5.3×10^{2}		HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V V X Q	 12 569 570, 571

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
omethoate $C_5H_{12}NO_4PS$ [1113-02-6] PZXOQEXFMJCDPG-UHFFFAOYSA-N	2.1×10^{8}		HSDB (2015)	Q	100
methidathion $C_6H_{11}N_2O_4PS_3$ [950-37-8] MEBQXILRKZHVCX-UHFFFAOYSA-N	1.4×10^{3} 5.8×10^{3} 5.8×10^{3}		HSDB (2015) Glotfelty et al. (1987) Burkhard and Guth (1981)	V V V	
fosthietan $C_6H_{12}NO_3PS_2$ [21548-32-3] RHJOIOVESMTJEK-UHFFFAOYSA-N	2.4×10^{5} 2.4×10^{5}		HSDB (2015) MacBean (2012a)	V ?	
formothion $C_6H_{12}NO_4PS_2$ [2540-82-1] AIKKULXCBHRFOS-UHFFFAOYSA-N	9.0×10^{4}		HSDB (2015)	V	
menazon $C_6H_{12}N_5O_2PS_2$ [78-57-9] SUYHYHLFUHHVJQ-UHFFFAOYSA-N	6.6×10^{3}		HSDB (2015)	V	
ethoate-methyl $C_6H_{14}NO_3PS_2$ [116-01-8] DICRHEJCQXFJBY-UHFFFAOYSA-N	3.5×10^{5}		HSDB (2015)	Q	100
glyphosate-trimesium $C_6H_{16}NO_5PS$ [81591-81-3] RUCAXVJJQQJZGU-UHFFFAOYSA-M	$>2.3\times10^{10}$		MacBean (2012a)	?	
phosfolan $C_7H_{14}NO_3PS_2$ (cyolane) [947-02-4] ILBONRFSLATCRE-UHFFFAOYSA-N	5.1×10^{4}		Ebert et al. (2023)	?	317
methylparathion $C_8H_{10}NO_5PS$ (parathion-methyl) [298-00-0] RLBIQVVOMOPOHC-UHFFFAOYSA-N	5.0×10^{1} 1.7×10^{1} 2.6×10^{2} 1.6×10^{2} 9.9×10^{1} 4.7×10^{1} 9.9×10^{1} 4.7×10^{1} 9.2×10^{1}		Mackay and Shiu (1981) Chao et al. (2017) Rice et al. (1997b) Fendinger and Glotfelty (1990) Metcalfe et al. (1980) Mackay et al. (2006d) Woodrow et al. (1990) Suntio et al. (1988) Glotfelty et al. (1987)	L M M M M V V V V	 12 12

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.1×10^{3}		Sanders and Seiber (1983)	V	88
	1.6×10^{2}		Metcalfe et al. (1980)	V	
	1.3×10^{-1}		Smith and Bomberger (1980)	V	24
	4.7×10^{-1}		Barcelo and Hennion (1997)	X	569
	2.1×10^{1}		Goodarzi et al. (2010)	Q	570
	1.5×10^{1}		Hilal et al. (2008)	Q	
zinophos $C_8H_{13}N_2O_3PS$ (thionazin) [297-97-2] IRVDMKJLOCGUBJ-UHFFFAOYSA-N	1.0×10^{1}		Mackay et al. (2006d)	V	
	1.2×10^{1}		Suntio et al. (1988)	V	12
	1.1×10^{1}		MacBean (2012a)	?	
vamidothion $C_8H_{18}NO_4PS_2$ [2275-23-2] LESVOLZBIFDZGS-UHFFFAOYSA-N	1.1×10^{10}		HSDB (2015)	Q	100
cyanophos $C_9H_{10}NO_3PS$ [2636-26-2] SCKHCCSZFPSHGR-UHFFFAOYSA-N	1.8		HSDB (2015)	V	
fenitrothion $C_9H_{12}NO_5PS$ [122-14-5] ZNOLGFHPUIJIMJ-UHFFFAOYSA-N	8.3×10^{1}		Watanabe (1993)	M	
	1.1×10^{1}		Metcalfe et al. (1980)	M	
	8.3×10^{2}		Mackay et al. (2006d)	V	
	2.8×10^{2}		Suntio et al. (1988)	V	12
	2.7×10^{1}		Mackay and Shiu (1981)	V	
	1.5×10^{1}		Metcalfe et al. (1980)	V	
	2.7		Barcelo and Hennion (1997)	X	569
	4.4×10^{1}		Goodarzi et al. (2010)	Q	570, 571
	5.3		Hilal et al. (2008)	Q	
fosthiazate-1 $C_9H_{18}NO_3PS_2$ [98886-44-3] DUFVKSUJRWYZQP-UHFFFAOYSA-N	7.5×10^{1}		MacBean (2012b)	X	352
	1.0×10^{5}		Keshavarz et al. (2022)	Q	
	5.7×10^{4}		Duchowicz et al. (2020)	Q	
	5.7×10^{4}		Duchowicz et al. (2020)	?	186, 21
	5.7×10^{4}		Maniere et al. (2011)	?	242, 166
prothoate $C_9H_{20}NO_3PS_2$ (trimethoate) [2275-18-5] QTXHFDHVLBDJIO-UHFFFAOYSA-N	1.5×10^{5}		HSDB (2015)	Q	100
amiton $C_{10}H_{24}NO_3PS$ [78-53-5] PJISLFCKHOHLLP-UHFFFAOYSA-N	3.5×10^{4}		Bartelt-Hunt et al. (2008)	?	21

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
azinphos-methyl	3.4×10^{3}		HSDB (2015)	V	
$C_{10}H_{12}N_3O_3PS_2$	3.2×10^{3}		Mackay et al. (2006d)	V	
[86-50-0]	3.1×10^{2}		Suntio et al. (1988)	V	12
CJJOSEISRRTUQB-UHFFFAOYSA-N	3.1		Barcelo and Hennion (1997)	X	569
	4.6×10^{1}		Goodarzi et al. (2010)	Q	570
parathion	1.2×10^{2}		Fendinger and Glotfelty (1990)	M	
$C_{10}H_{14}NO_5PS$	7.1×10^{1}		Mackay et al. (2006d)	V	
(E 605)	5.0×10^{1}		Siebers and Mattusch (1996)	V	12
[56-38-2]	5.0×10^{1}		Siebers et al. (1994)	V	
LCCNCVORNKJIRZ-UHFFFAOYSA-N	8.3×10^{1}		Suntio et al. (1988)	V	12
	4.2×10^{1}		Glotfelty et al. (1987)	V	
	1.6×10^{3}		Sanders and Seiber (1983)	V	88
	8.1		Mackay and Shiu (1981)	V	
	1.3×10^{1}		Burkhard and Guth (1981)	V	
	1.0×10^{1}		Chiou et al. (1980)	V	
	3.3×10^{1}		MacBean (2012b)	X	352
	8.0×10^{-1}		Barcelo and Hennion (1997)	X	569
	3.2×10^{-1}		Goodarzi et al. (2010)	Q	570
	6.5		Hilal et al. (2008)	Q	
	3.4×10^{1}		Bartelt-Hunt et al. (2008)	?	21
isoparathion	6.1×10^{1}		Ebert et al. (2023)	?	319
$C_{10}H_{14}NO_5PS$					
[597-88-6]					
BGWJTLLALYACOG-UHFFFAOYSA-N					
etrimfos	1.6×10^{1}		HSDB (2015)	V	
$C_{10}H_{17}N_2O_4PS$					
[38260-54-7]					
FGIWFCGDPUIBEZ-UHFFFAOYSA-N					
propetamphos	2.1×10^{2}		HSDB (2015)	V	
$C_{10}H_{20}NO_4PS$					
[31218-83-4]					
BZNDWPRGXNILMS-VQHVLOKHSA-N					
mecarbam	1.1×10^{4}		HSDB (2015)	Q	100
$C_{10}H_{20}NO_5PS_2$					
[2595-54-2]					
KLGMSAOQDHLCOS-UHFFFAOYSA-N					
phosmet	1.2×10^{3}		HSDB (2015)	V	
$C_{11}H_{12}NO_4PS_2$	1.3×10^{3}		Mackay et al. (2006d)	V	
[732-11-6]	1.1×10^{3}		Suntio et al. (1988)	V	12
LMNZTLDVJIUSHT-UHFFFAOYSA-N	1.0×10^{1}		Barcelo and Hennion (1997)	X	569
	3.8		Goodarzi et al. (2010)	Q	570
	7.4×10^{2}		Maniere et al. (2011)	?	166

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pirimiphos methyl $C_{11}H_{20}N_3O_3PS$ [29232-93-7] QHOQHJPRIBSPCY-UHFFFAOYSA-N	1.6×10^{1} 1.7×10^{1}		HSDB (2015) Maniere et al. (2011)	V ?	 242, 166
imicyafos $C_{11}H_{21}N_4O_2PS$ [140163-89-9] PPCUNNLZTNMXFO-UHFFFAOYSA-N	1.5×10^{9}		Ebert et al. (2023)	?	319
Agent VX $C_{11}H_{26}NO_2PS$ [50782-69-9] JJIUCEJQJXNMHV-UHFFFAOYSA-N	9.1×10^{2} 2.8×10^{3} 1.2×10^{3}		HSDB (2015) Bartelt-Hunt et al. (2008) Opresko et al. (1998)	V ? ?	 21
ditalimfos $C_{12}H_{14}NO_4PS$ [5131-24-8] MTBZIGHNGSTDJV-UHFFFAOYSA-N	2.3×10^{3}		Ebert et al. (2023)	?	317
quinalphos $C_{12}H_{15}N_2O_3PS$ [13593-03-8] JYQUHIFYBATCCY-UHFFFAOYSA-N	1.1×10^{2}		Ebert et al. (2023)	?	317
phoxim $C_{12}H_{15}N_2O_3PS$ [14816-18-3] ATROHALUCMTWTB-UHFFFAOYSA-N	5.0×10^{1}		Ebert et al. (2023)	?	317
triazophos $C_{12}H_{16}N_3O_3PS$ [24017-47-8] AMFGTOFWMRQMEM-UHFFFAOYSA-N	3.2×10^{2}		HSDB (2015)	V	
azinphos-ethyl $C_{12}H_{16}N_3O_3PS_2$ [2642-71-9] RQVGAIADHNPSME-UHFFFAOYSA-N	1.0×10^{2}		HSDB (2015)	V	
diazinon $C_{12}H_{21}N_2O_3PS$ (dimpylate) [333-41-5] FHIVAFMUCKRCQO-UHFFFAOYSA-N	4.6×10^{1} 9.2×10^{1} 1.5×10^{1} 1.1×10^{1} 8.4×10^{1} 8.8×10^{1} 2.5×10^{1} 1.5×10^{1} 6.7 1.0×10^{2}	 12000 	Muir et al. (2004) Muir et al. (2004) Feigenbrugel et al. (2004a) Watanabe (1993) Fendinger et al. (1989) Fendinger and Glotfelty (1988) Mackay et al. (2006d) Suntio et al. (1988) Glotfelty et al. (1987) Sanders and Seiber (1983)	L L M M M M V V V V	369 368 73 73 12 88

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.3×10^{1}		Burkhard and Guth (1981)	V	
	1.5×10^{-1}		Barcelo and Hennion (1997)	X	569
	1.7×10^{-1}		Goodarzi et al. (2010)	Q	570
	1.4×10^{2}		Meylan and Howard (1991)	Q	
isoxathion $C_{13}H_{16}NO_4PS$ [18854-01-8] SDMSCIWHRZJSRN-UHFFFAOYSA-N	1.6×10^{2}		HSDB (2015)	Q	100
butamifos $C_{13}H_{21}N_2O_4PS$ [36335-67-8] OEYOMNZEMCPTKN-UHFFFAOYSA-N	3.4×10^{1}		Ebert et al. (2023)	?	317
fenamiphos $C_{13}H_{22}NO_3PS$ [22224-92-6] ZCJPOPBZHLUFHF-UHFFFAOYSA-N	1.1×10^{3}		HSDB (2015)	V	
tebupirimfos $C_{13}H_{23}N_2O_3PS$ [96182-53-5] AWYOMXWDGWUJHS-UHFFFAOYSA-N	3.5		HSDB (2015)	V	
pirimiphos ethyl $C_{13}H_{24}N_3O_3PS$ [23505-41-1] TZBPRYIIJAJUOY-UHFFFAOYSA-N	1.8×10^{-1}		HSDB (2015)	V	
bensulide $C_{14}H_{24}NO_4PS_3$ [741-58-2] RRNIZKPFKNDSRS-UHFFFAOYSA-N	1.1×10^{3}		HSDB (2015)	V	
ethyl *p*-nitrophenyl benzenethiophosphonate $C_{14}H_{14}NO_4PS$ [2104-64-5] AIGRXSNSLVJMEA-UHFFFAOYSA-N	2.2×10^{1}		Duchowicz et al. (2020)	V	187
	2.2×10^{1}		HSDB (2015)	V	
	4.3×10^{7}		Duchowicz et al. (2020)	Q	
pyridaphenthion $C_{14}H_{17}N_2O_4PS$ [119-12-0] CXJSOEPQXUCJSA-UHFFFAOYSA-N	5.1×10^{4}		Ebert et al. (2023)	?	319
piperophos $C_{14}H_{28}NO_3PS_2$ [24151-93-7] UNLYSVIDNRIVFJ-UHFFFAOYSA-N	8.8×10^{2}		Ebert et al. (2023)	?	319

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
isofenphos	1.2×10^{2}		Mackay et al. (2006d)	V	
$C_{15}H_{24}NO_4PS$	2.4×10^{2}		MacBean (2012b)	X	352
[25311-71-1]	1.0×10^{3}		Barcelo and Hennion (1997)	X	569
HOQADATXFBOEGG-UHFFFAOYSA-N	6.9×10^{-1}		Goodarzi et al. (2010)	Q	570, 571
	2.4×10^{2}		MacBean (2012a)	?	12
chlormephos	3.4×10^{-2}		Duchowicz et al. (2020)	V	187
$C_5H_{12}ClO_2PS_2$	3.4×10^{-2}		HSDB (2015)	V	
[24934-91-6]	3.2×10^{5}		Duchowicz et al. (2020)	Q	
QGTYWWGEWOBMAK-UHFFFAOYSA-N					
chlorethoxyfos	2.3		HSDB (2015)	Q	100
$C_6H_{11}Cl_4O_3PS$					
[54593-83-8]					
XFDJMIHUAHSGKG-UHFFFAOYSA-N					
ronnel	4.8×10^{-1}		Mackay and Shiu (1981)	L	
$C_8H_8O_3Cl_3PS$	1.7×10^{-2}		Mackay et al. (2006d)	V	
[299-84-3]	3.1×10^{-1}		Suntio et al. (1988)	V	12
JHJOOSLFWRRSGU-UHFFFAOYSA-N	5.7×10^{-2}		Hilal et al. (2008)	Q	
tolclofos-methyl	1.7×10^{-2}		Mackay et al. (2006d)	V	
$C_9H_{11}Cl_2O_3PS$	2.7		Maniere et al. (2011)	?	12, 166
[57018-04-9]					
OBZIQQJJIKNWNO-UHFFFAOYSA-N					
methyl trithion	9.9×10^{1}		HSDB (2015)	Q	100
$C_9H_{12}ClO_2PS_3$					
[953-17-3]					
OUCCVXVYGFBXSV-UHFFFAOYSA-N					
trichloronate	8.8×10^{-1}		Duchowicz et al. (2020)	V	187
$C_{10}H_{12}Cl_3O_2PS$	9.0×10^{-1}		HSDB (2015)	V	
[327-98-0]	2.6×10^{4}		Duchowicz et al. (2020)	Q	
ANIAQSUBRGXWLS-UHFFFAOYSA-N	7.5×10^{1}		MacBean (2012a)	?	
dichlofenthion	1.0×10^{-2}		Duchowicz et al. (2020)	V	187
$C_{10}H_{13}Cl_2O_3PS$	1.0×10^{-2}		HSDB (2015)	V	
[97-17-6]	3.2×10^{-5}		Mackay et al. (2006d)	V	
WGOWCPGHOCIHBW-UHFFFAOYSA-N	3.2×10^{-5}		Suntio et al. (1988)	V	12
	1.5×10^{1}		Duchowicz et al. (2020)	Q	
prothiofos	3.4×10^{-1}		Ebert et al. (2023)	?	319
$C_{11}H_{15}Cl_2O_2PS_2$					
[34643-46-4]					
FITIWKDOCAUBQD-UHFFFAOYSA-N					

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chlorthiophos $C_{11}H_{15}Cl_2O_3PS_2$ [21923-23-9] JAZJVWLGNLCNDD-UHFFFAOYSA-N	8.2		HSDB (2015)	Q	100
carbophenothion $C_{11}H_{16}ClO_2PS_3$ [786-19-6] VEDTXTNSFWUXGQ-UHFFFAOYSA-N	4.9×10^{1} 2.2×10^{1}		HSDB (2015) Suntio et al. (1988)	V V	 12
coumaphos $C_{14}H_{16}ClO_5PS$ [56-72-4] BXNANOICGRISHX-UHFFFAOYSA-N	9.0×10^{1}		HSDB (2015)	V	
methylchlorpyrifos $C_7H_7NO_3Cl_3PS$ [5598-13-0] HRBKVYFZANMGRE-UHFFFAOYSA-N	4.1 2.5 2.9 3.3 6.5×10^{-1} 4.3		HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Mackay and Shiu (1981) Hilal et al. (2008) Maniere et al. (2011)	V V V V Q ?	 12 242, 166
dicapthon $C_8H_9NO_5ClPS$ [2463-84-5] OTKXWJHPGBRXCR-UHFFFAOYSA-N	1.0×10^{2} 4.2×10^{1} 4.2×10^{1} 4.4×10^{1} 6.5		HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Mackay and Shiu (1981) Hilal et al. (2008)	V V V V Q	 12
chlorthion $C_8H_9ClNO_5PS$ [500-28-7] NZNRRXXETLSZRO-UHFFFAOYSA-N	2.5×10^{2} 2.4×10^{2}		HSDB (2015) MacBean (2012a)	V ?	
azamethiphos $C_9H_{10}ClN_2O_5PS$ [35575-96-3] VNKBTWQZTQIWDV-UHFFFAOYSA-N	3.0×10^{5}		Ebert et al. (2023)	?	319
isazophos $C_9H_{17}ClN_3O_3PS$ [42509-80-8] XRHGWAGWAHHFLF-UHFFFAOYSA-N	1.9×10^{1} 1.1×10^{2} 7.2×10^{1}		HSDB (2015) Burkhard and Guth (1981) MacBean (2012a)	V V ?	
chlorpyrifos $C_9H_{11}Cl_3NO_3PS$ [2921-88-2] SBPBAQFWLVIOKP-UHFFFAOYSA-N	1.8 2.1 2.2×10^{-1} 3.1 2.4 9.2×10^{-1} 1.7 5.7×10^{-1}	 7800 	Muir et al. (2004) Muir et al. (2004) Cetin et al. (2006) Rice et al. (1997b) Fendinger and Glotfelty (1990) Mackay et al. (2006d) Siebers et al. (1994) Suntio et al. (1988)	L L M M M V V V	369 368 12 12

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.1×10^{-1}		Glotfelty et al. (1987)	V	
	5.6×10^{-3}		Barcelo and Hennion (1997)	X	569
	3.4		HSDB (2015)	C	
	1.4		Armbrust (2000)	C	
	1.0×10^{-1}		Goodarzi et al. (2010)	Q	570, 571
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	2.5×10^{2}		Meylan and Howard (1991)	Q	
	2.1		Maniere et al. (2011)	?	242, 166
chlorphoxim $C_{12}H_{14}ClN_2O_3PS$ [14816-20-7] GQKRUMZWUHSLJF-NTCAYCPXSA-N	$>2.3\times10^{10}$		MacBean (2012a)	?	
phosazetim $C_{14}H_{11}Cl_2N_2O_4PS$ [4104-14-7] XIBXUAZIZXDFTG-UHFFFAOYSA-N	2.1×10^{3}		HSDB (2015)	Q	100
dialifor $C_{14}H_{17}ClNO_4PS_2$ [10311-84-9] MUMQYXACQUZOFP-UHFFFAOYSA-N	5.5×10^{1}		HSDB (2015)	V	
	7.1		Mackay et al. (2006d)	V	
	7.1		Suntio et al. (1988)	V	12
pyraclofos $C_{14}H_{18}ClN_2O_3PS$ [77458-01-6] QHGVXILFMXYDRS-UHFFFAOYSA-N	2.3×10^{4}		Ebert et al. (2023)	?	319
bromophos $C_8H_8BrCl_2O_3PS$ [2104-96-3] NYQDCVLCJXRDSK-UHFFFAOYSA-N	1.0×10^{-1}		HSDB (2015)	V	
	1.1×10^{-1}		MacBean (2012a)	?	12
bromophos-ethyl $C_{10}H_{12}BrCl_2O_3PS$ [4824-78-6] KWGUFOITWDSNQY-UHFFFAOYSA-N	6.2×10^{-1}		HSDB (2015)	Q	100
profenofos $C_{11}H_{15}BrClO_3PS$ [41198-08-7] QYMMJNLHFKGANY-UHFFFAOYSA-N	4.5×10^{2}		HSDB (2015)	V	
	6.2×10^{2}		Mackay et al. (2006d)	V	
iodofenphos $C_8H_8Cl_2IO_3PS$ [18181-70-9] LFVLUOAHQIVABZ-UHFFFAOYSA-N	2.2		HSDB (2015)	V	
	$>2.3\times10^{10}$		MacBean (2012a)	?	

A11 Organic species with other elements

A11.1 Sodium (Na)

Table A11.1: Sodium (Na)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
sesone $C_8H_7Cl_2NaO_5S$ (2,4-dichlorophenoxyethyl sulfate) [136-78-7] KISFEBPWFCGRGN-UHFFFAOYSA-M	3.8×10^{5}		HSDB (2015)	Q	100
iodosulfuron-methyl-sodium $C_{14}H_{14}IN_5O_6SNa$ [144550-36-7] JUJFQMPKBJPSFZ-UHFFFAOYSA-M	4.4×10^{10}		Maniere et al. (2011)	?	12, 166
propoxycarbazone-sodium $C_{15}H_{17}N_4O_7NaS$ [181274-15-7] JRQGDDUXDKCWRF-UHFFFAOYSA-M	$>1.0\times10^{10}$		Maniere et al. (2011)	?	12, 166
dioctyl sulfosuccinatesodium salt $C_{20}H_{37}NaO_7S$ (bis(2-ethylhexyl) sodium sulfosuccinate) [577-11-7] APSBXTVYXVQYAB-UHFFFAOYSA-M	2.0×10^{6}		HSDB (2015)	Q	100
dodecylbenzenesulfonic acid sodium salt $C_{18}H_{29}NaO_3S$ (sodium dodecylbenzenesulfonate) [25155-30-0] BWUAQXVVJWAXHR-UHFFFAOYSA-M	1.6×10^{2}		HSDB (2015)	Q	100
D&C yellow 10 $C_{20}H_{17}NO_8Na_2S_2$ [8004-92-0] NYMFWSWVZMTZQO-UHFFFAOYSA-L	3.4×10^{14}		HSDB (2015)	Q	100
D&C yellow 8 $C_{20}H_{10}Na_2O_5$ (fluorescein sodium) [518-47-8] NJDNXYGOVLYJHP-UHFFFAOYSA-L	3.5×10^{10}		HSDB (2015)	Q	449
D&C black 1 $C_{22}H_{14}N_6Na_2O_9S_2$ (amido black 10B) [1064-48-8] HKBVRFLHNUEVRO-DWTBGCDMSA-L	8.2×10^{25}		HSDB (2015)	Q	100

Table A11.1: Sodium (Na) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
D&C green 5 $C_{28}H_{20}N_2Na_2O_8S_2$ [4403-90-1] FPAYXBWMYIMERV-UHFFFAOYSA-L	3.1×10^{23}		HSDB (2015)	Q	449
FD&C green 2 $C_{37}H_{34}N_2Na_2O_9S3$ [5141-20-8] DGOBMKYRQHEFGQ-UHFFFAOYSA-L	7.0×10^{30}		HSDB (2015)	Q	449

A11.2 Aluminum (Al)

Table A11.2: Aluminum (Al)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
fosetyl-aluminum $C_6H_{18}AlO_9P_3$ [39148-24-8] ZKZMJOFIHHZSRW-UHFFFAOYSA-K	3.1×10^9 $>3.1\times10^9$		HSDB (2015) Maniere et al. (2011)	V ?	 12, 166

A11.3 Silicon (Si)

Table A11.3: Silicon (Si)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tetramethylsilane $C_4H_{12}Si$ [75-76-3] CZDYPVPMEAXLPK-UHFFFAOYSA-N	2.3×10^{-6} 2.3×10^{-6} 1.4×10^{-3} 2.4×10^{-6}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Abraham et al. (1990)	V V Q ?	187
tetraethylsilane $C_8H_{20}Si$ [631-36-7] VCZQFJFZMMALHB-UHFFFAOYSA-N	3.8×10^{-6}		Abraham et al. (1990)	?	
trimethylsilanol $(CH_3)_3SiOH$ (TMS) [1066-40-6] AAPLIUHOKVUFCC-UHFFFAOYSA-N	7.0×10^{-2} 2.2×10^{-1}		Xu and Kropscott (2014) Mazzoni et al. (1997)	M V	
silicic acid $Si(OH)_4$ [10193-36-9] RMAQACBXLXPBSY-UHFFFAOYSA-N	2.3×10^{10}	14000	Plyasunov (2012)	M	820
dimethylsilanediol $C_2H_8O_2Si$ [1066-42-8] XCLIHDJZGPCUBT-UHFFFAOYSA-N	2.8×10^{3} 2.9×10^{-1}		Xu and Kropscott (2012) Mazzoni et al. (1997)	M V	12
tetramethyl silicate $C_4H_{12}O_4Si$ [681-84-5] LFQCEHFDDXELDD-UHFFFAOYSA-N	1.5		HSDB (2015)	Q	100
pentamethyldisiloxanol $C_5H_{16}O_2Si_2$ [56428-93-4] FGOLZCPMTWJPOU-UHFFFAOYSA-N	7.3×10^{-4}		Mazzoni et al. (1997)	V	
tetraethyl silicate $C_8H_{20}O_4Si$ [78-10-4] BOTDANWDWHJENH-UHFFFAOYSA-N	4.9×10^{-1}		HSDB (2015)	Q	100
trimethoxysilylpropyl methacrylate $C_{10}H_{20}O_5Si$ [2530-85-0] XDLMVUHYZWKMMD-UHFFFAOYSA-N	3.3×10^{1}		HSDB (2015)	Q	100

Table A11.3: Silicon (Si) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexamethyldisiloxane	1.3×10^{-6}		Xu and Kropscott (2014)	M	
$C_6H_{18}OSi_2$	1.7×10^{-4}		Kochetkov et al. (2001)	M	404, 332
(L2)	3.1×10^{-4}		Kochetkov et al. (2001)	M	404, 333
[107-46-0]	7.7×10^{-7}		David et al. (2000)	M	73
UQEAIHBTYFGYIE-UHFFFAOYSA-N	1.0×10^{-6}		Xu and Kropscott (2014)	V	
	1.0×10^{-6}		Kochetkov et al. (2001)	V	
	4.2×10^{-6}		Mazzoni et al. (1997)	V	
	2.2×10^{-4}		Keshavarz et al. (2022)	Q	
	1.9×10^{-4}		Duchowicz et al. (2020)	Q	
	2.2×10^{-4}		Duchowicz et al. (2020)	?	186, 21
octamethyltrisiloxane	3.4×10^{-7}		Xu and Kropscott (2014)	M	
$C_8H_{24}O_2Si_3$	3.3×10^{-6}		Kochetkov et al. (2001)	M	404, 332
(L3)	2.7×10^{-6}		Kochetkov et al. (2001)	M	404, 333
[107-51-7]	2.8×10^{-7}		Xu and Kropscott (2014)	V	
CXQXSVUQTKDNFP-UHFFFAOYSA-N	2.8×10^{-7}		Kochetkov et al. (2001)	V	
	1.2×10^{-6}		Mazzoni et al. (1997)	V	
	1.3×10^{-5}		Keshavarz et al. (2022)	Q	
	2.5×10^{-5}		Duchowicz et al. (2020)	Q	
	3.0×10^{-6}		Duchowicz et al. (2020)	?	186, 21
decamethyltetrasiloxane	1.4×10^{-7}		Xu and Kropscott (2014)	M	
$C_{10}H_{30}O_3Si_4$	5.8×10^{-7}		Kochetkov et al. (2001)	M	404, 332
(L4)	3.7×10^{-7}		Xu and Kropscott (2014)	V	
[141-62-8]	4.3×10^{-7}		Kochetkov et al. (2001)	V	
YFCGDEUVHLPRCZ-UHFFFAOYSA-N	3.1×10^{-7}		Mazzoni et al. (1997)	V	
	8.1×10^{-7}		Keshavarz et al. (2022)	Q	
	3.3×10^{-6}		Duchowicz et al. (2020)	Q	185
	5.8×10^{-7}		Duchowicz et al. (2020)	?	186, 21
dodecamethylpentasiloxane $C_{12}H_{36}O_4Si_5$ (L5) [141-63-9] FBZANXDWQAVSTQ-UHFFFAOYSA-N	8.7×10^{-8}		Mazzoni et al. (1997)	V	
silthiofam $C_{13}H_{21}NOSSi$ [175217-20-6] MXMXHPPIGKYTAR-UHFFFAOYSA-N	1.9		Maniere et al. (2011)	?	242, 166
tetradecamethylhexasiloxane $C_{14}H_{42}O_5Si_6$ (L6) [107-52-8] ADANNTOYRVPQLJ-UHFFFAOYSA-N	2.7×10^{-8}		Mazzoni et al. (1997)	V	

Table A11.3: Silicon (Si) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexadecamethylheptasiloxane $C_{16}H_{48}O_6Si_7$ (L7) [541-01-5] NFVSFLUJRHRSJG-UHFFFAOYSA-N	7.6×10^{-9}		Mazzoni et al. (1997)	V	
octadecamethyloctasiloxane $C_{18}H_{54}O_7Si_8$ (L8) [556-69-4] VWGDPBQTSZDFMX-UHFFFAOYSA-N	3.3×10^{-9}		Mazzoni et al. (1997)	V	
hexamethylcyclotrisiloxane $C_6H_{18}O_3Si_3$ (D3) [541-05-9] HTDJPCNNEPUOOQ-UHFFFAOYSA-N	5.6×10^{-6}		Mazzoni et al. (1997)	V	
	6.4×10^{-6}		Alton and Browne (2022)	Q	821
	1.6×10^{-5}		Alton and Browne (2022)	Q	822
	2.5×10^{-6}		Alton and Browne (2022)	Q	823
octamethylcyclotetrasiloxane $C_8H_{24}O_4Si_4$ (D4) [556-67-2] HMMGMWAXVFQUOA-UHFFFAOYSA-N	7.3×10^{-7}		Xu and Kropscott (2014)	M	
	8.3×10^{-7}		Xu and Kropscott (2012)	M	88
	1.7×10^{-5}		Kochetkov et al. (2001)	M	298, 332
	1.7×10^{-5}		Kochetkov et al. (2001)	M	298, 333
	1.2×10^{-4}		Hamelink et al. (1996)	M	12
	1.5×10^{-6}		Xu and Kropscott (2014)	V	
	1.6×10^{-6}		Kochetkov et al. (2001)	V	
	8.3×10^{-7}		Mazzoni et al. (1997)	V	
	2.7×10^{-6}		Hamelink et al. (1996)	V	12
	5.4×10^{-7}		Alton and Browne (2022)	Q	821
	1.3×10^{-6}		Alton and Browne (2022)	Q	822
	1.1×10^{-6}		Alton and Browne (2022)	Q	823
	1.3×10^{-5}		Keshavarz et al. (2022)	Q	
	4.2×10^{-5}		Duchowicz et al. (2020)	Q	
	8.4×10^{-5}		Duchowicz et al. (2020)	?	186, 21
decamethylcyclopentasiloxane $C_{10}H_{30}O_5Si_5$ (D5) [541-02-6] XMSXQFUHVRWGNA-UHFFFAOYSA-N	2.8×10^{-7}		Xu and Kropscott (2014)	M	
	3.0×10^{-7}		Xu and Kropscott (2012)	M	
	3.4×10^{-5}		Kochetkov et al. (2001)	M	374, 332
	3.1×10^{-5}		Kochetkov et al. (2001)	M	374, 333
	7.4×10^{-5}		David et al. (2000)	M	73
	2.3×10^{-6}		Xu and Kropscott (2014)	V	
	2.2×10^{-6}		Kochetkov et al. (2001)	V	
	1.5×10^{-6}		Mazzoni et al. (1997)	V	
	2.3×10^{-7}		Alton and Browne (2022)	Q	821
	1.2×10^{-6}		Alton and Browne (2022)	Q	822
	3.1×10^{-6}		Alton and Browne (2022)	Q	823

Table A11.3: Silicon (Si) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dodecamethylcyclohexasiloxane	4.0×10^{-7}		Xu and Kropscott (2012)	M	80
$C_{12}H_{36}O_6Si_6$	6.8×10^{-5}		Kochetkov et al. (2001)	M	374, 332
(D6)	1.5×10^{-4}		Kochetkov et al. (2001)	M	374, 333
[540-97-6]	3.9×10^{-6}		Kochetkov et al. (2001)	V	
IUMSDRXLFWAGNT-UHFFFAOYSA-N					
tetramethyldisiloxane-1,3-diol	1.8×10^{-1}		Mazzoni et al. (1997)	V	
$C_4H_{14}O_3Si_2$					
[1118-15-6]					
PFEAZKFNWPIFCV-UHFFFAOYSA-N					
hexamethyltrisiloxane-1,5-diol	3.4×10^{-3}		Mazzoni et al. (1997)	V	
$C_6H_{20}O_4Si_3$					
[3663-50-1]					
XYBQTTAROZGWOZ-UHFFFAOYSA-N					
octamethyltetrasiloxane-1,7-diol	2.7×10^{-3}		Mazzoni et al. (1997)	V	
$C_8H_{26}O_5Si_4$					
[3081-07-0]					
VERNMKKMBJGSQB-UHFFFAOYSA-N					
pentamethylcyclotrisiloxanol	1.1×10^{-3}		Mazzoni et al. (1997)	V	
$C_5H_{16}O_4Si_3$	1.2×10^{-1}		Alton and Browne (2022)	Q	821
(D3OH)	2.7×10^{-2}		Alton and Browne (2022)	Q	822
[106916-50-1]	1.5×10^{-3}		Alton and Browne (2022)	Q	823
OGNYSZJXUXVWRE-UHFFFAOYSA-N					
heptamethylcyclotetrasiloxanol	2.3×10^{-4}		Mazzoni et al. (1997)	V	
$C_7H_{22}O_5Si_4$	1.1×10^{-2}		Alton and Browne (2022)	Q	821
(D4OH)	1.1×10^{-2}		Alton and Browne (2022)	Q	822
[5290-02-8]	1.3×10^{-5}		Alton and Browne (2022)	Q	823
MLGUQSFCJNMKPT-UHFFFAOYSA-N					
nonamethylcyclopentasiloxanol	7.0×10^{-5}		Mazzoni et al. (1997)	V	
$C_9H_{28}O_6Si_5$	4.6×10^{-3}		Alton and Browne (2022)	Q	821
(D5OH)	2.0×10^{-2}		Alton and Browne (2022)	Q	822
[5290-04-0]	4.4×10^{-5}		Alton and Browne (2022)	Q	823
DKTKKERLEMHMHS-UHFFFAOYSA-N					
D3FormEst	2.8×10^{-4}		Alton and Browne (2022)	Q	821
$C_6H_{16}O_5Si_3$	3.2×10^{-4}		Alton and Browne (2022)	Q	822
TZIXLALHTGGYNZ-UHFFFAOYSA-N	1.7×10^{-3}		Alton and Browne (2022)	Q	823
D3OHFormEst	5.4		Alton and Browne (2022)	Q	821
$C_5H_{14}O_6Si_3$	9.9		Alton and Browne (2022)	Q	822
RMJPVGNUQFKGPC-UHFFFAOYSA-N	1.2×10^{-2}		Alton and Browne (2022)	Q	823
D3Hydroperoxide	6.9×10^{-2}		Alton and Browne (2022)	Q	821
$C_6H_{18}O_5Si_3$	1.9×10^{-3}		Alton and Browne (2022)	Q	822
JKDUHABXPCJOJB-UHFFFAOYSA-N	8.9×10^{-6}		Alton and Browne (2022)	Q	823

Table A11.3: Silicon (Si) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
D3EtherHydroperoxide	8.4×10^{-1}		Alton and Browne (2022)	Q	821
$C_6H_{18}O_6Si_3$	1.9×10^{-2}		Alton and Browne (2022)	Q	822
LHGAYMWHCKTFJV-UHFFFAOYSA-N	1.7×10^{-2}		Alton and Browne (2022)	Q	823
D3FormEst2	1.2×10^{-2}		Alton and Browne (2022)	Q	821
$C_6H_{14}O_7Si_3$	9.2×10^{-3}		Alton and Browne (2022)	Q	822
WKTLUKWDJJZJCN-UHFFFAOYSA-N	2.0×10^{-2}		Alton and Browne (2022)	Q	823
D3OH2O1	2.4×10^{3}		Alton and Browne (2022)	Q	821
$C_4H_{14}O_5Si_3$	2.9		Alton and Browne (2022)	Q	822
UGEQNRIYBONGCP-UHFFFAOYSA-N	1.8×10^{-1}		Alton and Browne (2022)	Q	823
D4FormEst	2.4×10^{-5}		Alton and Browne (2022)	Q	821
$C_8H_{22}O_6Si_4$	8.5×10^{-5}		Alton and Browne (2022)	Q	822
PWVQOGDRWKITJQ-UHFFFAOYSA-N	8.8×10^{-5}		Alton and Browne (2022)	Q	823
D4OHFormEst	4.6×10^{-1}		Alton and Browne (2022)	Q	821
$C_7H_{20}O_7Si_4$	3.1		Alton and Browne (2022)	Q	822
AXBVNNKTZSENOJ-UHFFFAOYSA-N	1.2×10^{-4}		Alton and Browne (2022)	Q	823
1,1,1,3,5,5,5- heptamethyltrisiloxane $C_7H_{22}O_2Si_3$ [1873-88-7] QNWOFLWXQGHSRH-UHFFFAOYSA-N	1.1×10^{-7}		Ebert et al. (2023)	?	319
D4Hydroperoxide	5.8×10^{-3}		Alton and Browne (2022)	Q	821
$C_8H_{24}O_6Si_4$	4.4×10^{-4}		Alton and Browne (2022)	Q	822
IEOAKTNTPADFJB-UHFFFAOYSA-N	1.8×10^{-6}		Alton and Browne (2022)	Q	823
D4EtherHydroperoxide	7.1×10^{-2}		Alton and Browne (2022)	Q	821
$C_8H_{24}O_7Si_4$	4.5×10^{-3}		Alton and Browne (2022)	Q	822
BKBHFCQPJIYNBR-UHFFFAOYSA-N	1.5×10^{-5}		Alton and Browne (2022)	Q	823
D4FormEst2	1.0×10^{-3}		Alton and Browne (2022)	Q	821
$C_8H_{20}O_8Si_4$	1.8×10^{-3}		Alton and Browne (2022)	Q	822
WJOJQLFAIHHNFX-UHFFFAOYSA-N	2.9×10^{-4}		Alton and Browne (2022)	Q	823
D4OH2	2.1×10^{2}		Alton and Browne (2022)	Q	821
$C_6H_{20}O_6Si_4$	1.0		Alton and Browne (2022)	Q	822
ONAQLRRZBYFKLA-UHFFFAOYSA-N	8.3×10^{-5}		Alton and Browne (2022)	Q	823
D5FormEst	1.0×10^{-5}		Alton and Browne (2022)	Q	821
$C_{10}H_{28}O_7Si_5$	1.2×10^{-4}		Alton and Browne (2022)	Q	822
IGERVNZEGVJPED-UHFFFAOYSA-N	6.4×10^{-5}		Alton and Browne (2022)	Q	823
glycidoxypropyltrimethoxysilane $C_9H_{20}O_5Si$ [2530-83-8] BPSIOYPQMFLKFR-UHFFFAOYSA-N	1.4×10^{2}		Ebert et al. (2023)	?	319

Table A11.3: Silicon (Si) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
D5OHFormEst	2.0×10^{-1}		Alton and Browne (2022)	Q	821
$C_9H_{26}O_8Si_5$	5.6		Alton and Browne (2022)	Q	822
KNIXZSAQQHGMJX-UHFFFAOYSA-N	4.7×10^{-5}		Alton and Browne (2022)	Q	823
D5Hydroperoxide	2.5×10^{-3}		Alton and Browne (2022)	Q	821
$C_{10}H_{30}O_7Si_5$	6.3×10^{-4}		Alton and Browne (2022)	Q	822
VGMLSGIAATVHBV-UHFFFAOYSA-N	1.1×10^{-6}		Alton and Browne (2022)	Q	823
D5EtherHydroperoxide	3.1×10^{-2}		Alton and Browne (2022)	Q	821
$C_{10}H_{30}O_8Si_5$	6.8×10^{-3}		Alton and Browne (2022)	Q	822
GSAPDUDDTPAQSH-UHFFFAOYSA-N	1.1×10^{-5}		Alton and Browne (2022)	Q	823
D5FormEst2	4.5×10^{-4}		Alton and Browne (2022)	Q	821
$C_{10}H_{26}O_9Si_5$	2.5×10^{-3}		Alton and Browne (2022)	Q	822
QFORSIVEJZTNKQ-UHFFFAOYSA-N	2.0×10^{-4}		Alton and Browne (2022)	Q	823
isobutyltriethoxysilane $C_{10}H_{24}O_3Si$ [17980-47-1] ALVYUZIFSCKIFP-UHFFFAOYSA-N	5.5×10^{-3}		Ebert et al. (2023)	?	317
methyltris(trimethylsiloxy)silane $C_{10}H_{30}O_3Si_4$ [17928-28-8] RGMZNZABJYWAEC-UHFFFAOYSA-N	2.9×10^{-8}		Ebert et al. (2023)	?	317
vinyltris(2-methoxyethoxy)silane $C_{11}H_{24}O_6Si$ [1067-53-4] WOXXJEVNDJOOLV-UHFFFAOYSA-N	5.9×10^{2}		Ebert et al. (2023)	?	319
tetrakis(trimethylsiloxy)silane $C_{12}H_{36}O_4Si_5$ [3555-47-3] VNRWTCZXQWOWIG-UHFFFAOYSA-N	2.6×10^{-8}		Ebert et al. (2023)	?	319
2-(3,4-epoxycyclohexyl) ethyltriethoxysilane $C_{14}H_{28}O_4Si$ [10217-34-2] UDUKMRHNZZLJRB-UHFFFAOYSA-N	9.9		Ebert et al. (2023)	?	319
D5OH2	8.9×10^{1}		Alton and Browne (2022)	Q	821
$C_8H_{26}O_7Si_5$	2.5		Alton and Browne (2022)	Q	822
AGIASGIZCMBNMT-UHFFFAOYSA-N	1.3×10^{-4}		Alton and Browne (2022)	Q	823
hexamethyldisilazane $C_6H_{19}NSi_2$ [999-97-3] FFUAGWLWBBFQJT-UHFFFAOYSA-N	1.1×10^{-1}		HSDB (2015)	Q	100

Table A11.3: Silicon (Si) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
D3Organonitrate	2.4×10^{-3}		Alton and Browne (2022)	Q	821
$C_6H_{17}NO_6Si_3$	1.6×10^{-4}		Alton and Browne (2022)	Q	822
WGZJMUDCTAXYSF-UHFFFAOYSA-N	1.0×10^{-4}		Alton and Browne (2022)	Q	823
D3EtherOrganonitrate	2.9×10^{-2}		Alton and Browne (2022)	Q	821
$C_6H_{17}NO_7Si_3$	1.7×10^{-3}		Alton and Browne (2022)	Q	822
CJWFNCZCCFYEKP-UHFFFAOYSA-N	1.4×10^{-3}		Alton and Browne (2022)	Q	823
D4Organonitrate	2.0×10^{-4}		Alton and Browne (2022)	Q	821
$C_8H_{23}NO_7Si_4$	4.1×10^{-5}		Alton and Browne (2022)	Q	822
CYMCLGYPZZKOOI-UHFFFAOYSA-N	7.5×10^{-6}		Alton and Browne (2022)	Q	823
D4EtherOrganonitrate	2.4×10^{-3}		Alton and Browne (2022)	Q	821
$C_8H_{23}NO_8Si_4$	3.8×10^{-4}		Alton and Browne (2022)	Q	822
XHFUWVKWVPBCDO-UHFFFAOYSA-N	1.6×10^{-5}		Alton and Browne (2022)	Q	823
(3-aminopropyl)triethoxysilane $C_9H_{23}NO_3Si$ [919-30-2] WYTZZXDRDKSJID-UHFFFAOYSA-N	1.2×10^{2}		Ebert et al. (2023)	?	319
D5Organonitrate	8.7×10^{-5}		Alton and Browne (2022)	Q	821
$C_{10}H_{29}NO_8Si_5$	4.9×10^{-5}		Alton and Browne (2022)	Q	822
KWHVDACCYNMOAR-UHFFFAOYSA-N	1.2×10^{-5}		Alton and Browne (2022)	Q	823
D5EtherOrganonitrate	1.1×10^{-3}		Alton and Browne (2022)	Q	821
$C_{10}H_{29}NO_9Si_5$	5.7×10^{-4}		Alton and Browne (2022)	Q	822
BQINUVFPZWRRBW-UHFFFAOYSA-N	2.9×10^{-5}		Alton and Browne (2022)	Q	823
silafluofen $C_{25}H_{29}FO_2Si$ [105024-66-6] HPYNBECUCCGGPA-UHFFFAOYSA-N	4.0×10^{-1}		Ebert et al. (2023)	?	319
flusilazole	2.7×10^{1}		Barcelo and Hennion (1997)	X	569
$C_{16}H_{15}F_2N_3Si$	4.4×10^{2}		Goodarzi et al. (2010)	Q	570, 573
[85509-19-9] FQKUGOMFVDPBIZ-UHFFFAOYSA-N					
simeconazole $C_{14}H_{20}FN_3OSi$ [149508-90-7] YABFPHSQTSFWQB-UHFFFAOYSA-N	4.0×10^{3}		Ebert et al. (2023)	?	319
dichloromethylsilane CH_4Cl_2Si (methyldichlorosilane) [75-54-7] NWKBSEBOBPHMKL-UHFFFAOYSA-N	7.6×10^{-4}		HSDB (2015)	Q	100

Table A11.3: Silicon (Si) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
etacelasil $C_{11}H_{25}O_6ClSi$ [37894-46-5] SLZWEMYSYKOWCG-UHFFFAOYSA-N	2.9×10^3		MacBean (2012a)	?	

A11.4 Calcium (Ca)

Table A11.4: Calcium (Ca)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
prohexadione-calcium $C_{20}H_{22}O_{10}Ca$ [127277-53-6] VQIYODJWCVPJRC-UHFFFAOYSA-N	5.2×10^4		Maniere et al. (2011)	?	242, 166

A11.5 Zinc (Zn)

Table A11.5: Zinc (Zn)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
zineb	2.7×10^3		Mackay et al. (2006d)	V	
$C_4H_6N_2S_4Zn$	$>3.7\times10^3$		MacBean (2012b)	X	352
[12122-67-7]	$>1.9\times10^2$		Maniere et al. (2011)	?	12, 166
AMHNZOICSMBGDH-UHFFFAOYSA-L					
ziram	1.6×10^4		HSDB (2015)	V	
$C_6H_{12}N_2S_4Zn$	2.1×10^5		Mackay et al. (2006d)	V	
[137-30-4]	1.8×10^2		Maniere et al. (2011)	?	166
DUBNHZYBDBBJHD-UHFFFAOYSA-L					
mancozeb	1.6×10^1		Maniere et al. (2011)	?	12, 166
$C_8H_{12}MnN_4S_8Zn$					
[8018-01-7]					
CHNQZRKUZPNOOH-UHFFFAOYSA-J					

A11.6 Arsenic (Sn)

Table A11.6: Arsenic (Sn)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methylarsine CH_5As [593-52-2] IDDBICIFODFKQO-UHFFFAOYSA-N	9.0×10^{-6}		Ebert et al. (2023)	?	319
ethylarsine C_2H_7As [593-59-9] OSAGMAAQMRQLLW-UHFFFAOYSA-N	1.5×10^{-5}		Ebert et al. (2023)	?	317
diethyl arsine $C_4H_{11}As$ [692-42-2] JZCIYTSNUPIOMK-UHFFFAOYSA-N	2.2×10^{-5}		HSDB (2015)	Q	100
phenylarsine oxide C_6H_5AsO [637-03-6] BQVCCPGCDUSGOE-UHFFFAOYSA-N	9.0×10^{-1}		Bartelt-Hunt et al. (2008)	?	21
diphenylarsanylformonitrile $C_{13}H_{10}AsN$ [23525-22-6] BDHNJKLLVSRGDK-UHFFFAOYSA-N	1.1×10^{3}		Ebert et al. (2023)	?	319
dichloro(methyl)arsane CH_3AsCl_2 [593-89-5] VXRMBBLRHSRVDK-UHFFFAOYSA-N	5.1×10^{-3}		Ebert et al. (2023)	?	319
lewisite $C_2H_2AsCl_3$ [541-25-3] GIKLTQKNOXNBNY-OWOJBTEDSA-N	4.5×10^{-2} 3.1×10^{-2} 5.2×10^{-3} 3.7×10^{-2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Bartelt-Hunt et al. (2008)	V V Q ?	187 21
diphenylchloroarsine $C_{12}H_{10}AsCl$ [712-48-1] YHHKGKCOLGRKKB-UHFFFAOYSA-N	6.1×10^{1}		Ebert et al. (2023)	?	319
lewisite oxide C_2H_2AsClO [3088-37-7] MVCVAGFCWDFQQX-OWOJBTEDSA-N	5.2×10^{-3}		Bartelt-Hunt et al. (2008)	?	21

Table A11.6: Arsenic (Sn) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
phenyldichloroarsine $C_6H_5AsCl_2$ [696-28-6] UDHDFEGCOJAVRE-UHFFFAOYSA-N	3.3×10^{-1}		HSDB (2015)	Q	100
adamsite $C_{12}H_9AsClN$ [578-94-9] PBNSPNYJYOYWTA-UHFFFAOYSA-N	3.0×10^{2}		HSDB (2015)	Q	100

A11.7 Selenium (Se)

Table A11.7: Selenium (Se)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dimethyl selenide C_2H_6Se [593-79-3] RVIXKDRPFPUUOO-UHFFFAOYSA-N	1.2×10^{-2} 4.3×10^{-3} 5.7×10^{-3}		Keshavarz et al. (2022) Duchowicz et al. (2020) Duchowicz et al. (2020)	Q Q ?	 186, 21
dimethyl diselenide $C_2H_6Se_2$ [7101-31-7] VLXBWPOEOIIREY-UHFFFAOYSA-N	1.4×10^{-3}		Ebert et al. (2023)	?	319
2-amino-4-(methylselenyl)butyric acid $C_5H_{11}NO_2Se$ (selenium methionine) [1464-42-2] RJFAYQIBOAGBLC-UHFFFAOYSA-N	2.9×10^{5}		HSDB (2015)	Q	100

A11.8 Tin (Sn)

Table A11.8: Tin (Sn)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tetramethylstannane $C_4H_{12}Sn$ (tetramethyltin) [594-27-4] VXKWYPOMXBVZSJ-UHFFFAOYSA-N	9.4×10^{-6} 9.7×10^{-6} 1.2×10^{-5}	3800	Abraham and Nasehzadeh (1981) Abraham et al. (1990) Abraham (1979)	M ? ?	
tetraethylstannane $C_8H_{20}Sn$ (tetraethyltin) [597-64-8] RWWNQEOPUOCKGR-UHFFFAOYSA-N	1.6×10^{-5} 6.1×10^{-6} 5.7×10^{-6} 1.1×10^{-5}	6100	HSDB (2015) Abraham et al. (1990) Abraham and Nasehzadeh (1981) Abraham (1979)	Q ? ? ?	100 824
tetrabutylstannane $C_{16}H_{36}Sn$ (tetra-butyl tin) [1461-25-2] AFCAKJKUYFLYFK-UHFFFAOYSA-N	1.6×10^{-6}		HSDB (2015)	Q	100
triphenyltin hydroxide $C_{18}H_{16}OSn$ [76-87-9] BFWMWWXRWVJXSE-UHFFFAOYSA-M	2.3×10^{1} 3.8×10^{-1}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187
hexabutyldistannoxane $C_{24}H_{54}OSn_2$ (bis(tributyltin)oxide) [56-35-9] APQHKWPGGHMYKJ-UHFFFAOYSA-N	7.6×10^{1}		HSDB (2015)	V	
hexakis(2-methyl-2-phenylpropyl)distannoxane $C_{60}H_{78}OSn_2$ (fenbutatin oxide) [13356-08-6] HOXINJBQVZWYGZ-UHFFFAOYSA-N	4.9×10^{3}		HSDB (2015)	V	
fentin acetate $C_{20}H_{18}O_2Sn$ [900-95-8] WDQNIWFZKXZFAY-UHFFFAOYSA-M	2.0×10^{3}		Ebert et al. (2023)	?	367
1-(tricyclohexylstannyl)1H-1,2,4-triazole $C_{20}H_{35}N_3Sn$ (azocyclotin) [41083-11-8] ONHBDDJJTDTLIR-UHFFFAOYSA-N	4.6×10^{6} 4.6×10^{6} 1.2		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	187

A11.9 Mercury (Hg)

Table A11.9: Mercury (Hg)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dimethylmercury	1.3×10^{-3}	2700	Talmi and Mesmer (1975)	M	
C_2H_6Hg	2.1×10^{-3}		Abraham et al. (2008)	C	
[593-74-8]	1.3×10^{-3}	2700	WHO (1990)	C	
ATZBPOVXVPIOMR-UHFFFAOYSA-N	1.0×10^{-3}	3000	Abraham et al. (2008)	Q	219
	1.5×10^{-3}		Schroeder and Munthe (1998)	?	21
	1.3×10^{-3}	2700	Schroeder and Munthe (1998)	?	21
	3.1×10^{-3}		Iverfeldt and Persson (1985)	?	220
diethylmercury $C_4H_{10}Hg$ [627-44-1] SPIUPAOJDZNUJH-UHFFFAOYSA-N	1.0×10^{-3}	3800	Abraham et al. (2008)	Q	219
dipropylmercury $C_6H_{14}Hg$ [628-85-3] UZTYYBPPVOXULF-UHFFFAOYSA-N	5.6×10^{-4}	4600	Abraham et al. (2008)	Q	219
diisopropylmercury $C_6H_{14}Hg$ [1071-39-2] UVUGOJQWNVFTRT-UHFFFAOYSA-N	3.9×10^{-4}	4600	Abraham et al. (2008)	Q	219
dibutylmercury $C_8H_{18}Hg$ [629-35-6] CCYKQVBIPYDCKS-UHFFFAOYSA-N	2.9×10^{-4}	5400	Abraham et al. (2008)	Q	219
diphenylmercury $C_{12}H_{10}Hg$ [587-85-9] HWMTUNCVVYPZHZ-UHFFFAOYSA-N	2.8×10^{2}	8800	Abraham et al. (2008)	Q	219
hydroxymethylmercury	9.8×10^{2}	7700	Iverfeldt and Persson (1985)	M	
CH_3HgOH	1.5×10^{3}		Shon et al. (2005)	?	825
[1184-57-2]					
KRZWEBVPFGCYMY-UHFFFAOYSA-M					
phenyl mercuric ethanoate $C_8H_8HgO_2$ [62-38-4] XEBWQGVWTUSTLN-UHFFFAOYSA-M	1.5×10^{4}		Suntio et al. (1988)	V	12
(3-cyanoguanidino)methylmercury $C_3H_6N_4Hg$ (methylmercuric dicyanamide) [502-39-6] JVJUWCMBRUMDDQ-UHFFFAOYSA-N	7.0×10^{4}		HSDB (2015)	Q	100

Table A11.9: Mercury (Hg) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chloromethylmercury	2.2×10^{1}	1800	Iverfeldt and Lindqvist (1982)	M	33, 826
CH_3HgCl	1.5×10^{1}		Talmi and Mesmer (1975)	M	88
[115-09-3]	2.0×10^{1}	4100	WHO (1990)	C	33
BABMCXWQNSQAOC-UHFFFAOYSA-M		5300	Abraham et al. (2008)	Q	215
	2.6×10^{1}		Schroeder and Munthe (1998)	?	81, 21
	1.5×10^{1}		Iverfeldt and Persson (1985)	?	220
chloroethylmercury	1.5×10^{1}	5600	Abraham et al. (2008)	Q	219
C_2H_5HgCl					
[107-27-7]					
QWUGXIXRFGEYBD-UHFFFAOYSA-M					
chloropropylmercury	1.2×10^{1}	5900	Abraham et al. (2008)	Q	219
C_3H_7HgCl					
[2440-40-6]					
ZLAYJSKLDWSALK-UHFFFAOYSA-M					
chloroisopropylmercury	9.9	6000	Abraham et al. (2008)	Q	219
C_3H_7HgCl					
[30615-19-1]					
YOKZNQICWABELX-UHFFFAOYSA-M					
chlorobutylmercury	8.8	6300	Abraham et al. (2008)	Q	219
C_4H_9HgCl					
[543-63-5]					
OKPMTXZRMGMMOO-UHFFFAOYSA-M					
chloropentylmercury	7.0	6700	Abraham et al. (2008)	Q	219
$C_5H_{11}HgCl$					
[544-15-0]					
UHFZINPMKCNPQL-UHFFFAOYSA-M					
chlorophenylmercury	3.8×10^{2}		Abraham et al. (2008)	V	
C_6H_5HgCl	9.2×10^{2}	7400	Abraham et al. (2008)	Q	219
[100-56-1]					
AWGTVRDHKJQFAX-UHFFFAOYSA-M					
2-methoxyethylmercury chloride	3.9×10^{3}	8600	Abraham et al. (2008)	Q	219
$CH_3OC_2H_4HgCl$					
(aretan)					
[123-88-6]					
VJTAZCKMHINUKO-UHFFFAOYSA-M					
bromomethylmercury		4800	Abraham et al. (2008)	Q	215
CH_3HgBr	3.7		Iverfeldt and Persson (1985)	?	220
[506-83-2]					
ZDHHIJSLJCLMPX-UHFFFAOYSA-M					

Table A11.9: Mercury (Hg) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bromoethylmercury C_2H_5HgBr [107-26-6] UREACWLAXSOUKG-UHFFFAOYSA-M	3.0	5200	Abraham et al. (2008)	Q	219
bromophenylmercury C_6H_5HgBr [1192-89-8] PUPHNPSAIJQNEE-UHFFFAOYSA-M	1.8×10^{2}	6900	Abraham et al. (2008)	Q	219
iodomethylmercury CH_3HgI [143-36-2] JVDIOYBHEYUIBM-UHFFFAOYSA-M	2.0 5.8×10^{-1}	4800	Abraham et al. (2008) Iverfeldt and Persson (1985)	Q ?	219 220
iodoethylmercury C_2H_5HgI [2440-42-8] BYIGJUQTUPMNMF-UHFFFAOYSA-M	2.5	5200	Abraham et al. (2008)	Q	219
iodophenylmercury C_6H_5HgI [823-04-1] BISBXZWWFIOZSX-UHFFFAOYSA-M	9.0×10^{1}	6700	Abraham et al. (2008)	Q	219

A11.10 Lead (Pb)

Table A11.10: Lead (Pb)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tetramethyl lead $C_4H_{12}Pb$ [75-74-1] XOOGZRUBTYCLHG-UHFFFAOYSA-N	1.6×10^{-5}		HSDB (2015)	V	
ethyltrimethylplumbane $C_5H_{14}Pb$ [1762-26-1] KHQJREYATBQBHY-UHFFFAOYSA-N	2.8×10^{-5}		HSDB (2015)	Q	100
diethyldimethylplumbane $C_6H_{16}Pb$ (diethyldimethyl lead) [1762-27-2] OLOAJSHVLXNSQV-UHFFFAOYSA-N	2.1×10^{-5}		HSDB (2015)	Q	100
triethylmethylplumbane $C_7H_{18}Pb$ (methyltriethyl lead) [1762-28-3] KGFRUGHBHNUHOS-UHFFFAOYSA-N	1.6×10^{-5}		HSDB (2015)	Q	100
tetraethyl lead $C_8H_{20}Pb$ [78-00-2] MRMOZBOQVYRSEM-UHFFFAOYSA-N	1.3×10^{-5} 1.3×10^{-5}	6400	Feldhake and Stevens (1963) Abraham (1979)	M ?	
trimethyl lead chloride C_3H_9ClPb [1520-78-1] HPQRSQFZILKRDH-UHFFFAOYSA-M	2.5		Ebert et al. (2023)	?	317
triethyl lead chloride $C_6H_{15}ClPb$ [1067-14-7] UQWYUMLFPUILRT-UHFFFAOYSA-M	2.1×10^{5} 1.1×10^{-3}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	187

Appendix: Notes

1) A detailed temperature dependence with more than one parameter is available in the original publication. Here, only the temperature dependence at 298.15 K according to the van 't Hoff equation is presented.

2) Clever et al. (2014) recommend the data from Rettich et al. (2000).

3) The vapor pressure for water from Wagner and Pruss (1993) was used to calculate H_s.

4) The data from Millero et al. (2002a) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-130.91491 + 6700.12242/T + 17.04684 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

5) Almost the same data were also published in Millero et al. (2002b).

6) The data from Millero et al. (2002b) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-118.73105 + 6163.97787/T + 15.22401 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

7) Almost the same data were also published in Millero et al. (2002a).

8) The data from Rettich et al. (2000) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-179.13831 + 8707.17767/T + 24.33473 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

9) The data from Sherwood et al. (1991) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-197.67462 + 9515.09306/T + 27.11204 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

10) The data from Rettich et al. (1981) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-178.21340 + 8672.23354/T + 24.19307 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

11) Measured at high temperature and extrapolated to $T^{\ominus} = 298.15$ K.

12) Value at $T = 293$ K.

13) Value at $T = 273$ K.

14) Value at $T = 310$ K.

15) The data from Murray and Riley (1969) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-180.22078 + 8760.50130/T + 24.49289 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

16) The data from Shoor et al. (1969) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-91.44799 + 4548.67245/T + 11.38821 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

17) The data from Carpenter (1966) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-130.04464 + 6687.45227/T + 16.90114 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

18) The data from Morrison and Billett (1952) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-167.89288 + 8254.02144/T + 22.62741 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

19) The data from Winkler (1891b) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-155.30315 + 7638.78869/T + 20.77945 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

20) Calculated using machine learning matrix completion methods (MCMs).

21) Several references are given in the list of Henry's law constants but not assigned to specific species.

22) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-161.84252 + 7966.66767/T + 21.73409 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

23) The partial pressure of water vapor (needed to convert some Henry's law constants) was calculated using the formula given by Buck (1981). The quantities A and α from Dean and Lange (1999) were assumed to be identical.

24) Value at "room temperature".

25) Clever et al. (2014) recommend the data from Battino (1981).

26) Battino (1981) concludes that ozone aqueous chemistry needs further clarification. Data from Roth and Sullivan (1981) are recommended, in spite of limitations and assumptions of the data.

27) Roth and Sullivan (1981) found that H_s depends on the concentration of OH^-.

28) Value at $T = 291$ K.

29) Value given here as quoted by Durham et al. (1981).

30) Lide and Frederikse (1995) present an unusually low value for the Henry solubility of ozone. They refer to Battino (1981) as the source, but the quoted value cannot be found there.

31) Parker (1992) assumes that the free energy of solvation of atomic hydrogen is equal to that of He because of a similar van der Waals radius.

32) Roduner and Bartels (1992) say that the free energy of solvation $\Delta G^{\mathrm{H}}_{\mathrm{solv}}$ (and therefore Henry's law constant) of atomic hydrogen is approximated well by that of molecular hydrogen. However, they apparently do not give a value for $\Delta G^{\mathrm{H}}_{\mathrm{solv}}$.

33) Fitting the temperature dependence $\mathrm{d}\ln H/\mathrm{d}(1/T)$ produced a low correlation coefficient ($r^2 < 0.9$). The data should be treated with caution.

34) Data digitized from Figs. 2 and 3 in Schmidt (1979).

35) The data from Gordon et al. (1977) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-158.95051 + 6959.76267/T + 21.73478 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

36) The data from Crozier and Yamamoto (1974) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-129.44163 + 5676.58091/T + 17.31002 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

37) The data presented for hydrogen in Table II of Shoor et al. (1969) appear to be incorrect and are not reproduced here.

38) Value at $T = 303$ K.

39) The data from Morrison and Billett (1952) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-94.36490 + 4110.23880/T + 12.07743 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

40) The data from Braun (1900) were fitted to the three-parameter equation: $H_s^{cp} = \exp(171.59451 - 6856.02728/T - 28.14739 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

41) The data from Winkler (1891a) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-103.47250 + 4506.63123/T + 13.44160 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

42) Fitting the temperature dependence $\mathrm{d}\ln H/\mathrm{d}(1/T)$ produced a very low correlation coefficient ($r^2 < 0.5$). The data should be treated with caution.

43) The paper by Bunsen (1855a) was written in German. English versions with the same data were published by Bunsen (1855b) and Bunsen (1855c).

44) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-98.78036 + 4298.15060/T + 12.74131 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

45) Young (1981a) recommend the data from Muccitelli and Wen (1978).

46) The data from Muccitelli and Wen (1978) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-103.11330 + 4676.56978/T + 13.28348 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

47) The free energy of solution was calculated based on electrochemical reduction potentials and related free energies.

48) Calculated from correlation between the polarizabilities and solubilities of stable gases. The temperature dependence is an estimate of the upper limit.

49) Jacob (1986) assumed the temperature dependence to be the same as for water.

50) In the abstract, Schwartz (1984) gives a range of 9.9 mol m^{-3} Pa^{-1} $< H_s^{cp} < 3.0\times10^{1}$ mol m^{-3} Pa^{-1}. The mean value of this range (2.0×10^{1} mol m^{-3} Pa^{-1}) has been used by Lelieveld and Crutzen (1991), Pandis and Seinfeld (1989), and Jacob (1986).

51) The value of $H_s^{\ominus}$ was taken from Schwartz (1984).

52) Erratum for page 264 of Fogg and Sangster (2003): the second value from their Ref. [10] refers to 291.15 K, not 281.15 K.

53) This value is a correction of the solubility published by Lind and Kok (1986).

54) This value was measured at low pH. It is superseded by a later publication of the same group (Lind and Kok, 1994).

55) Pandis and Seinfeld (1989) cite an incorrect value from Lind and Kok (1986); see erratum by Lind and Kok (1994).

56) The data from Rettich et al. (1984) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-187.67954 + 8903.42524/T + 25.60079 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

57) The data from Murray et al. (1969) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-174.95275 + 8370.22025/T + 23.67878 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

58) The data from Morrison and Billett (1952) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-193.68175 + 9249.63150/T + 26.45117 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

59) Value at $T = 311$ K.

60) The data from Braun (1900) were fitted to the three-parameter equation: $H_s^{cp} = \exp(291.66324 - 11637.66767/T - 46.44134 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

61) The data from Winkler (1891b) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-164.15156 + 7906.86704/T + 22.05399 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

62) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-163.64571 + 7887.30480/T + 21.97696 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

63) Tsuji et al. (1990) provide effective Henry's law constants at several pH values. Here, only the value at pH = 5.8 is shown for the (acidic) S compounds and the value at pH = 8.6 for the alkaline N compounds.

64) Value given here as quoted by Betterton (1992).

65) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(206.08500 - 7165.18642/T - 32.18383 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

66) Bone et al. (1983) give Carter et al. (1968) as the source. However, no data were found in that reference.

67) There is a typo in Sander et al. (2011): the value for A should be -10.19 not 10.19.

68) Modarresi et al. (2007) use different descriptors for their calculations. They conclude that a genetic algorithm/radial basis function network (GA/RBFN) is the best QSPR model. Only these results are shown here.

69) Incorrect data are given by Burkholder et al. (2019) for HN_3. The correct parameter for the temperature dependence is $A = -10.19$ (Robert E. Huie, personal communication, 2021).

70) Incorrect data are given by Burkholder et al. (2015) for HN_3. The correct parameter for the temperature dependence is $A = -10.19$ (Robert E. Huie, personal communication, 2021).

71) Solubility in sea water.

72) The data from Weiss and Price (1980) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-180.63611 + 9824.20147/T + 24.46112\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

73) Value at $T = 296\,\mathrm{K}$.

74) The data from Roth (1897) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-125.17909 + 7706.80638/T + 15.96486\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

75) Value given here as quoted by Gabel and Schultz (1973).

76) Value given here as quoted by Sy and Hasbrouck (1964).

77) The H298 and A, B, C data listed in Table 5.4 of Sander et al. (2011) are inconsistent, with 94 % difference.

78) The H298 and A, B, C data listed in Table 5.4 of Sander et al. (2006) are inconsistent, with 94 % difference.

79) A minus sign is missing in the fitting parameter presented by Young (1981b). It should be -62.8086, not 62.8086.

80) Value at $T = 297\,\mathrm{K}$.

81) Value at $T = 288\,\mathrm{K}$.

82) The data from Winkler (1901) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-184.00012 + 8924.34832/T + 25.13228\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

83) The data from Loomis (1928) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-223.88313 + 10620.37030/T + 31.13453\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

84) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-160.19223 + 7888.02642/T + 21.56401\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

85) Incorrect data are given by Burkholder et al. (2019) for NO. The correct parameters for the temperature dependence are $A = -163.86$, $B = 8234$, $C = 22.816$ (Robert E. Huie, personal communication, 2021).

86) Incorrect data are given by Burkholder et al. (2015) for NO. The correct parameters for the temperature dependence are $A = -163.86$, $B = 8234$, $C = 22.816$ (Robert E. Huie, personal communication, 2021).

87) The fitting parameters A, B, C, and D in Table I of Wilhelm et al. (1977) do not reproduce the data in their Table III.

88) Value at $T = 295\,\mathrm{K}$.

89) Pandis and Seinfeld (1989) refer to Schwartz (1984) as the source, but the quoted value cannot be found there.

90) Value obtained by estimating the diffusion coefficient for NO_3 to be $D = 1.0\times10^{-5}\,\mathrm{cm^2/s}$.

91) Jacob (1986) assumes that NO_3 has the same Henry's law constant as HNO_3.

92) Seinfeld and Pandis (1997) probably refer to the incorrect value given by Pandis and Seinfeld (1989).

93) Calculated from the solvation free energy.

94) Calculated from the solvation free energy.

95) Calculated from the solvation free energy.

96) This value was extrapolated from data at $T = 230\,\mathrm{K}$ and $T = 273\,\mathrm{K}$.

97) Robinson et al. (1997) applied an empirical correlation between Henry's law solubilities and boiling points from Schwartz and White (1981).

98) Estimate based on the relation between boiling points and Henry's law constants for other nitrogen oxides from Schwartz and White (1981).

99) Fast, irreversible hydrolysis is assumed, which is equivalent to an infinite effective Henry's law constant.

100) Calculated based on the method by Meylan and Howard (1991).

101) Lelieveld and Crutzen (1991) assume the temperature dependence to be the same as for $a(H^+)a(NO_3^-)/p(HNO_3)$ in Schwartz and White (1981).

102) $H_s' = 2.6\times10^7\times\exp\left(8700\,\mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

103) $H_s' = 2.4\times10^7\times\exp\left(8700\,\mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

104) Pandis and Seinfeld (1989) refer to Schwartz (1984) as the source, but it is probably from Schwartz and White (1981).

105) The value is incorrect. See erratum by Brimblecombe and Clegg (1989).

106) Möller and Mauersberger (1992) assumed the solubility of HNO_4 to be comparable to that of HNO_3.

107) $H'_s = 9.4 \times 10^1 \times \exp\left(7400\,\mathrm{K}\left(\frac{1}{T} - \frac{1}{T^\ominus}\right)\right) \frac{\mathrm{mol}^2}{\mathrm{m}^6\,\mathrm{Pa}}$

108) The data from Dean et al. (1973) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-164.52717 + 8214.77776/T + 21.97482\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

109) The data from Ashton et al. (1968) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-279.21972 + 13536.60588/T + 38.97386\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

110) The data from Dean et al. (1973) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-318.29953 + 15733.17858/T + 44.55320\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

111) The value presented here appears to be the total solubility of chlorine (i.e., the sum of Cl_2 and HOCl) at a partial pressure of $p(Cl_2) = 101325\,\mathrm{Pa}$. This is different from Henry's law constant, which is defined at extrapolation to infinite dilution.

112) Young (1983) recommends values calculated from Table 1 of Adams and Edmonds (1937). Thus, the data refer to effective values that take into account the hydrolysis in the aqueous phase:

$$H_{s,\mathrm{eff}} = ([Cl_2] + [HOCl])/p(Cl_2).$$

In addition, the values apply to a partial pressure of $p(Cl_2) = 101325\,\mathrm{Pa}$, and not to infinite dilution.

113) The same experimental data were also published by Whitney and Vivian (1941b).

114) The data from Yakovkin (1900) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-122.31264 + 7690.40834/T + 15.63947\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

115) Leaist (1986) converted the total solubility of chlorine in pure water from Adams and Edmonds (1937) to an intrinsic Henry's law constant.

116) Adams and Edmonds (1937) re-analyzed the data from Yakovkin (1900) and Arkadiev (1918), considering deviations from the perfect gas law. They calculated the total solubility of chlorine (i.e., the sum of Cl_2 and HOCl) at several partial pressures of Cl_2. This is different from Henry's law constant, which is defined at extrapolation to infinite dilution.

117) Arkadiev (1918) re-analyzed the measurements of Yakovkin (1900). In addition to the data between 15 °C and 83.4 °C, he also analyzed the experimental results at 0 °C and obtained a dimensionless Henry solubility of $H_s^{cc} = 4.115$ at that temperature.

118) The value of ΔH° listed in Table 2 of Bartlett and Margerum (1999) is incorrect. The correct value can be found in the text on page 3411.

119) Wilhelm et al. (1977) present a fitting function for Cl_2 based on four papers which are cited in the footnotes of Table I. However, Bunsen (1855b) and Bunsen (1855c) do not contain any data for Cl_2, and the data from Whitney and Vivian (1941a) and Whitney and Vivian (1941b) are inconsistent with the fitting function.

120) Calculated from the free energy of solution by Schwarz and Dodson (1984).

121) $H'_s = 2.0 \times 10^7\ \frac{\mathrm{mol}^2}{\mathrm{m}^6\,\mathrm{Pa}}$

122) $H'_s = 2.0 \times 10^7 \times \exp\left(9000\,\mathrm{K}\left(\frac{1}{T} - \frac{1}{T^\ominus}\right)\right) \frac{\mathrm{mol}^2}{\mathrm{m}^6\,\mathrm{Pa}}$

123) $H'_s = 2.0 \times 10^7 \times \exp\left(9000\,\mathrm{K}\left(\frac{1}{T} - \frac{1}{T^\ominus}\right)\right) \frac{\mathrm{mol}^2}{\mathrm{m}^6\,\mathrm{Pa}}$

124) $H'_s = 2.0 \times 10^7 \times \exp\left(9000\,\mathrm{K}\left(\frac{1}{T} - \frac{1}{T^\ominus}\right)\right) \frac{\mathrm{mol}^2}{\mathrm{m}^6\,\mathrm{Pa}}$

125) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(9.16427 + 45.13997/T - 1.92853\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

126) Pandis and Seinfeld (1989) refer to Marsh and McElroy (1985) as the source, but the quoted value cannot be found there.

127) This value was extrapolated from data at $T = 215\,\mathrm{K}$ and $T = 263\,\mathrm{K}$.

128) Value at pH = 6.5.

129) Value at $T = 200\,\mathrm{K}$.

130) Secoy and Cady (1941) measured the gas–aqueous equilibrium constant $p(Cl_2O)/c(HOCl)^2$ but not the intrinsic Henry's law constant of Cl_2O.

131) Ourisson and Kastner (1939) measured the gas–aqueous equilibrium constant $p(Cl_2O)/c(HOCl)^2$ but not the intrinsic Henry's law constant of Cl_2O.

132) The data from this work were fitted to the three-parameter equation: $H_s^{cp} = \exp(1680.49677 - 69933.08019/T - 254.37188\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

133) The gas–aqueous equilibrium constant $p(Cl_2O)/c(HOCl)^2$ was combined with the temperature-dependent aqueous-phase hydration constant $c(HOCl)^2/c(Cl_2O)$ from Roth (1929) in order to calculate the intrinsic Henry's law constant of Cl_2O.

134) Data for the equilibrium between gaseous Cl_2O and aqueous HOCl were taken from Secoy and Cady (1941).

135) Data for the equilibrium between gaseous Cl_2O and aqueous HOCl were taken from Ourisson and Kastner (1939).

136) Value at $T = 277\,\mathrm{K}$.

137) The recommended value from Wilhelm et al. (1977) appears to be dubious as it refers to Secoy and Cady (1941), who do not provide a value for the intrinsic Henry's law constant of Cl_2O.

138) Young (1983) cites data from Secoy and Cady (1941). However, that paper only describes the equilibrium between gas-phase Cl_2O and aqueous-phase HOCl. A Henry's law constant of Cl_2O is not provided. In addition, the values given by Young (1983) are not extrapolated to infinite dilution but to 1 atm partial pressure of Cl_2O. It is not explained how the nonlinear pressure dependence was extrapolated to 1 atm.

139) Wilhelm et al. (1977) cite Secoy and Cady (1941) as the source for their value. However, that paper only describes the equilibrium between gas-phase Cl_2O and aqueous-phase HOCl. A Henry's law constant of Cl_2O is not provided.

140) Even though Haller and Northgraves (1955) have been cited several times as the source of the ClO_2 solubility data, they did not perform any measurements. They took the data from the 1952 edition of the Kirk-Othmer Encyclopedia of Chemical Technology which apparently reproduced data from Holst (1944).

141) Derived as a fitting parameter used in numerical modeling.

142) Robinson et al. (1997) assumed that the entropy of vaporization is the same for HOCl and $ClNO_3$ according to Trouton's rule. On their page 3592, they mention a value of $7\,\mathrm{M\,atm^{-1}}$ at 250 K. However, checking their Fig. 9 and applying the temperature-dependence equation from their Table 3, it seems that the value of $7\,\mathrm{M\,atm^{-1}}$ refers to 298 K, not 250 K.

143) Dubik et al. (1987) measured the solubility in concentrated salt solutions (natural brines).

144) Value given here as quoted by McCoy et al. (1990).

145) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-148.75612 + 9709.79389/T + 19.53402\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

146) $H_s' = 8.2\times10^9 \times \exp\left(10000\,\mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

147) $H_s' = 1.3\times10^{10} \times \exp\left(10000\,\mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

148) $H_s' = 7.0\times10^9 \times \exp\left(10000\,\mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

149) Chameides and Stelson (1992) give a value of $H_s' = 7.1\times10^9 \times \exp\left(6100\,\mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$. They refer to Jacob (1986) and Chameides (1984) as the source, but this value cannot be found there.

150) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-60.28318 + 2830.41867/T + 8.66642\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

151) The value is from Table 1 of the paper. However, *J. Geophys. Res.* forgot to print the tables, and I received them directly from the author.

152) The value presented for HOBr is incorrect. A corrected version was later published by Burkholder et al. (2019).

153) Fickert (1998) extracted a value from wetted-wall flow tube experiments. However, it was later discovered that under the experimental conditions no evaluation of H_s is possible (John Crowley, personal communication, 1999).

154) Value at $T = 275\,\mathrm{K}$.

155) Value at $T = 290\,\mathrm{K}$.

156) Calculated using data from Wagman et al. (1982) and the aqueous-phase equilibrium $Cl_2 + Br_2 \rightleftharpoons 2\,BrCl$ from Wang et al. (1994).

157) Thompson and Zafiriou (1983) quote a paper as the source that gives only the solubility but not the Henry's law constant.

158) Calculated from the free energy of solution by Schwarz and Bielski (1986).

159) $H_s' = 2.5\times10^{10} \times \exp\left(9800\,\mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

160) $H_s' = 2.1\times10^{10} \times \exp\left(9800\,\mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

161) Saiz-Lopez et al. (2014) refer to Saiz-Lopez et al. (2008) as the source, but the quoted value cannot be found there.

162) It is unclear to which isomer the value of the Henry's law constant refers to.

163) Assumed to be infinity by analogy with INO_3.

164) Thompson and Zafiriou (1983) assume that H_s^{cp}(HOI) is between $4.4\times10^{-1}\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$ and $4.4\times10^{2}\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$.

165) Badia et al. (2019) assume that INO_2 has the same Henry's law constant as $BrNO_2$.

166) Data taken from the AGRITOX database file agritox-20210608.zip.

167) Fogg and Young (1988) provide two different fitting functions: one for $T < 283.2$ K and one for $T > 283.2$ K. At $T = 283.2$ K, the functions have different values and different slopes. Here, only the function that is valid at $T^{\ominus}$ is used.

168) The data from Clarke and Glew (1971) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-133.37135 + 7422.07576/T + 17.82903 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

169) The data from Schoenfeld (1855) were fitted to the three-parameter equation: $H_s^{cp} = \exp(98.96644 - 3021.28876/T - 16.78233 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

170) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-122.57010 + 6962.28299/T + 16.20245 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

171) The parameter fit for the temperature dependence is incorrect. A corrected version was later presented by Iliuta and Larachi (2007).

172) The data from Clarke and Glew (1971) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-152.96053 + 8324.82999/T + 20.73129 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

173) Obtained with D_2O as solvent.

174) Value at $T = 353$ K.

175) The data from Schoenfeld (1855) were fitted to the three-parameter equation: $H_s^{cp} = \exp(265.79241 - 9131.99684/T - 42.01987 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

176) Value given here as quoted by Rodríguez-Sevilla et al. (2002).

177) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(153.05871 - 4328.05304/T - 25.05397 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

178) Marti et al. (1997) give partial pressures of H_2SO_4 over a concentrated solution (e.g., 2.6×10^{-9} Pa for 54.1 wt % at 298 K). Extrapolating this to dilute solutions can only be considered an order-of-magnitude approximation for H_s.

179) Ayers et al. (1980) give partial pressures of H_2SO_4 over concentrated solutions at high temperatures. Extrapolating this to dilute solutions can only be considered an order-of-magnitude approximation for H_s.

180) Gmitro and Vermeulen (1964) give partial pressures of H_2SO_4 over a concentrated solution (e.g., 10^{-7} mmHg for 70 wt % at 298 K). Extrapolating this to dilute solutions can only be considered an order-of-magnitude approximation for H_s.

181) Clegg et al. (1998) estimate a Henry's law constant of 5×10^{11} atm^{-1} at 303.15 K for the reaction $H_2SO_4(g) \rightleftharpoons 2\ H^+(aq) + SO_4^{2-}(aq)$ but do not give a definition for it. Probably it is defined as $x^2(H^+) \times x(SO_4^{2-})/p(H_2SO_4)$, where x is the aqueous-phase mixing ratio.

182) The data from Bullister et al. (2002) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-281.50843 + 14256.43847/T + 38.73689 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

183) The data presented for SF6 in Table II of Shoor et al. (1969) appear to be incorrect and are not reproduced here.

184) The data from Ashton et al. (1968) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-431.90650 + 20715.81650/T + 61.33841 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

185) Value from the validation set for checking whether the model is satisfactory for compounds that are absent from the training set.

186) Experimental value, extracted from HENRYWIN.

187) Estimation based on the quotient between vapor pressure and water solubility, extracted from HENRYWIN.

188) The data presented for helium in Table II of Shoor et al. (1969) appear to be incorrect and are not reproduced here.

189) The data from Morrison and Johnstone (1954) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-267.15298 + 11440.04263/T + 37.95994 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

190) The data from Lannung (1930) were fitted to the three-parameter equation: $H_s^{cp} = \exp(84.35043 - 4135.59197/T - 14.55881 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

191) Calculated employing molecular force field models for the solutes from Warr et al. (2015).

192) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-153.15219 + 6434.36008/T + 20.89911 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

193) The data from Morrison and Johnstone (1954) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-171.84866 + 7492.61303/T + 23.58966 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

194) The data from Lannung (1930) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-40.04033 + 1266.80589/T + 4.12574 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

195) The data from Dean and Lange (1999) were fitted to the three-parameter equation:

$H_s^{cp} = \exp(-150.94728 + 6639.96438/T + 20.42365 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

196) The data from Rettich et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-178.55165 + 8674.63293/T + 24.26764 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

197) The data from Murray and Riley (1970) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-151.84230 + 7548.13106/T + 20.24085 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

198) The data from Shoor et al. (1969) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-177.19900 + 8740.49327/T + 23.99118 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

199) The data from Ashton et al. (1968) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-160.52023 + 7898.05096/T + 21.56102 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

200) The data from Morrison and Johnstone (1954) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-159.49603 + 7859.86242/T + 21.39868 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

201) The data from Lannung (1930) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-183.19260 + 8856.79081/T + 24.97248 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

202) Calculated employing molecular force field models for the solutes from Vrabec et al. (2001).

203) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-143.77232 + 7158.59719/T + 19.05403 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

204) The data from Morrison and Johnstone (1954) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-153.87925 + 7855.39037/T + 20.51280 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

205) Two series of measurements with considerably different results are presented by von Antropoff (1910) for krypton.

206) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-220.92114 + 10903.79433/T + 30.49407 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

207) The value b for Xe given by Himmelblau (1960) in their Table III is incorrect. Most likely, only a minus sign is missing.

208) The data from Morrison and Johnstone (1954) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-165.83721 + 8808.62019/T + 22.15186 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

209) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-199.40126 + 10306.10786/T + 27.18844 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

210) The data from Lewis et al. (1987) were fitted to the three-parameter equation: $H_s^{cp} = \exp(5.03587 + 1555.37916/T - 3.42648 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

211) Calculated employing molecular force field models for the solutes from Mick et al. (2016).

212) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-240.66156 + 12686.97685/T + 33.12171 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

213) The data from Sisi et al. (1971) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-81.82525 + 4954.57763/T + 10.19950 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

214) Solubility in natural sea water. Measurements at different salinities were also performed but only at a fixed temperature of 296.15 K.

215) Temperature dependence calculated using linear free energy relationships (LFERs).

216) Petersen et al. (1998) give the invalid unit "mol L^{-1} ppm^{-1}". Here, it is assumed that "ppm" is used as a synonym for "10^{-6} atm".

217) Shon et al. (2005) refer to Petersen et al. (1998) as the source, but a different value is listed there.

218) Value at $T = 333$ K.

219) Calculated using linear free energy relationships (LFERs).

220) More than one reference is given as the source of this value.

221) Hedgecock et al. (2005) refer to Hedgecock and Pirrone (2004) as the source, but this value cannot be found there.

222) Clever and Young (1987) recommend the data from Rettich et al. (1981).

223) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-133.87728 + 6629.97157/T + 17.62624 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

224) The data from Scharlin and Battino (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-206.41168 + 10058.77208/T + 28.34417 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

225) The data from Shoor et al. (1969) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-201.05778 + 9920.37989/T + 27.48020 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

226) The same value was also published in McAuliffe (1963).

227) The same value was also published in McAuliffe (1966).

228) The data from Morrison and Billett (1952) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-195.92072 + 9624.37184/T + 26.74976 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

229) The data from Winkler (1901) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-203.15902 + 9951.75251/T + 27.82679 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

230) Yao et al. (2002) compared two QSPR methods and found that radial basis function networks (RBFNs) are better than multiple linear regression. In their paper, they provide neither a definition nor the unit of their Henry's law constants. Comparing the values with those that they cite from Yaws (1999), it is assumed that they use the variant H_v^{px} and the unit atm.

231) English and Carroll (2001) provide several calculations. Here, the preferred value with explicit inclusion of hydrogen bonding parameters from a neural network is shown.

232) Value from the training dataset.

233) Calculated with a principal component analysis (PCA); see Suzuki et al. (1992) for details.

234) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-185.72813 + 9197.97387/T + 25.21142 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

235) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-109.51433 + 6313.03876/T + 13.60483 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

236) The data from Morrison and Billett (1952) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-215.51394 + 10861.98666/T + 29.50128 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

237) The data from Winkler (1901) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-277.60377 + 13887.90452/T + 38.63046 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

238) Value given here as quoted by Gharagheizi et al. (2010).

239) Calculated using linear free energy relationships (LFERs).

240) Calculated using SPARC Performs Automated Reasoning in Chemistry (SPARC).

241) Calculated using COSMOtherm.

242) Temperature is not specified.

243) Value from the training dataset.

244) Calculated using the GROMHE model.

245) Calculated using the SPARC approach.

246) Calculated using the HENRYWIN method.

247) Calculated using a combination of a group contribution method and neural networks.

248) Modarresi et al. (2005) use different descriptors for the QSPR models. They conclude that their "COSA" method and the artificial neural network (ANN) are best. However, as COSA is not ideal for hydrocarbons with low solubility, only results obtained with ANN are shown here.

249) Yaffe et al. (2003) present QSPR results calculated with the fuzzy ARTMAP (FAM) and with the back-propagation (BK-Pr) method. They conclude that FAM is better. Only the FAM results are shown here.

250) Value from the training set.

251) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-249.13770 + 12672.58357/T + 34.34947 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

252) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-275.67877 + 14048.75446/T + 38.16041 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

253) The data from Morrison and Billett (1952) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-257.69118 + 13189.22089/T + 35.51019 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

254) The H298 and A, B, C data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 14 % difference.

255) The H298 and A, B, C data listed in Table 5-4 of Burkholder et al. (2015) are inconsistent, with 14 % difference.

256) The H298 and A, B, C data listed in Table 5.4 of Sander et al. (2011) are inconsistent, with 14 % difference.

257) The H298 and A, B, C data listed in Table 5.4 of Sander et al. (2006) are inconsistent, with 14 % difference.

258) The data from Morrison and Billett (1952) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-257.40529 + 13425.82235/T + 35.27658 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

259) Value given here as quoted by Dupeux et al. (2022).

260) Calculated using the COSMO-RS method.

261) Value from the validation dataset.

262) The H298 and A, B, C data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 6 % difference.

263) The H298 and A, B, C data listed in Table 5-4 of Burkholder et al. (2015) are inconsistent, with 6 % difference.

264) The H298 and A, B, C data listed in Table 5.4 of Sander et al. (2011) are inconsistent, with 6 % difference.

265) The H298 and A, B, C data listed in Table 5.4 of Sander et al. (2006) are inconsistent, with 6 % difference.

266) Fogg and Sangster (2003) cite an incorrect fitting function from Hayduk (1986).

267) The fitting function and the data in the table on page 34 of Hayduk (1986) are inconsistent by a factor of about 3. A comparison with the original measurements by Wetlaufer et al. (1964) shows that the data in the table are correct. Refitting the data suggests that the third fitting parameter should be 52.4651, not 53.4651.

268) Value from the test set.

269) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 15 % difference.

270) The data from Jou and Mather (2000) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-400.38105 + 20169.61328/T + 56.35286\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

271) The paper by Jou and Mather (2000) also contains high-temperature data. However, only data up to 373.2 K were used here to calculate the temperature dependence.

272) Value from the validation dataset.

273) Value from the test set.

274) The data from Shoor et al. (1969) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-311.59148 + 15699.27148/T + 43.32183\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

275) Value from the test dataset.

276) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

277) Apparently, the values in Table 2 of Park et al. (1997) show $\log_{10}(K_{aw})$ and not K_{aw} as their figure caption states.

278) Extrapolated from data measured between 40 °C and 80 °C.

279) Data are taken from the report by Howe et al. (1987).

280) Value from the training set.

281) In their Table 8, Staudinger and Roberts (1996) incorrectly cite a value given by Ashworth et al. (1988).

282) The same data were also published in Hansen et al. (1995).

283) Hansen et al. (1993) found that the solubility of 2-methylhexane increases with temperature.

284) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 5 % difference.

285) The data from Dohányosová et al. (2004) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-670.94997 + 33188.34075/T + 95.95541\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

286) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 21 % difference.

287) The data from Dohányosová et al. (2004) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-792.29258 + 38089.35992/T + 114.36667\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

288) Data taken from the Supplement.

289) Calculated using the EPI Suite (v4.0) method.

290) Calculated using the SPARC (v4.2) method.

291) Calculated using the COSMOtherm (v2.1) method.

292) Calculated using the ABSOLV (ADMEBoxes v4.1) method.

293) Mackay et al. (2006a) list a vapor pressure p, a solubility c, and a Henry's law constant calculated as p/c. However, the data are internally inconsistent and deviate by more than 10 %.

294) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 23 % difference.

295) Value at $T = 294$ K.

296) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 13 % difference.

297) The data listed in Tables 2 and 3 of Dewulf et al. (1999) are inconsistent, with 5 % difference.

298) Value at $T = 301$ K.

299) Value given here as quoted by Staudinger and Roberts (1996).

300) Value from the test set for true external validation.

301) The data from Dohányosová et al. (2004) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-365.40645 + 19821.40051/T + 50.78223\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

302) The data from Dohányosová et al. (2004) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-383.72514 + 20514.87228/T + 53.42859\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

303) The data from Dohányosová et al. (2004) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-369.42853 + 19642.40603/T + 51.34116\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

304) Haynes (2014) refers to Mackay and Shiu (1981), but that article lists this value for 1,4-dimethylcyclohexane, not for 1,2-dimethylcyclohexane.

305) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

306) The data from Dohányosová et al. (2004) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-346.32561 + 18710.63122/T + 47.87398 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

307) The data from Maaßen (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-187.57836 + 9639.75245/T + 25.50544 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

308) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-166.44394 + 8613.39266/T + 22.39721 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

309) The data from Morrison and Billett (1952) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-175.14997 + 9028.26949/T + 23.67675 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

310) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-221.00286 + 11107.47493/T + 30.50401 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

311) The data from Maaßen (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-168.51157 + 9378.22622/T + 22.33127 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

312) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-241.54655 + 12718.75981/T + 33.18333 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

313) The data from Serra and Palavra (2003) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-261.78355 + 13728.91505/T + 36.10688 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

314) According to Donahue and Prinn (1993), the value is incorrect.

315) Wang et al. (2017) provide separate data for *cis* and *trans*. However, since both isomers are identified by the same SMILES string in their study, it is unclear how the stereochemistry has been taken into account.

316) Values for the Henry's law constants shown in Fig. 3 of Martins et al. (2017) were obtained from Simão Pinho (personal communication, 2022).

317) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from multiple sources and obtained from experimental vapor pressure and water solubility.

318) The data from Dohányosová et al. (2004) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-169.70973 + 10843.51763/T + 21.91320 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

319) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from a single database or data collection and obtained from experimental vapor pressure and water solubility.

320) Approximate value extracted from Fig. 1 of Maillard and Rosenthal (1952).

321) The same article was also published in *Monatshefte für Chemie* 23, 489–501 (1902).

322) Value given here as quoted by Fogg et al. (2002).

323) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-143.25283 + 7542.89338/T + 19.33269 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

324) Incorrect data are given by Burkholder et al. (2019) for 1-butyne. The number in their table should probably be 0.0569, not 0.569.

325) Regression and individual data points of Simpson and Lovell (1962) are inconsistent, with 5 % difference.

326) Using the theoretical initial concentration (H_0); see Zhang et al. (2013) for details.

327) Average of all duplicates (H_1); see Zhang et al. (2013) for details.

328) Sieg et al. (2009) also provide data for supercooled water. Here, only data above 0 °C were used to calculate the temperature dependence.

329) Extrapolated from data above 298 K.

330) It was found that H_s changes with the concentration of the solution.

331) The data from Görgényi et al. (2002) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-346.88030 + 18421.52810/T + 48.91393 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

332) Value obtained by applying a modified batch air-stripping method, otherwise called the vapor entry loop (VEL) method; see Kochetkov et al. (2001) for details.

333) Value obtained by applying the static head space (HS) method; see Kochetkov et al. (2001) for details.

334) The data from Khalfaoui and Newsham (1994b) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-129.36095 + 8999.48627/T + 16.29087 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

335) The data from Robbins et al. (1993) were fitted to the three-parameter equation: $H_s^{cp} = \exp(189.41389 - 5855.10843/T - 30.90289 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

336) Value at $T = 302$ K.

337) The data from Cooling et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-231.38331 + 13640.47358/T + 31.46504 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

338) Calculated using G_h and H_h from Table 2 in Andon et al. (1954). Note that the thermodynamic functions in that table are not based on their α in Table 1. Instead, the expression $\exp(-G_h/(RT))$ yields the Henry's law constant H_s^{xp} in the unit 1/atm.

339) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 11 % difference.

340) Values for salt solutions are also available from this reference.

341) The data from Görgényi et al. (2002) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-468.28203 + 24099.39947/T + 66.85565 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

342) Value obtained by applying the EPICS method; see Ayuttaya et al. (2001) for details.

343) Value obtained by applying the static cell (linear form) method; see Ayuttaya et al. (2001) for details.

344) Value obtained by applying the direct phase concentration ratio method; see Ayuttaya et al. (2001) for details.

345) Value obtained by applying the static cell (nonlinear form) method; see Ayuttaya et al. (2001) for details.

346) The data from Robbins et al. (1993) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-573.76928 + 28956.65188/T + 82.51911 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

347) The temperature dependence is recalculated using the data in Table 4 of Lamarche and Droste (1989) and not taken from their Table 5.

348) Apparently, the vapor pressure of toluene was used to calculate its Henry's law constant. However, no source is provided.

349) Value given here as quoted by Dewulf et al. (1995).

350) The data from Robbins et al. (1993) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-1350.74178 + 64760.28328/T + 197.85937 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

351) The data from Schwardt et al. (2021) were fitted to the three-parameter equation: $H_s^{cp} = \exp(100.47045 - 2603.76722/T - 17.31043 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

352) Value given here as quoted by HSDB (2015).

353) The regression parameters for ethylbenzene in Table 1 of Schwardt et al. (2021) are wrong. Corrected values from Schwardt et al. (2022) are used here.

354) The data from Schwardt et al. (2021) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-176.88587 + 11290.74921/T + 23.22869 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

355) Different types of Henry's law constants of Ryu and Park (1999) are inconsistent, with 14 % difference.

356) The data from Robbins et al. (1993) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-371.46947 + 20514.07888/T + 51.95086 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

357) The value listed as A for diethylbenzene is probably not A but the Henry's law volatility constant H_v^{px} at 298 K.

358) Yaffe et al. (2003) list this species twice in their table, with different values. As it is unclear which is correct, the data are not reproduced here.

359) Erratum for page 365 of Fogg and Sangster (2003): data from Kondoh and Nakajima (1997) are cited incorrectly, giving the same values at 308.2 K and 318.2 K, respectively.

360) Value from the external prediction set.

361) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 8 % difference.

362) Because of discrepancies between the values shown in Tables 4 and 5 of Shiu and Ma (2000), the data are not used here.

363) Effective Henry's law constants at several pH values are provided by van Ruth and Villeneuve (2002). Here, only the value at pH = 3 is shown.

364) The values of Dewulf et al. (1999) are not used here because, according to them, the calculated regression does not match the theoretical expectation for this species.

365) Calculated using the COSMO-RS method.

366) Value given here as quoted by Haynes (2014).

367) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from a single database or data collection and measured directly.

368) Literature-derived value.

369) Final adjusted value.

370) Value given here as quoted by Petrasek et al. (1983).

371) Calculated using COSMOtherm.

372) Calculated using the COSMO-RS method.

373) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from a single original paper and obtained from experimental vapor pressure and water solubility.

374) Value at $T = 299\,\mathrm{K}$.

375) Value at $T = 283\,\mathrm{K}$.

376) Cargill (1990) recommends the data from Rettich et al. (1982).

377) The data from Rettich et al. (1982) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-188.21737 + 8974.05844/T + 25.72558\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

378) The data from Douglas (1967) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-180.92848 + 8514.05914/T + 24.68060\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

379) Solubility in sea water at 20.99 % chlorinity.

380) The data from Winkler (1901) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-163.07031 + 7890.85881/T + 21.94517\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

381) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-161.93492 + 7852.78262/T + 21.76812\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

382) The data from Zheng et al. (1997) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-144.44443 + 8071.06186/T + 19.20040\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

383) The data from Murray and Riley (1971) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-167.86941 + 9146.24434/T + 22.67331\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

384) The data from Morrison and Billett (1952) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-126.83009 + 7302.88179/T + 16.55553\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

385) The data from Bohr (1899) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-140.70007 + 7951.73013/T + 18.60961\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

386) As mentioned by Fogg and Sangster (2003), the fitting equation by Scharlin (1996) is erroneous. It appears that a correction factor of about 10^6 is necessary for consistency with their own data in Table 1.

387) The data from Dean and Lange (1999) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-138.54120 + 7859.16351/T + 18.28486\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

388) Keßel et al. (2017) provide data at several pH values. Here, only the value at pH = 2 is shown because hydrolysis occurs in more alkaline solutions.

389) The H298 and A, B, C data listed in Table 5.4 of Sander et al. (2011) are inconsistent, with 92 % difference.

390) This paper supersedes earlier work with more concentrated solutions (Butler et al., 1933).

391) Value given here as quoted by Gaffney et al. (1987).

392) Value given here as quoted by Hine and Weimar (1965).

393) The H298 and A, B, C data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 10 % difference.

394) The H298 and A, B, C data listed in Table 5-4 of Burkholder et al. (2015) are inconsistent, with 10 % difference.

395) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 8 % difference.

396) The H298 and A, B, C data listed in Table 5.4 of Sander et al. (2011) are inconsistent, with 10 % difference.

397) Extrapolated from data above 298 K.

398) Koga (1995) found that *tert*-butanol does not obey Henry's law at $c > 3.8\,\mathrm{mM}$.

399) Incorrect data are given by Burkholder et al. (2019) for 2-methyl-2-propanol. The correct parameter for the temperature dependence is $C = 37.98$ (Robert E. Huie, personal communication, 2021).

400) Incorrect data are given by Burkholder et al. (2015) for 2-methyl-2-propanol. The correct parameter for the temperature dependence is $C = 37.98$ (Robert E. Huie, personal communication, 2021).

401) Calculated for an aqueous solution containing 60 % ethanol by volume as the solvent.

402) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

403) Value obtained by Saxena and Hildemann (1996) using the group contribution method.

404) Value at $T = 300\,\mathrm{K}$.

405) The error given by Suzuki et al. (1992) is not the difference between the observed and the calculated value, as it should be. It is unclear which of the numbers is wrong.

406) The species is probably 2,3-dimethyl-2-butanol and not 2,3-dimethylbutanol as listed in Hine and Mookerjee (1975).

407) Rumble (2021) refers to Moore et al. (1995) as the source, but this value cannot be found there.

408) It is assumed here that entry number 72 in Table 1 of Yaws et al. (1997) refers to 2-methyl-1-heptanol, not 2-methyl-2-heptanol.

409) KWAC and KAWp from Table 2 of Lei et al. (2007) are inconsistent, with 10 % difference.

410) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 8 % difference.

411) Different types of Henry's law constants of Yaws and Yang (1992) are inconsistent, with 16 % difference.

412) Different types of Henry's law constants of Yaws and Yang (1992) are inconsistent, with 10 % difference.

413) Value at $T = 307\,\mathrm{K}$.

414) Value given here as quoted by Mackay et al. (1995).

415) Calculated using SPARC Performs Automated Reasoning in Chemistry (SPARC). It is assumed here that the value refers to $T = 298.15\,\mathrm{K}$.

416) Value given here as quoted by Hine and Mookerjee (1975).

417) Value at $T = 373\,\mathrm{K}$.

418) Value at $T = 281\,\mathrm{K}$.

419) It is assumed here that the thermodynamic data refer to the units [mol dm^{-3}] and [atm] as standard states.

420) Value given here as quoted by Shiu et al. (1994).

421) HSDB (2015) refers to Abraham et al. (1994b) as the source, but this value cannot be found there. Maybe the value is taken from Abraham et al. (1990).

422) Mackay et al. (2006c) list a vapor pressure p, a solubility c, and a Henry's law constant calculated as p/c. However, the data are internally inconsistent and deviate by more than 10 %.

423) Betterton (1992) gives Buttery et al. (1969) as the source. However, no data were found in that reference.

424) Intermediate of estimates employing the bond method from the EPI HENRYWIN software.

425) Although Mansfield (2020) writes that his "Table 6 summarizes numerical calculations for formaldehyde and acetaldehyde assuming the values given in Tables 4 and 5", different values for the Henry's law constants are shown in these tables.

426) Saxena and Hildemann (1996) say that this value is unreliable.

427) Calculated using the free energy perturbation (FEP) method.

428) Calculated using the thermodynamic integration (TI) method.

429) Calculated using the Bennett acceptance ratio (BAR) method.

430) Saxena and Hildemann (1996) give a range of $9.9\times10^{2}\,\mathrm{mol\,m^{-3}\,Pa^{-1}} < H_\mathrm{s}^{cp} < 5.9\times10^{4}\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$.

431) Saxena and Hildemann (1996) give a range of $5.9\times10^{6}\,\mathrm{mol\,m^{-3}\,Pa^{-1}} < H_\mathrm{s}^{cp} < 3.9\times10^{9}\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$.

432) The formula of 1,2-butanediol is incorrectly given as "HOCH(OH)C_2H_5" by Burkholder et al. (2019).

433) The formula of 1,2-butanediol is incorrectly given as "HOCH(OH)C_2H_5" by Burkholder et al. (2015).

434) Saxena and Hildemann (1996) give a range of $9.9\times10^{2}\,\mathrm{mol\,m^{-3}\,Pa^{-1}} < H_\mathrm{s}^{cp} < 4.9\times10^{4}\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$.

435) Saxena and Hildemann (1996) give a range of $3.9\times10^{2}\,\mathrm{mol\,m^{-3}\,Pa^{-1}} < H_\mathrm{s}^{cp} < 3.9\times10^{4}\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$.

436) Calculated based on atmospheric measurements.

437) Calculated using EPI.

438) Calculated using SPARC.

439) Henry's law constants calculated using the GROMHE model. Temperature dependences calculated with the method of Kühne et al. (2005).

440) Isaacman-VanWertz et al. (2016) refer to Raventos-Duran et al. (2010) as the source, but the quoted value cannot be found there.

441) Calculated using GROMHE.

442) Isaacman-VanWertz et al. (2016) refer to a paper by Hilal et al. as the source, but the quoted value cannot be found there.

443) Calculated using SPARC.

444) Calculated using the bond contribution of HENRYWIN.

445) Compernolle and Müller (2014b) recommend H_s^{cp} for 1,7-heptanediol in the range of $4.5\times10^{4}\,\mathrm{mol\,m^{-3}\,Pa^{-1}} < H_\mathrm{s}^{cp} < 8.3\times10^{4}\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$.

446) Compernolle and Müller (2014b) recommend H_s^{cp} for 1,9-nonanediol in the range of $2.4\times10^{4}\,\mathrm{mol\,m^{-3}\,Pa^{-1}} < H_\mathrm{s}^{cp} < 3.9\times10^{4}\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$.

447) Compernolle and Müller (2014b) recommend H_s^{cp} for 1,10-decanediol in the range of $2.5\times10^{4}\,\mathrm{mol\,m^{-3}\,Pa^{-1}} < H_\mathrm{s}^{cp} < 3.0\times10^{4}\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$.

448) Value given here as quoted by Hilal et al. (2008).

449) Calculated using the EPI Suite method at https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface (last access: 18 September 2023).

450) Value for the temperature range from 261 K to 281 K.

451) Value at $T = 278\,\mathrm{K}$.

452) Leriche et al. (2000) assume $H_s(\mathrm{ROO}) = H_s(\mathrm{ROOH}) \times H_s(\mathrm{HO_2})/H_s(\mathrm{H_2O_2})$.

453) Lelieveld and Crutzen (1991) assume $H_s(\mathrm{CH_3OO}) = H_s(\mathrm{HO_2})$.

454) Jacob (1986) assumes $H_s(\mathrm{CH_3OO}) = H_s(\mathrm{CH_3OOH}) \times H_s(\mathrm{HO_2})/H_s(\mathrm{H_2O_2})$.

455) Calculated using EVAPORATION and AIOMFAC.

456) Calculated using the GROMHE model.

457) Effective value that takes into account the hydration of HCHO:

$$H_s = ([\mathrm{HCHO}] + [\mathrm{CH_2(OH)_2}])/p(\mathrm{HCHO}).$$

458) Data from Table 1 by Zhou and Mopper (1990) were used to redo the regression analysis. The data for acetone in their Table 2 are incorrect.

459) Dong and Dasgupta (1986) found that the Henry's law constant for HCHO is not a true constant but that it increases with increasing concentration. Note that their expression does not converge asymptotically to a constant value at infinite dilution.

460) Ledbury and Blair (1925) (and also Blair and Ledbury (1925)) measured the solubility of HCHO at very high concentrations around 5 to 15 M. Their value of H_s increases with HCHO concentration. Lelieveld and Crutzen (1991), Hough (1991), and Pandis and Seinfeld (1989) all use these solubility data but do not specify how they extrapolated to lower concentrations. Since the concentration range is far from typical values in atmospheric chemistry, the value is not reproduced here.

461) Value given here as quoted by Möller and Mauersberger (1992).

462) Effective value that takes into account the hydration of the aldehyde:

$$H_s = ([\mathrm{RCHO}] + [\mathrm{RCH(OH)_2}])/p(\mathrm{RCHO}).$$

463) The data from Wieland et al. (2015) were fitted to the three-parameter equation: $H_s^{cp} = \exp(25.01220 + 3596.11696/T - 6.81730\ln(T))\ \mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

464) Value given here as quoted by Bone et al. (1983).

465) Value suitable for the conditions of a case study in Mexico City.

466) Volkamer et al. (2009) found average effective Henry's law constants for CHOCHO in the range $1.6\times10^6\ \mathrm{mol\,m^{-3}\,Pa^{-1}} < H_s^{cp} < 5.9\times10^6\ \mathrm{mol\,m^{-3}\,Pa^{-1}}$ for solutions containing ammonium sulfate and/or fulvic acid. A salting-in effect by fulvic acid was observed even in the absence of sulfate.

467) Solubility in sulfate aerosol.

468) Woo and McNeill (2015) say that the Henry's law constant was updated based on advances in the literature since McNeill et al. (2012) but do not provide further details.

469) Value at $T = 372\,\mathrm{K}$.

470) The data from Wieland et al. (2015) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-176.35942 + 12895.73116/T + 22.70566\ln(T))\ \mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

471) The formula of propenal is incorrectly given as "CH_2CHO" by Burkholder et al. (2019).

472) The temperature dependence parameter C for 2-butenal is missing in Burkholder et al. (2019). The correct value is $C = 24.42$ (Robert E. Huie, personal communication, 2021).

473) The data from Buttery et al. (1971) for *trans*-2-octenal are incorrectly cited by Betterton (1992).

474) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

475) Calculated under the assumption that ΔG and ΔH are based on [mol $\mathrm{L^{-1}}$] and [atm] as the standard states.

476) Calculated using the experimental value adjusted (EVA) method; see McFall et al. (2020) for details.

477) Value at $T = 359\,\mathrm{K}$.

478) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 5 % difference.

479) Calculated from the slope of $y_{ac}P$ vs x_{ac}, using data from Table VIII in Lichtenbelt and Schram (1985).

480) Value at $T = 313\,\mathrm{K}$.

481) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

482) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 7 % difference.

483) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

484) Table S2 in the Supplement of Wu et al. (2022a) contains incorrect data for 3-octanone. Here, the corrected data (Shuang Wu, personal communication, 2022) were used: 2.88×10^{-2} and 1.52×10^{-2} at 25 °C and 35 °C, respectively.

485) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 7 % difference.

486) The value listed as A for 2,6,8-trimethyl-4-nonanone is probably not A but the Henry's law volatility constant H_v^{px} at 298 K.

487) The data from Wieland et al. (2015) were fitted to the three-parameter equation: $H_s^{cp} = \exp(116.85779 -$

$1341.05519/T - 19.91967 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

488) The data from Wieland et al. (2015) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-74.84087 + 9452.88617/T + 7.41865 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

489) The value given here was measured at a liquid-phase mixing ratio of 1 µmol mol^{-1}. Servant et al. (1991) found that the Henry's law constant changes at higher concentrations.

490) Abraham (1984) smoothed the values from a plot of enthalpy against carbon number.

491) The value of $H_s^{\ominus}$ was taken from Keene and Galloway (1986).

492) Calculated using thermodynamic data from Latimer (1952).

493) Value at pH = 4.

494) Calculated using HENRYWIN 3.2 (bond contribution method).

495) At pH = 7.

496) At pH = 10.8.

497) Value at T = 289 K.

498) Value at T = 338 K.

499) Pecsar and Martin (1966) are quoted as the source. However, only activity coefficients and no vapor pressures are listed there.

500) The H298 and A, B, C data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 6 % difference.

501) The formula of methyl ethanoate is incorrectly given as "$CH_3C(O)CH_3$" by Burkholder et al. (2015).

502) The H298 and A, B data listed in Table 5-4 of Burkholder et al. (2015) are inconsistent, with 74 % difference.

503) The same data were also published in Kieckbusch and King (1979a).

504) The H298 and A, B, C data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 7 % difference.

505) The formula of propyl ethanoate is incorrectly given as "$CH_3C(O)C_3H_8$" by Burkholder et al. (2019).

506) Katritzky et al. (1998) list this species twice in their table, with different values. As it is unclear which of them is correct, the data are not reproduced here.

507) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 5 % difference.

508) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

509) The value listed as A for n-heptyl acetate is probably not A but the Henry's law volatility constant H_v^{px} at 298 K.

510) The value listed as A for n-octyl acetate is probably not A but the Henry's law volatility constant H_v^{px} at 298 K.

511) Betterton (1992) gives Kieckbusch and King (1979b) as the source. However, no data were found in that reference.

512) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

513) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 5 % difference.

514) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

515) The data from Wieland et al. (2015) were fitted to the three-parameter equation: $H_s^{cp} = \exp(34.46832 + 3269.29552/T - 8.76905 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

516) Burkholder et al. (2019) refer to Dohnal et al. (2010) but the quoted value cannot be found there.

517) Burkholder et al. (2015) refer to Dohnal et al. (2010) but the quoted value cannot be found there.

518) Dipropyl phthalate is listed twice with different values.

519) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 9 % difference.

520) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 17 % difference.

521) Hwang et al. (2010) present regression parameters in their Table 6 and values extrapolated to 298.15 K in their Table 5. However, I was not able to reproduce their calculation. The data shown here are from my own regression of the measured data between 318.15 K and 333.15 K.

522) The data from Haimi et al. (2006) were fitted to the three-parameter equation: $H_s^{cp} = \exp(752.39274 - 29351.83448/T - 115.55407 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

523) Different types of Henry's law constants of Arp and Schmidt (2004) are inconsistent, with 5 % difference.

524) The data from Robbins et al. (1993) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-4264.16032 + 202439.46180/T + 628.54371 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

525) The data from Haimi et al. (2006) were fitted to the three-parameter equation: $H_s^{cp} = \exp(224.10069 - 4205.03828/T - 37.65761 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

526) The data from Haimi et al. (2006) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-780.30940 + 40758.59752/T + 112.07468 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

527) The data from Haimi et al. (2006) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-565.00561 + 31411.46240/T + 79.73748 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

528) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from a single original paper and obtained from experimental vapor pressure and the infinite-dilution activity coefficient.

529) The data from Haimi et al. (2006) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-1125.52184 + 56732.54277/T + 163.04749 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

530) The data from Haimi et al. (2006) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-1315.53726 + 64110.36765/T + 191.89554 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

531) The value listed as A for di-n-pentyl ether is probably not A but the Henry's law volatility constant H_v^{px} at 298 K.

532) The value listed as A for di-n-hexyl ether is probably not A but the Henry's law volatility constant H_v^{px} at 298 K.

533) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 5 % difference.

534) The data from Wieland et al. (2015) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-157.10556 + 10203.60762/T + 20.42555 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

535) Betterton (1992) gives Hine and Weimar (1965) as the source. However, no data were found in that reference.

536) Betterton (1992) gives Vitenberg et al. (1975) as the source. However, no data were found in that reference.

537) Based on gas chromatograph retention indices (GC-RIs).

538) Warneck (2005) refers to Saxena and Hildemann (1996) as the source, but the quoted value cannot be found there.

539) The formula of hydroxyethanoic acid is incorrectly given as "HC(OH)C(O)OH" by Burkholder et al. (2019).

540) The formula of hydroxyethanoic acid is incorrectly given as "HC(OH)C(O)OH" by Burkholder et al. (2015).

541) Temperature dependencies in Tables 1 and 2 of Ashworth et al. (1988) are inconsistent, with 31 % difference.

542) Compernolle and Müller (2014a) recommend H_s^{cp} for tartaric acid in the range of 6.9×10^{14} mol m^{-3} Pa^{-1} $< H_s^{cp} < 9.2\times10^{15}$ mol m^{-3} Pa^{-1}.

543) Chan et al. (2010) give a range of 1.9×10^{5} mol m^{-3} Pa^{-1} $< H_s^{cp} <$ 9.5×10^{6} mol m^{-3} Pa^{-1}.

544) Calculated using the HENRYWIN program and calibration to 1,3-propanediol.

545) The value was chosen for a model study because it gave the best agreement with measurements.

546) Center of the range (2.3...4.0) mol m^{-3} Pa^{-1}.

547) Calculated based on the method by Hine and Mookerjee (1975).

548) Compernolle and Müller (2014a) recommend H_s^{cp} for citric acid in the range of 2.0×10^{14} mol m^{-3} Pa^{-1} $< H_s^{cp} < 5.9\times10^{15}$ mol m^{-3} Pa^{-1}.

549) The data from Wieland et al. (2015) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-96.39127 + 11107.87195/T + 10.76466 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

550) In their Fig. 5b, Kish et al. (2013) apply an unspecified factor to the Henry's law constant, and it is not clear if the temperature dependence shown there is correct (Yong Liu, personal communication, 2014).

551) Calculated using the method from Nguyen (2013).

552) Calculated from the slope of $y_1 P$ vs x_1, using the tabulated VLE data from Kim et al. (2008) between 40 °C and 100 °C. Only dilute solutions with $x_1 \le 0.1$ were considered.

553) Value at $T = 309$ K.

554) The data from Christie and Crisp (1967) for dipropylamine are incorrectly cited by Betterton (1992).

555) Value at $T = 323$ K.

556) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

557) Value at $T = 308$ K.

558) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 5 % difference.

559) Value at $T = 285$ K.

560) Mackay et al. (2006d) list a vapor pressure p, a solubility c, and a Henry's law constant calculated as p/c. However, the data are internally inconsistent and deviate by more than 10 %.

561) Calculated using $\Delta G_s^{g\to H_2O}$ and $\Delta H_s^{g\to H_2O}$ from Table IV of Arnett and Chawla (1979). Since some of the values in this table are taken directly from Andon et al. (1954), it is assumed that the thermodynamic properties are defined in the same way. Since $\Delta H_s^{g\to H_2O}$ is defined relative to pyridine, a value of $-11.93\,\mathrm{kcal\,mol^{-1}}$ from Arnett et al. (1977) was added.

562) Due to an apparently incorrect definition of the Henry's law constant by Andon et al. (1954), Staudinger and Roberts (2001) quote incorrect values from that paper.

563) The data from Wieland et al. (2015) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-12.48322 + 7833.96799/T - 2.23379\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

564) Value given here as quoted by Feigenbrugel and Le Calvé (2021).

565) Value calculated from the solubility of $9.4\times10^{-3}\,\mathrm{mol\,L^{-1}}$ and the vapor pressure of 0.255 mmHg, as shown on pages 7142-7143 of Arnett and Chawla (1979). It is inconsistent with the entry in Table IV of that paper.

566) Value given here as quoted by Ma et al. (2010a).

567) Nguyen (2013) refer to Kim et al. (2008) as the source, but this value cannot be found there.

568) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 7 % difference.

569) Value given here as quoted by Goodarzi et al. (2010).

570) Goodarzi et al. (2010) compared several QSPR methods and found that the Levenberg–Marquardt algorithm with Bayesian regularization produces the best results. Values obtained with other methods can be found in their Supplement.

571) Value from the validation set.

572) At pH = 5.

573) Value from the test set.

574) At pH = 10.

575) At pH = 9.

576) At pH = 5.2.

577) At pH = 7.4.

578) At pH = 9.3.

579) At pH = 4.

580) Kames and Schurath (1992) were unable to assign the values to the isomers.

581) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from a single original paper and measured directly.

582) The same data were also published in Fischer and Ballschmiter (1998a).

583) The formula of 1,3-propanediol dinitrate is incorrectly given as "$O_2NO_2CH_2CH_2CH_2ONO_2$" by Burkholder et al. (2019).

584) The formula of 1,3-propanediol dinitrate is incorrectly given as "$O_2NO_2CH_2CH_2CH_2ONO_2$" by Burkholder et al. (2015).

585) Comparing the value with that from the cited publication (Kames and Schurath, 1995), it can be seen that the unit and the temperature listed in Table 3 of Warneck et al. (1996) are incorrect.

586) The data from Kames and Schurath (1995) for peroxyacetyl nitrate are incorrectly cited by Schurath et al. (1996).

587) The data from Kames and Schurath (1995) for peroxypropionyl nitrate are incorrectly cited by Schurath et al. (1996).

588) The data from Kames and Schurath (1995) for peroxy-*n*-butyl nitrate are incorrectly cited by Schurath et al. (1996).

589) The data from Kames and Schurath (1995) for peroxymethacryloyl nitrate are incorrectly cited by Schurath et al. (1996).

590) The data from Kames and Schurath (1995) for peroxy-*i*-butyl nitrate are incorrectly cited by Schurath et al. (1996).

591) Estimate based on Raventos-Duran et al. (2010).

592) The value at $T^{\ominus}$ is the intrinsic Henry's law constant, but the temperature dependence refers to the effective Henry's law constant at pH = 3.0.

593) The value at $T^{\ominus}$ is the intrinsic Henry's law constant, but the temperature dependence refers to the effective Henry's law constant at pH = 3.08.

594) Burkholder et al. (2019) refer to Borduas et al. (2016), but the quoted temperature dependence cannot be found there.

595) The values for nitroethane in Tables VI and VIII of Friant and Suffet (1979) differ by a factor of 10. Apparently, the value in Table VIII is wrong.

596) The data listed in Tables 2 and 3 of Dewulf et al. (1999) are inconsistent, with 27 % difference.

597) Mackay et al. (2006d) list two values for dinoseb which differ by a factor of 1000. It is unclear which number is correct (if any), and the data are not reproduced here.

598) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

599) The data from Glew and Moelwyn-Hughes (1953) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-135.82151 + 7593.40134/T + 18.05983 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

600) The data from Maaßen (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-163.70243 + 8973.31702/T + 22.17142 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

601) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-142.70480 + 8025.53525/T + 19.04459 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

602) The data from Zheng et al. (1997) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-190.61883 + 10088.26604/T + 25.94088 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

603) The data from Maaßen (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-177.44258 + 9554.69077/T + 23.94054 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

604) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-350.64777 + 16708.21486/T + 49.40261 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

605) The data from Scharlin and Battino (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-552.21779 + 25529.81258/T + 79.59510 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

606) The data from Scharlin and Battino (1994) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-552.21779 + 25529.81258/T + 79.59510 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

607) The data from Wen and Muccitelli (1979) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-356.93310 + 16943.80173/T + 50.37092 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

608) The data from Ashton et al. (1968) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-320.94892 + 15261.58540/T + 45.04995 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

609) The data from Morrison and Johnstone (1954) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-174.44927 + 8434.85415/T + 23.34667 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

610) The H298 and A, B data listed in Table 5-7 of Burkholder et al. (2019) are inconsistent, with 8 % difference.

611) The H298 and A, B data listed in Table 5-7 of Burkholder et al. (2015) are inconsistent, with 8 % difference.

612) The data from Zheng et al. (1997) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-203.78636 + 11097.46295/T + 27.89781 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

613) The data from Maaßen (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-184.82864 + 10260.68840/T + 25.06659 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

614) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-175.64793 + 9805.36391/T + 23.71997 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

615) The data from Zheng et al. (1997) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-244.13803 + 12963.44791/T + 33.68869 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

616) The data from Maaßen (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-225.56576 + 12186.49271/T + 30.88527 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

617) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-208.89051 + 11387.65726/T + 28.42219 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

618) The data from Chang and Criddle (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-1003.84803 + 45506.40253/T + 147.89569 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

619) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-164.25882 + 9381.26592/T + 21.50848 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

620) The data from Wen and Muccitelli (1979) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-499.57565 + 23563.38593/T + 71.28478 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

621) Value at $T = 287$ K.

622) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-78.74672 + 5836.90728/T + 8.41930 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

623) The data from Clever et al. (2005) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-588.11467 + 28143.61522/T + 84.26598 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

624) In their Table 13, Clever et al. (2005) list Ostwald coefficients that are probably incorrect by a factor of 100. Therefore, these values are not used. Instead, H_s is calculated using the amount fraction x_1 from the same table.

625) The data from Scharlin and Battino (1994) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-630.69809 + 30309.09484/T + 90.46889 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

626) The data from Wen and Muccitelli (1979) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-673.45393 + 31915.35190/T + 97.01332 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

627) The data from Maaßen (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-197.14327 + 10473.25304/T + 26.34780 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

628) Calculated using the COSMO-RS method.

629) Value given here as quoted by Kanakidou et al. (1995).

630) Comparing with Abraham et al. (1994a), it seems that the compound called "trifluoroethanol" by Goss (2005) refers to 2,2,2-trifluoroethanol.

631) Comparing with Abraham et al. (1994a), it seems that the compound called "hexafluoropropanol" by Goss (2005) refers to 1,1,1,3,3,3-hexafluoro-2-propanol.

632) Value at $T = 284$ K.

633) Measured in aqueous hydrochloric acid and extrapolated to pure water as the solvent at 25 °C. Measurements were also made at other temperatures; however, those were not extrapolated to pure water as the solvent.

634) Calculated using the EPI Suite Bond estimation method.

635) Calculated using the new SPARC method; see Arp et al. (2006) for details.

636) Calculated using the COSMOtherm method; see Arp et al. (2006) for details.

637) A refit yields $A = -18.99$, $B = 5493$, and $H(298\,\mathrm{K}) = 0.57$ M atm^{-1} (Robert E. Huie, personal communication, 2021).

638) A refit yields $A = -18.99$, $B = 5493$, and $H(298\,\mathrm{K}) = 0.57$ M atm^{-1} (Robert E. Huie, personal communication, 2021).

639) A refit yields $A = -21.67$, $B = 5776$, and $H(298\,\mathrm{K}) = 0.10$ M atm^{-1} (Robert E. Huie, personal communication, 2021).

640) The H298 and A, B data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 29 % difference.

641) A refit yields $A = -21.67$, $B = 5776$, and $H(298\,\mathrm{K}) = 0.10$ M atm^{-1} (Robert E. Huie, personal communication, 2021).

642) The H298 and A, B data listed in Table 5-4 of Burkholder et al. (2015) are inconsistent, with 29 % difference.

643) The H298 and A, B data listed in Table 5.4 of Sander et al. (2011) are inconsistent, with 29 % difference.

644) The data from Clever et al. (2005) were fitted to the three-parameter equation: $H_s^{cp} = \exp(289.52696 - 11352.27202/T - 46.16631 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

645) The Ostwald coefficient given by Clever et al. (2005) at 313.2 K is probably incorrect. Therefore, the Ostwald coefficients are not used. Instead, H_s is calculated using the amount fraction x_1 from the same table.

646) Extrapolated based on number of carbons.

647) Measured with the wetted-wall column at room temperature.

648) The H298 and A, B data listed in Table 5.4 of Sander et al. (2011) are inconsistent, with 9 % difference.

649) The H298 and A, B data listed in Table 5.4 of Sander et al. (2006) are inconsistent, with 9 % difference.

650) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-251.05500 + 13259.10200/T + 35.01685 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

651) The same data were also published in McConnell et al. (1975).

652) The data from Glew and Moelwyn-Hughes (1953) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-171.13914 + 9743.00524/T + 23.09616 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

653) Values at different temperatures are from different sources. Thus a temperature dependence was not calculated.

654) Chiang et al. (1998) show vinyl chloride in their Table 2 but most probably they meant to refer to dichloromethane instead.

655) The data from Wright et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-444.17924 + 22456.73010/T + 63.76504 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

656) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 7 % difference.

657) The data from Görgényi et al. (2002) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-378.59438 + 20174.67146/T + 53.50889 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

658) The data from Moore et al. (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(32.52949 + 1878.33965/T - 7.88669 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

659) The data from Wright et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-109.09283 + 8000.75665/T + 13.39152 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

660) Probably an interpolation of the data from Balls (1980).

661) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 5 % difference.

662) The data from Bullister and Wisegarver (1998) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-704.15798 + 34144.64622/T + 102.06046 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

663) The data from Wright et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-426.63883 + 22457.44484/T + 60.22986 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

664) The data from Maaßen (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-221.58683 + 12291.19608/T + 30.42274 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

665) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-233.85465 + 12927.81251/T + 32.20905 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

666) The data from Görgényi et al. (2002) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-372.18420 + 19566.35271/T + 52.67600 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

667) The data from Wright et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-1295.59488 + 61538.96732/T + 190.02999 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

668) The data from Wright et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-309.75754 + 17275.24359/T + 43.35857 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

669) The data from Robbins et al. (1993) were fitted to the three-parameter equation: $H_s^{cp} = \exp(313.50875 - 12121.71831/T - 49.20602 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

670) The data from Wright et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(255.46482 - 8896.18926/T - 40.90189 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

671) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 5 % difference.

672) The data from Schwardt et al. (2021) were fitted to the three-parameter equation: $H_s^{cp} = \exp(200.57633 - 7128.32092/T - 31.87111 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

673) The data from Wright et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-304.31063 + 17046.46392/T + 42.59182 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

674) The data from Schwardt et al. (2021) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-1784.40256 + 88283.19114/T + 260.26556 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

675) The data from Wright et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(608.52671 - 23622.70039/T - 93.86675 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

676) The value for A in the table of Kondoh and Nakajima (1997) is incorrect. Recalculating the regression, it can be seen that it should be 13.95 and not 1.395.

677) The data from Wright et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(2638.58362 - 114985.14319/T - 396.08684 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

678) The H298 and A, B data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 9 % difference.

679) The data from Wright et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-573.71583 + 28877.33987/T + 82.70652 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

680) The data from Sarraute et al. (2006) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-503.53929 + 28223.72051/T + 70.89539 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

681) As explained by Miller and Stuart (2003), the measurements were performed at 296 K.

682) Value for T = 295…298 K.

683) Value for T = 293…298 K.

684) The data from Schwardt et al. (2021) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-20.66741 + 2604.13624/T + 0.71646 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

685) Mackay et al. (2006b) list a vapor pressure p, a solubility c, and a Henry's law constant calculated as p/c. However, the data are internally inconsistent and deviate by more than 10 %.

686) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

687) The data from Schwardt et al. (2021) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-214.72727 + 12076.60512/T + 29.20360 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

688) A typo in Ashworth et al. (1988) has been corrected by Howe et al. (1987).

689) The data from Wright et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-332.68901 + 17925.88529/T + 46.77838 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

690) The data from Schwardt et al. (2021) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-6.68864 + 2211.35284/T - 1.35565 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

691) The data from Khalfaoui and Newsham (1994b) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-593.56757 + 30300.79738/T + 85.11672 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

692) The data from Wright et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-294.54970 + 16409.35487/T + 40.82700 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

693) The data from Cooling et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-511.78322 + 26710.11950/T + 72.88403 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

694) The data from Schwardt et al. (2021) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-265.05147 + 15058.79780/T + 36.44507 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

695) The data from Görgényi et al. (2002) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-480.92432 + 24776.46284/T + 68.60174 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

696) The data from Knauss et al. (2000) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-389.28726 + 21123.08804/T + 54.69871 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

697) The data from Khalfaoui and Newsham (1994b) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-511.93773 + 26713.30359/T + 72.90551 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

698) The data from Robbins et al. (1993) were fitted to the three-parameter equation: $H_s^{cp} = \exp(176.56015 - 5511.47473/T - 28.96682 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

699) The data from Wright et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(681.41357 - 27448.54898/T - 104.63745 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

700) The data from Cooling et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-574.03630 + 29404.80442/T + 82.22224 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

701) The data from Schwardt et al. (2021) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-330.94781 + 18207.73829/T + 46.05991 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

702) The data from Knauss et al. (2000) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-281.09217 + 15955.08953/T + 38.60107 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

703) The data from Robbins et al. (1993) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-1145.60543 + 55089.35358/T + 167.32916 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

704) The data from Wright et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-224.85290 + 13463.70772/T + 30.65123 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

705) Henry's law constants were evaluated using data from Florida sandy field soil.

706) According to Thomas et al. (2006), theoretical Henry's law constants were calculated using the "normal boiling point, the critical temperature, and the enthalpy of volatilization at the normal boiling point".

707) Haynes (2014) refers to Mackay and Shiu (1981), but that article lists this value for 1-chloro-2-methylpropane (the saturated compound), not for 1-chloro-2-methylpropene.

708) The regression parameters for chlorobenzene in Table 1 of Schwardt et al. (2021) are wrong. Corrected values from Schwardt et al. (2022) are used here.

709) The data from Schwardt et al. (2021) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-266.69788 + 14811.78372/T + 37.00246 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

710) The data from Khalfaoui and Newsham (1994b) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-757.46460 + 35956.18738/T + 110.75693 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

711) The data from Cooling et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-820.00716 + 38880.20610/T + 120.01460 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

712) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 8 % difference.

713) Erratum for page 344 of Fogg and Sangster (2003): their reference [89] does not contain 1,2-dichlorobenzene.

714) The data listed in Tables 2 and 3 of Dewulf et al. (1999) are inconsistent, with 7 % difference.

715) The data listed in Tables 2 and 3 of Dewulf et al. (1999) are inconsistent, with 7 % difference.

716) Rumble (2021) refers to Oliver (1985) as the source, but this value cannot be found there.

717) Value for T = 298…303 K.

718) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from multiple sources and obtained from the experimental octanol–water partition coefficient and the octanol–air partition coefficient.

719) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from a single database or data collection and obtained from the experimental octanol–water partition coefficient and the octanol–air partition coefficient.

720) Odabasi and Adali (2016) provide the parameters A and B for an equation to calculate temperature-dependent Henry's law constants. Values calculated with this equation at 298 K are slightly different than those measured at 298 K and given as H in their Table 1. Here, the values H and B are used.

721) Modified gas-stripping method (MGSM); see Lau et al. (2006) for details.

722) Integrated gas-stripping method (IGSM); see Lau et al. (2006) for details.

723) Calculated with the principal component regression (PCR) method; see Lee (2007) for details.

724) Calculated with the partial least-square regression (PLSR) method; see Lee (2007) for details.

725) The same data were also published in Dunnivant et al. (1988).

726) Value given here as quoted by Dunnivant et al. (1988).

727) Calculated using the EPICS method.

728) Calculated using the "Direct" method.

729) Westcott et al. (1981) give a range of $1.9\times10^{-2}\,\mathrm{mol\,m^{-3}\,Pa^{-1}} < H_s^{cp} < 3.2\times10^{-2}\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$.

730) Westcott et al. (1981) give a range of $2.8\times10^{-2}\,\mathrm{mol\,m^{-3}\,Pa^{-1}} < H_s^{cp} < 9.0\times10^{-2}\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$.

731) Erratum for page 350 of Fogg and Sangster (2003): the equation describing the recommended temperature-dependent data appears to be incorrect and is not used here.

732) Value at pH = 4.

733) When comparing H in Table 4 with K_{gw} in Table 5 of Pfeifer et al. (2001), it can be seen that the values refer to $K_{gw}\times100$ and not $K_{gw}/100$.

734) Measured at pH = 1.

735) The same data were also published in Brandsch et al. (1993).

736) Erratum for page 376 of Fogg and Sangster (2003): data from Santl et al. (1994) are cited incorrectly; it should be 3.64, not 3.84.

737) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 8 % difference.

738) Although pronamide and propyzamide are the same species, Mackay et al. (2006d) list two different values for them. It is unclear which number is correct (if any), and the data are not reproduced here.

739) The value at 20 °C was calculated from published values of vapor pressure and water solubility. Data between 25 °C and 40 °C were calculated from the measured evaporation rate.

740) At pH = 5.4.

741) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from multiple sources and measured directly.

742) The data from Zheng et al. (1997) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-206.94328 + 11372.60160/T + 28.22232\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

743) The data from Maaßen (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-200.57402 + 11192.93914/T + 27.21798\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

744) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-208.06388 + 11491.48483/T + 28.35421\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

745) The data from Chang and Criddle (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-1756.79407 + 80807.02552/T + 259.24906\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

746) The data from McLinden (1989) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-387.81156 + 19950.78638/T + 54.91348\ln(T))\,\mathrm{mol\,m^{-3}\,Pa^{-1}}$, with T in K.

747) The temperature dependence was recalculated from the data on p. 20 of McLinden (1989).

748) The data from McLinden (1989) for HCFC-22 are incorrectly cited by Kanakidou et al. (1995).

749) The H298 and A, B data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 5 % difference.

750) The H298 and A, B data listed in Table 5-4 of Burkholder et al. (2015) are inconsistent, with 5 % difference.

751) The H298 and A, B data listed in Table 5.4 of Sander et al. (2011) are inconsistent, with 5 % difference.

752) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(100.23590 - 3339.68982/T - 17.66849 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

753) The data from Scharlin and Battino (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-291.40685 + 14224.53456/T + 40.73325 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

754) The data from Scharlin and Battino (1994) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-291.40685 + 14224.53456/T + 40.73325 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

755) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-147.53824 + 8643.05363/T + 18.97752 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

756) The data from Scharlin and Battino (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-211.99699 + 11400.41036/T + 28.66283 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

757) The data from Scharlin and Battino (1994) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-211.99699 + 11400.41036/T + 28.66283 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

758) The data from Maaßen (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-278.68448 + 15169.41095/T + 38.36974 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

759) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-129.78084 + 8533.77911/T + 16.20428 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

760) The data from Bu and Warner (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-415.59157 + 21411.24346/T + 58.50528 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

761) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(0.13353 + 5070.08549/T - 4.84639 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

762) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-113.07654 + 6884.36758/T + 13.75470 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

763) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-149.62353 + 7869.46528/T + 19.40044 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

764) The data from Chang and Criddle (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-402.28495 + 20229.16189/T + 57.28419 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

765) The data from Maaßen (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-277.88370 + 14905.51805/T + 38.38688 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

766) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-195.56650 + 11207.08869/T + 26.12575 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

767) The data from Maaßen (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-249.15404 + 13774.89590/T + 34.23234 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

768) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-210.55601 + 11968.42846/T + 28.54087 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

769) The data from Maaßen (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-155.04312 + 9704.04801/T + 20.06575 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

770) The data from Maaßen (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-270.78344 + 14413.03953/T + 37.48366 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

771) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-184.96240 + 10541.13831/T + 24.70437 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

772) The data from Chang and Criddle (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-190.58060 + 10602.65774/T + 25.66197 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

773) The data from Maaßen (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-237.50724 + 13032.41274/T + 32.48569 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

774) The data from Reichl (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-200.95912 + 11406.81841/T + 27.03092 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

775) The data from Smith et al. (1981b) were fitted to the three-parameter equation: $H_s^{cp} = \exp(678.00770 - 27346.39638/T - 103.92351 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

776) Kanakidou et al. (1995) assume $H_s(\mathrm{CClF_2OONO_2}) = H_s(\mathrm{PAN})$.

777) The H298 and A, B data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 11 % difference.

778) The data from De Bruyn and Saltzman (1997) were fitted to the three-parameter equation:

$H_s^{cp} = \exp(-521.17646 + 25057.64644/T + 75.60914 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

779) The data from Glew and Moelwyn-Hughes (1953) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-184.73597 + 10636.09284/T + 25.03175 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

780) Values at 298 K in Tables C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

781) The data from Moore et al. (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-395.20167 + 20638.03484/T + 56.40082 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

782) The data from Wright et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-82.06673 + 6867.92071/T + 9.56720 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

783) The data from Moore et al. (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-408.59491 + 21699.59623/T + 58.19801 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

784) The data from Wright et al. (1992) were fitted to the three-parameter equation: $H_s^{cp} = \exp(1124.79951 - 46767.40872/T - 170.54217 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

785) Erratum for page 274 of Fogg and Sangster (2003): the value in the table is k_H, not $\ln k_H$.

786) Value at $T = 50$ K.

787) Rumble (2021) refers to Hiatt (2013) as the source, but this value cannot be found there.

788) Haynes (2014) refers to Mackay et al. (1993) as the source, but this value cannot be found there.

789) The data from Sarraute et al. (2006) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-370.06283 + 22192.71634/T + 51.12683 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

790) Erratum for page 321 of Fogg and Sangster (2003): data from Yates and Gan (1998) are cited with a typo. The value at 313.2 K should probably be 4.78×10^{-6}, not 4.78×10^{-2}.

791) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from a single original paper and obtained from the experimental octanol–water partition coefficient and the octanol–air partition coefficient.

792) Diaz et al. (2005) also cite a Henry's law constant from Pfeifer et al. (2001) even though this species is not mentioned there. There might be a mix up of the different haloanisoles.

793) Erratum for page 285 of Fogg and Sangster (2003): data in their table look strange (9.70R) and are not used here.

794) The data from Moore et al. (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-76.31131 + 7250.73360/T + 8.15388 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

795) The data from Moore et al. (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-265.18008 + 15516.80509/T + 36.54803 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

796) The data from Moore et al. (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-229.06923 + 13418.39257/T + 31.15669 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

797) The data from Glew and Moelwyn-Hughes (1953) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-384.31677 + 19391.25580/T + 54.93602 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

798) The data from Moore et al. (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-247.93525 + 14910.30572/T + 34.08071 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

799) The regression given by Fogg and Sangster (2003) does not produce the data in their table. Thus the regression was recalculated.

800) The value listed as A for iodobenzene is probably not A but the Henry's law volatility constant H_v^{px} at 298 K. For the value of B, a minus sign is probably missing.

801) The data from Moore et al. (1995) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-242.58767 + 14043.89458/T + 33.48497 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

802) Karagodin-Doyennel et al. (2021) probably assume that CH_2BrI has the same Henry's law constant as CH_2ClI.

803) The data from Haimi et al. (2006) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-266.45850 + 15036.99733/T + 36.80758 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

804) Yaws et al. (2003) present Henry's law constants based on water solubility and vapor pressure. The water solubility is calculated using a correlation to the boiling point. For the vapor pressures, no references are provided.

805) The data from Zin et al. (2016) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-419.66332 + 22034.35758/T + 59.55571 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

806) The data from Haimi et al. (2006) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-166.97891 +$

$10357.07398/T + 22.04420 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

807) The data from Haimi et al. (2006) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-406.56800 + 21428.82541/T + 57.60207 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

808) The data from Zin et al. (2016) were fitted to the three-parameter equation: $H_s^{cp} = \exp(10.26074 + 2303.75755/T - 4.36399 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

809) Presumably, the species called "42-methyl-2-butanethiol" in Table 1 of Yao et al. (2002) should be 2-methyl-2-butanethiol.

810) Schäfer and Lax (1962) present data based on Booth and Jolley (1943). However, these data appear to be incorrect.

811) Booth and Jolley (1943) converted data from Rex (1906) to another unit. However, this was apparently not done correctly.

812) Booth and Jolley (1943) present data from Chancel and Parmentier (1885). However, in that paper only the solubility at an unknown partial pressure of CS_2 was measured.

813) Value extracted from their Fig. 46.

814) The data from Haimi et al. (2006) were fitted to the three-parameter equation: $H_s^{cp} = \exp(-233.39763 + 13839.16150/T + 31.85189 \ln(T))$ mol m^{-3} Pa^{-1}, with T in K.

815) $H_s' = 6.4 \times 10^{14} \frac{\text{mol}^2}{\text{m}^6\,\text{Pa}}$

816) It is unclear how Fogg and Sangster (2003) obtained the data. Apparently, limiting activity coefficients γ^∞ were taken from Trampe and Eckert (1993), but a source for vapor pressure data is not mentioned. Also, the γ^∞ values listed in the table are different from those found in the original paper.

817) At pH = 3.9.

818) At pH = 4.8.

819) Mackay et al. (2006d) list two values for thiobencarb which differ by a large factor. It is unclear which number is correct (if any), and the data are not reproduced here.

820) Extrapolated from data at elevated temperatures.

821) Calculated using HENRYWIN 3.21.

822) Calculated using vapor pressures and water solubilities from HENRYWIN 3.21.

823) Calculated using vapor pressures and water solubilities from the EPA Toxicity Estimation Software Tool (TEST).

824) Wilhelm et al. (1977) and Abraham (1979) are quoted as the source. However, the data cannot be found there.

825) Shon et al. (2005) refer to Petersen et al. (1998) as the source, but this value cannot be found there.

826) The value from their experiment 7 at 10 °C is not used in the determination of the temperature dependence because of very different ionic strengths and concentrations for that experiment.

Code and data availability. All code and data related to the Henry's law database can be found in the Supplement and at https://www.henrys-law.org (Sander, 2023).

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