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Supplement of

Compilation and evaluation of gas phase diffusion coefficients of reactive trace gases in the atmosphere: Volume 2. Diffusivities of organic compounds, pressure-normalised mean free paths, and average Knudsen numbers for gas uptake calculations

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1 Alkanes and cycloalkanes

1.1 CH$_4$ (methane), C$_2$H$_6$ (ethane), and C$_3$H$_8$ (propane)

Last evaluated: 10 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
Methane	Coward and Georgeson, 1937	273	149	174	138	-7
	Muller and Cahill, 1964	298	164	164	161	-2
		353	218		217	-1
		382	252		249	-1
	Cowie and Watts, 1970	298	165	165	161	-2
ethane	Boyd et al., 1951	298	112	112	109	-3
	Elliott and Watts, 1972	298	116	116	109	-6
propane	Barr and Watts, 1972	298	87	87	86	-1

Comments:

methane: The diffusivities of methane measured at 298 K by Muller and Cahill (1964) and Cowie and Watts (1970) agree well with that extrapolated to 298 K from that at 273 K measured by Coward and Georgeson (1937). The measured diffusivities by the three studies agree well with the estimated values using Fuller's method over 273-382 K.

ethane: The diffusivities of ethane measured at 298 K by Boyd et al. (1951) and Elliot and Watts (1972) agree well, and are only a few percentages larger than the estimated value using Fuller's method.

propane: Only one study (Barr and Watts, 1972) measured the diffusivity of propoane (at 298 K), and the reported value is only 1% larger than the estimated value using Fuller's method.

Preferred value in N$_2$ (or air/O$_2$) at 298 K:

methane: (168±5) Torr cm^2 s^{-1}

The preferred diffusivity of methane at 298 K, (168±5) Torr cm^2 s^{-1}, is the average of those reported by Muller and Cahill (1965) at 298 K, Cowie and Watts (1970) at 298 K, and that extrapolated to 298 K from that measured at 273 K by Coward and Georgeson (1937).

ethane: (114±5) Torr cm^2 s^{-1}

The preferred diffusivity of ethane at 298 K, (114±5) Torr cm^2 s^{-1}, is the average of those reported at 298 K by Boyd et al. (1951) and Elliot and Watts (1972), and the given uncertainty reflects the difference between the preffered value and the estimated value using Fuller's method.

propane: (87±5) Torr cm^2 s^{-1}

The preferred diffusivity of propane at 298 K, (87±5) Torr cm^2 s^{-1}, is based on that reported by Barr and Watts (1972). Though the relative difference between the measured and estimated values is only 1%, a 5% uncertainty is given to the preferred value.

Last change in the preferred value: 10 July 2014

References:

Barr, J. K., and Sawyer, D. T.: Studies of the Liquid Phase Mass-Transfer Term in Gas Chromatography, *Anal. Chem.*, 36, 1753-1759, 1964.

Boyd, C. A., Stein, N., Steingrimsson, V., and Rumpel, W. F.: An Interferometric Method of Determining Diffusion Coefficients in Gaseous Systems, *J. Chem. Phys.*, 19, 548-553, 1951.

Coward, H. F., and Georgeson, E. H. M.: The diffusion coefficient of methane and air, *J. Chem. Soc.*, 1085-1087, 1937.

Cowie, M., and Watts, H.: Diffusion of Methane and Chloromethanes in Air, *Can. J. Chem.*, 49, 74-77, 1971.

Elliott, R. W., and Watts, H.: Diffusion of some Hydrocarbons in Air: a Regularity in the Diffusion Coefficients of a Homologous Series, *Can. J. Chem.*, 50, 31-34, 1972.

Muller, C. R., and Cahill, R. W.: Mass Spectrometric Measurement of Diffusion Coefficients, *J. Chem. Phys.*, 40, 651-654, 1964.

1.2 C$_4$H$_{10}$ (butane, methyl propane)

Last evaluated: 10 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
n-butane	Boyd et al., 1951	298	73	73	74	1
	Hargrove and Sawyer, 1967	298	73	73	74	2
	Fuller et al., 1969	302	76	74	75	-1
	Elliott and Watts, 1972	298	78	78	75	-3
	Gotoh et al., 1974	298	77	77	75	-3
		378	121		112	-8
		438	160		144	-10
methyl propane	Boyd et al., 1951	298	69	69	74	7
	Barr and Watts, 1972	298	73	73	74	1

Comments:

n-butane: The diffusivities measured at 298 K by Boyd et al. (1951), Hargrove and Sawyer (1967), Elliot and Watts (1972) and Gotoh et al. (1974) all agree well with that extrapolated to 298 K from that measured at 303 K by Fuller et al. (1969). The difference between the measured diffusivities and the estimated values over 298-438 K are not larger than 10%.

methyl propane: The diffusivities of methyl propane measurd by the two studies (Boyd et al., 1951; Barr and Watts, 1972) at 298 K agree well, and are only a few percentages smaller than the estimated value using Fuller's method.

Preferred value in N$_2$ (or air/O$_2$) at 298 K:

n-butane: (75 ± 3) Torr cm^2 s^{-1}

The preferred diffusivity of n-butane, (75 ± 3) Torr cm^2 s^{-1}, is the average of those reported by all the studies at 298 K (or extrapolated to 298 K if the measurement was not carried out at 298 K).

methyl propane: (71 ± 3) Torr cm^2 s^{-1}

The preferred diffusivity of methyl propane, (71 ± 3) Torr cm^2 s^{-1}, is the average reported by Boyd et al. (1951) and Barr and Watts (1972).

Last change in the preferred value: 10 July 2014

References:

Barr, J. K., and Sawyer, D. T.: Studies of the Liquid Phase Mass-Transfer Term in Gas Chromatography, *Anal. Chem.*, 36, 1753-1759, 1964.

Boyd, C. A., Stein, N., Steingrimsson, V., and Rumpel, W. F.: An Interferometric Method of Determining Diffusion Coefficients in Gaseous Systems, *J. Chem. Phys.*, 19, 548-553, 1951.

Elliott, R. W., and Watts, H.: Diffusion of some Hydrocarbons in Air: a Regularity in the Diffusion Coefficients of a Homologous Series, *Can. J. Chem.*, 50, 31-34, 1972.

Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. The effect of structure on collision cross sections, *J. Phys. Chem.*, 73, 3679-3685, 1969.

Gotoh, S., Manner, M., Sorensen, J. P., and Stewart, W. E.: Binary diffusion coefficients of low-density gases. I. Measurements by modified Loschmidt method, *J. Chem. Eng. Data*, 19, 169-171, 1974.

Hargrove, G. L., and Sawyer, D. T.: Determination of gaseous interdiffusion coefficients for solute vapor-carrier gas pairs, *Anal. Chem.*, 39, 244-246, 1967.

Muller, C. R., and Cahill, R. W.: Mass Spectrometric Measurement of Diffusion Coefficients, *J. Chem. Phys.*, 40, 651-654, 1964.

1.3 C_5H_{12} (n-pentane, methyl butane, dimethyl butane)

Last evaluated: 10 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
n-pentane	Lugg, 1968	298	64	64	65	2
	Arnikar and Ghule, 1969	353	103	77	88	-15
	Barr and Watts, 1972	298	65	65	65	0
	Nagasaka, 1973	258	51		51	-1
		263	53		52	-3
		268	56		54	-3
		273	57		56	-2
		278	59		58	-1
		283	61		59	-3
		288	63		61	-3
		293	65		63	-3
		298	67	67	65	-2
methyl butane	Elliott and Watts, 1972	298	71	71	65	-9
dimethyl propane	Elliott and Watts, 1972	298	67	67	65	-2

Comments:

n-pentane: The diffusivities of n-pentane at 298 K reported by Lugg (1968), Barr and Watts (1972), Nagasaka (1973) are in good agreement. The differencs between the reported diffusivities reported by these three studies and the estimated values using Fuller's method are <5%. Arnikar and Ghule (1969) measured its diffusivity at 353 K, 15% larger than the estimated value, and if extrapolated to 298 K, it is significantly larger than those reported by the other three studies. This may suggest that the value reported by Arnikar and Ghule (1969) is not reliable.

methyl butane: The diffusivity of methyl butane measured at 298 K by Elliott and Watts (1972) is 9% larger than the estimated value.

dimethyl propane: The diffusivity of dimethyl propane measured at 298 K by Elliott and Watts (1972) is 2% larger than the estimated value.

Preferred value in N_2 (or air/O_2) at 298 K:

n-pentane: (65±2) Torr cm^2 s^{-1}

The preferred diffusivity of n-pentane, (65±2) Torr cm^2 s^{-1}, is the average of those reported by Lugg (1968), Barr and Watts (1972), and Nagasaka (1973).

methyl butane: (71 ± 6) Torr cm^2 s^{-1}

The preferred diffusivity of methyl butane, (71 ± 6) Torr cm^2 s^{-1}, is based on the value reported by Elliott and Watts (1972), and the given uncertainty reflects the difference between the measured and estimated diffusivities.

dimethyl propane: (67 ± 2) Torr cm^2 s^{-1}

The preferred diffusivity of dimethyl propane, (71 ± 6) Torr cm^2 s^{-1}, is based on the value reported by Elliott and Watts (1972), and the given uncertainty reflects the difference between the measured and estimated diffusivities.

Last change in the preferred value: 10 July 2014

References:

Arnikar, H. J., and Ghule, H. M.: Electrodeless discharge as detector in the rapid determination of binary diffusion coefficient of gases, *Int. J. Electronics.*, 26, 159-162, 1969.

Barr, J. K., and Sawyer, D. T.: Studies of the Liquid Phase Mass-Transfer Term in Gas Chromatography, *Anal. Chem.*, 36, 1753-1759, 1964.

Elliott, R. W., and Watts, H.: Diffusion of some Hydrocarbons in Air: a Regularity in the Diffusion Coefficients of a Homologous Series, *Can. J. Chem.*, 50, 31-34, 1972.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

Nagasaka, M.: Binary diffusion coefficients of n-pentane in gases, *J. Chem. Eng. Data.*, 18, 388-390, 1973.

1.4 C_6H_{14} (n-hexane, 2,3-dimethyl butane)

Last evaluated: 10 July 2014

Species	Reference	T (K)	$D_m(T)$	$D_m(298)$	$D_e(T)$	(D_e/D_m-1) (%)
n-hexane	Cummings and Ubbelohde, 1953	289	58	61	56	-3
	Altshuller and Cohen, 1960	298	61	61	59	-3
		303	62		61	-1
		322	69		67	-2
	Lugg, 1968	298	56	56	59	6
	Arnikar and Ghule, 1969	353	133	99	79	-41
2,3-dimethyl butane	Cummings and Ubbelohde, 1953	289	57	60	56	-2

Comments:

n-hexane: The diffusivities measured at 298 K by Altshuller and Cohen (1960) and Lugg (1968) agree well, and are also in good agreement with that extrapolated to 298 K from that measured at 289 K by Cummings and Ubbelohde (1953). The difference between the diffusivities measured by these three studies and the estimated values is not larger than 6%. Arnikar and Ghule (1969) measured the diffusivity at 353 K, 41% larger than the estimated value using Fuller's method, and if extrapolated to 298 K, it is >50% larger than those reported by the other three studies. This may suggest that the value reported by Arnikar and Ghule (1969) is not reliable.

2,3-dimethyl butane: The diffusivity measured at 289 K by Cummings and Ubbelohde (1953) shows excellent agreement with the estimated value.

Preferred value in N_2 (or air/O_2) at 298 K:

n-hexane: (59±3) Torr cm^2 s^{-1}

The preferred diffusivity of n-hexane, (59±3) Torr cm^2 s^{-1}, is the average of those reported by Cummings and Ubbelohde (1953), Altshuller and Coehn (1960) and Lugg (1968) at 298 K (or extrapolated to 298 K if the measurement was not carried out at 298 K).

2,3-dimethyl butane: (60±2) Torr cm^2 s^{-1}

The preferred diffusivity of 2,3-dimethyl butane, (60±2) Torr cm^2 s^{-1}, is extrapolated to 298 K from the measurement of Cummings and Ubbelohde (1953) at 289 K. The given

uncertainty reflects the normalized difference between the measured and estimated diffusivities at 289 K.

Last change in the preferred value: 10 July 2014

References:

Altshuller, A. P., and Cohen, I. R.: Application of Diffusion Cells to Production of Known Concentration of Gaseous Hydrocarbons, *Anal. Chem.*, 32, 802-810, 1960.

Arnikar, H. J., and Ghule, H. M.: Electrodeless discharge as detector in the rapid determination of binary diffusion coefficient of gases, *Int. J. Electronics.*, 26, 159-162, 1969.

Cummings, G. A. M., and Ubbelohde, A. R.: Collision diameters of flexible hydrocarbon molecules in the vapour phase : the "hydrogen effect.", *J. Chem. Soc.*, 3751-3755, 1953.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

1.5 C$_7$H$_{16}$ (n-heptane, 2,4-dimethyl pentane)

Last evaluated: 10 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
n-heptane	Cummings et al., 1955	303	56	55	56	-1
	Clarke and Ubbelohde, 1957	303	56	55	56	0
	Altshuller and Cohen, 1960	290	54	56	52	-3
		338	64		68	6
2,4-dimethyl pentane	Clarke and Ubbelohde, 1957	303	57	55	56	-1

Comments:

n-heptane: The measured diffusvities (Cummings et al., 1955; Clarke and Ubbelohde, 1957; Altshuller and Cohen) over 290-338 K show excellent agreement with the estimated values. If extrapolated to 298 K, all three studies agree well with each other.

2,4-dimethyl pentane: The only measurement by Clarke and Ubbelohde (1957) shows excellent agreement with the estimation.

Preferred value in N$_2$ (or air/O$_2$) at 298 K:

n-heptane: (55±2) Torr cm^2 s^{-1}

The preferred diffusivity of n-heptane, (59±2) Torr cm^2 s^{-1}, is the average of those extrapolated to 298 K from those measured at 303 K by Cuymmings et al. (1955) and Clarke and Ubbelohde (1957) and at 290 K by Altshuller and Cohen (1960). The given uncertainty reflects the difference between the measurement and estimation.

2,4-dimethyl pentane: (55±2) Torr cm^2 s^{-1}

The measurement by Clark and Ubbelohde (1957) at 303 K is preferred, and it gives a lue of 55 Torr cm^2 s^{-1} after being extrapolated to 298 K.

Last change in the preferred value: 10 July 2014

References:

Altshuller, A. P., and Cohen, I. R.: Application of Diffusion Cells to Production of Known Concentration of Gaseous Hydrocarbons, *Anal. Chem.*, 32, 802-810, 1960.

Clarke, J. K., and Ubbelohde, A. R.: Isotope effects in diffusion cross-sections for flexible hydrocarbons, *J. Chem. Soc.*, 2050-2055, 1957.

Cummings, G. A. M., McLaughlin, E., and Ubbelohde, A. R.: Collision parameters of C6-C9 hydrocarbons in the vapour phase: the hydrogen effect, *J. Chem. Soc.*, 1141-1144, 1955.

1.6 C_8H_{18} (n-octane, 2,2,4-trimethyl pentane)

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
n-octane	Mack, 1925	298	46	46	50	9
	Cummings and Ubbelohde, 1953	303	54	52	52	-4
	Clarke and Ubbelohde, 1957	303	55	54	52	-6
	Lugg, 1968	298	47	47	50	7
2,2,4-trimethyl pentane	Cummings and Ubbelohde, 1953	303	54	53	52	-4
	Clarke and Ubbelohde, 1957	303	54	53	52	-3

Comments:

n-octane: The measured diffusvities at 298 K by the two studies (Mack, 1925; Lugg, 1968) agree well. The other two studies (Cummings and Ubbelohde, 1953; Clarke and Ubbelohde) measured it at 303 K, and the reported values, after being extrapolated to 298 K, show good agreement with these reported by Mack (1925) and Lugg (1968). The differences between the measured and estimated diffusivities at 298 and 303 K are <10%.

2,2,4-trimethyl pentane: The measured diffusivities at 303 K, reported by Cummings and Ubbelohde (1953) and Clarke and Ubbelohde (1957) are in good agreement, and are only 4% different from the estimated values using Fuller's method.

Preferred value in N_2 (or air/O_2) at 298 K:

n-octane: (50 ± 4) Torr cm^2 s^{-1}

The preferred diffusivity of n-octane at 298 K, (50 ± 4) Torr cm^2 s^{-1}, is the average of these reported by all the four studies (extrapolated to 298 K if the measurement was not performed at 298 K).

2,2,4-trimethyl pentane: (53 ± 2) Torr cm^2 s^{-1}

The preferred diffusivity of n2,2,4-trimethyl pentane at 298 K, (53 ± 2) Torr cm^2 s^{-1}, is based on the values measured by Cummings and Ubbelohde (1953) and Clarke and Ubbelohde (1957). The given uncertainty reflects the difference between the measurement and estimation.

References:

Clarke, J. K., and Ubbelohde, A. R.: Isotope effects in diffusion cross-sections for flexible hydrocarbons, *J. Chem. Soc.*, 2050-2055, 1957.

Cummings, G. A. M., McLaughlin, E., and Ubbelohde, A. R.: Collision parameters of C6-C9 hydrocarbons in the vapour phase: the hydrogen effect, *J. Chem. Soc.*, 1141-1144, 1955.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

Mack, E.: Average cross-sectional areas of molecules by gaseous diffusion methods, *J. Am. Chem. Soc.*, 47, 2468-2482, 1925.

1.7 C_9H_{20} (n-nonane), $C_{10}H_{22}$ (n-decane, 2,3,3-trimethyl heptane) and $C_{12}H_{26}$ (n-dodecane)

Last evaluated: 11 July 2014

Species	Reference	T (K)	$D_m(T)$	$D_m(298)$	$D_e(T)$	(D_e/D_m-1) (%)
n-nonane	Cummings et al., 1955	340	56	44	60	7
n-decane	Cummings and Ubbelohde, 1953	364	64	45	64	0
	Altshuller and Cohen, 1960	313	46	42	49	6
		334	52		55	5
		357	59		61	4
		391	66		72	10
		422	71		82	16
2,3,3-trimethyl heptane	Cummings and Ubbelohde, 1953	303	54	52	46	-14
n-dodecane	Cummings and Ubbelohde, 1953	399	62	37	68	10

Comments:

n-nonane: The diffusivity of n-nonane was measured only measured by one study (Cummings et al., 1955) at 340 K, and the agreement with the estimated value is good.

n-decane: Both studies (Cummings and Ubbelohde, 1953; Altshuller and Cohen, 1960) were carried out above 310 K. The measured diffusivities over 313-422 K agree well with the estimated values, though it appears that the difference becomes larger at higher temperature. If extrapolated to 298 K, the two measurements show good agreement.

2,3,3-trimethyl heptane: The diffusivity of 2,3,3-trimethyl heptane was only measured by one study (Cummings and Ubbelohde, 1953) at 309 K, and the reported value is 14% larger than the estimated one.

n-dodecane: The diffusivity of n-dodecane was only measured by one study (Cummings and Ubbelohde, 1953) at 399 K, and the reported value is 10% lower than the estimated one.

Preferred value in N_2 (or air/O_2) at 298 K:

n-nonane: (44±4) Torr cm^2 s^{-1}

The diffusivity of n-nonane, measured by Cumming et al. (1955) at 340 K, (56±4) Torr cm^2 s^{-1}, is preffered. It gives a value of (44±4) Torr cm^2 s^{-1} when extrapolated

to 298 K. The given uncertainty reflects the difference between the measurement and estimation.

n-decane: (44 ± 2) Torr cm^2 s^{-1}

The preferred value, (44 ± 2) Torr cm^2 s^{-1}, is the average of those extrapolated to 298 K from those measured at 364 K by Cummings and Ubbelohde (1953) and at 313 K by Altshuller and Cohen (1960).

2,3,3-trimethyl heptane: (52 ± 8) Torr cm^2 s^{-1}

The measurement by Cummings and Ubbelohde (1953) is preferred, giving recommended values of (54 ± 8) Torr cm^2 s^{-1} at 303 K and (52 ± 8) Torr cm^2 s^{-1} at 298 K. The given uncertainty reflects the difference between the measurement and estimation.

n-dodecane: (37 ± 4) Torr cm^2 s^{-1}

The measurement by Cummings and Ubbelohde (1953) is preferred, giving recommended values of (62 ± 7) Torr cm^2 s^{-1} at 399 K and (37 ± 4) Torr cm^2 s^{-1} at 298 K.

Last change in the preferred value: 11 July 2014

References:

Altshuller, A. P., and Cohen, I. R.: Application of Diffusion Cells to Production of Known Concentration of Gaseous Hydrocarbons, *Anal. Chem.*, 32, 802-810, 1960.

Cummings, G. A. M., McLaughlin, E., and Ubbelohde, A. R.: Collision parameters of C6-C9 hydrocarbons in the vapour phase: the hydrogen effect, *J. Chem. Soc.*, 1141-1144, 1955.

Cummings, G. A. M., and Ubbelohde, A. R.: Collision diameters of flexible hydrocarbon molecules in the vapour phase : the "hydrogen effect.", *J. Chem. Soc.*, 3751-3755, 1953.

1.8 $C_{16}H_{34}$ (n-hexadecane), $C_{17}H_{36}$ (n-heptadecane) and $C_{18}H_{38}$ (n-octadecane)

Last evaluated: 11 July 2014

Species	Reference	T (K)	$D_m(T)$	$D_m(298)$	$D_e(T)$	(D_e/D_m-1) (%)
n-hexadecane	Bradley and Shellard, 1949	288	29		33	13
		290	30		33	11
		293	30		34	14
		298	31	31	35	15
		303	32		36	11
		308	33		37	12
n-heptadecane	Bradley and Shellard, 1949	288	31		32	4
		293	32		33	3
		298	32	32	34	6
		303	33		35	6
		308	34		36	5
		313	35		37	5
n-octadecane	Bradley and Shellard, 1949	288	29		31	5
		293	30		32	6
		298	32	32	33	4
		303	31		34	10
		308	32		35	9
		313	35		36	4

Comments:

n-hexadecane, n-heptadecane, n-octadecane: The diffusivities of n-hexadecane, n-heptadecane and n-octadecane were only measured by one study (Bradley and Shellard, 1949) over 299-313 K. The differences between the measurements and estimations are usually <15%.

Preferred value in N_2 (or air/O_2) at 298 K:

n-hexadecane: (31 ± 5) Torr cm^2 s^{-1}

n-heptadecane: (32 ± 5) Torr cm^2 s^{-1}

n-octadecane: (32 ± 5) Torr cm^2 s^{-1}

The preferred diffusivities of of n-hexadecane, n-heptadecane and n-octadecane are based on the measurements at 298 K by Bradley and Shellard (1949). The given uncertainties reflects the difference between the measurement (Bradley and Shellard, 1949) and the estimation over the temperature range investigated by Bradley and Shellard (1949).

Last change in the preferred value: 11 July 2014

References:

Bradley, R. S., and Shellard, A. D.: The Rate of Evaporation of Droplets. III. Vapour Pressures and Rates of Evaporation of Straight-Chain Paraffin Hydrocarbons, ***Proc. Roy. Soc. A***, 198, 239-251, 1949.

1.9 C_3H_6 (cyclopropane), C_5H_{10} (cyclopentane) and C_6H_{12} (cyclohexane, methyl cyclopentane)

Last evaluated: 11 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
cyclopropane	Elliott and Watts, 1972	298	97	97	90	-7
cyclopentane	Elliott and Watts, 1972	298	70	70	62	-11
cyclohexane	Cummings and Ubbelohde, 1953	289	58	61	57	-1
	Hudson et al., 1960	289	57	60	57	1
	Nagata and Hasegawa, 1970	363	94	67	85	-10
		383	102		93	-9
		403	113		102	-10
methyl cyclopentane	Cummings and Ubbelohde, 1953	286	58	62	56	-3

Comments:

cyclopropane and cyclopentane: The diffusivities of cyclopropane and cyclppentane were measured at 298 K by Elliott and Watts (1972), and the measurements agree well with estimation.

cyclonehexane: The diffusivities of cyclohexane were measured at 289 K by Cummings and Ubbelohde (1953) and Hudson et al. (1960) and over 363-403 K by Nagata and Hasegawa (1970). All the measurements agree well with estimation. If extrapolated to 298 K, the measurements by the three studies show good agreement.

methyl cyclopentane: The diffusivity of methyl cyclopentane was only measured by one study (Cummings and Ubbelohde, 1953) at 286 K, and the reported value agrees very well with the estimated one.

Preferred value in N_2 (or air/O_2) at 298 K:

cyclopropane: (97±7) Torr cm^2 s^{-1}

cyclopentane: (70±8) Torr cm^2 s^{-1}

The measured diffusivities of cyclopropane and cyclopentane at 298 K by Elliott and Watts (1972) are preferred. The given uncertainties reflects the differences between the measurements and estimations.

cyclonehexane: (63±4) Torr cm^2 s^{-1}

The preferred diffusivity of cyclohexane, is the average of those extrapolated to 298 K of those measured at 289 K by Cummings and Ubbelohde (1953) and Hudson et al. (1960) and at 363 K by Nagata and Hasegawa (1970).

methyl cyclopentane: (62 ± 2) Torr cm^2 s^{-1}

The measurement by Cummings and Ubbelohde (1953) is preffered. The recommended diffusivities are (58 ± 2) Torr cm^2 s^{-1} at 286 K and thus (62 ± 2) Torr cm^2 s^{-1} at 298 K. The given uncertainties reflects the difference between the measurement and estimation.

Last change in the preferred value: 11 July 2014

References:

Clarke, J. K., and Ubbelohde, A. R.: Isotope effects in diffusion cross-sections for flexible hydrocarbons, *J. Chem. Soc.*, 2050-2055, 1957.

Elliott, R. W., and Watts, H.: Diffusion of some Hydrocarbons in Air: a Regularity in the Diffusion Coefficients of a Homologous Series, *Can. J. Chem.*, 50, 31-34, 1972.

Hudson, G. H., McCoubrey, J. C., and Ubbelohde, A. R.: Vapour diffusion coefficients and collision parameters for cyclic molecules, *Trans. Faraday Soc.*, 56, 1144-1151, 1960.

Nagata, I., and Hasegawa, T.: Gaseous interdiffusion coefficients, **J. Chem. Eng. Japan**, 3, 143-145, 1970.

2 Alkenes and alkynes

2.1 C_2H_4 (ethene) and C_3H_6 (propnene)

Last evaluated: 11 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
ethene	Boyd et al., 1951	298	124	124	115	-7
	Knox and McLaren, 1964	291	124	129	110	-11
	Muller and Cahill, 1964	298	129	129	115	-11
		373	192		170	-12
	Evans and Kenney, 1965	287	109	117	108	-1
		291	114	119	110	-3
	Fuller et al., 1969	303	129	125	118	-9
	Elliott and Watts, 1972	298	126	126	115	-9
propene	Elliott and Watts, 1972	298	100	100	90	-10

Comments:

ethene: The diffusivities of ethene were measured over 287-373 K (Boyd et al., 1951; Knox and McLaren, 1964; Muller and Cahill, 1964; Evans and Kenney, 1965; Fuller et al., 1969; Elliott and Watts, 1972), and the differences between the measured and estimated diffusivities are not larger than 12%. If extrapolated to 298 K, all the five measurements agree well.

propene: The diffusivity of propene was only measured by one study (Elliott and Watts, 1972) at 298 K, and the difference between the measured and estimated diffusivities is ~10%.

Preferred value in N_2 (or air/O_2) at 298 K:

ethene: (124±5) Torr cm^2 s^{-1}

The preferred diffusivity of ethene at 298 K, (124±5) Torr cm^2 s^{-1}, is the average of those measured at or extrapolated to this tempearture by all the five studies (Boyd et al., 1951; Knox and McLaren, 1964; Muller and Cahill, 1964; Evans and Kenney, 1965; Fuller et al., 1969; Elliott and Watts, 1972).

propene: (100±10) Torr cm^2 s^{-1}

The measurement at 298 K by Elliott and Watts (1972) is preferred, and the given uncertainty reflects the difference between the measured and estimated diffusivities.

Last change in the preferred value: 11 July 2014

References:

Boyd, C. A., Stein, N., Steingrimsson, V., and Rumpel, W. F.: An Interferometric Method of Determining Diffusion Coefficients in Gaseous Systems, *J. Chem. Phys.*, 19, 548-553, 1951.

Elliott, R. W., and Watts, H.: Diffusion of some Hydrocarbons in Air: a Regularity in the Diffusion Coefficients of a Homologous Series, *Can. J. Chem.*, 50, 31-34.

Evans, E. V., and Kenney, C. N.: Gaseous Dispersion in Laminar Flow Through a Circular Tube, *Proc. Roy. Soc. A*, 284, 540-550, 1965.

Fuller, E. N., Ensley, K., and Giddings, J. C.: Diffusion of halogenated hydrocarbons in helium. The effect of structure on collision cross sections*, J. Phys. Chem.*, 73, 3679-3685, 1969.

Knox, J. H., and McLaren, L.: A New Gas Chromatographic Method for Measuring Gaseous Diffusion Coefficients and Obstructive Factors, *Anal. Chem.*, 36, 1477-1482, 1964.

Muller, C. R., and Cahill, R. W.: Mass Spectrometric Measurement of Diffusion Coefficients, *J. Chem. Phys.*, 40, 651-654, 1964.

2.2 C$_4$H$_8$ (1-butene, cis-2-butene, trans-2-butene, 2-methyl propene)

Last evaluated: 11 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
1-butene	Elliott and Watts, 1972	298	83	83	76	-8
cis-2-butene	Elliott and Watts, 1972	298	83	83	76	-8
trans-2-butene	Elliott and Watts, 1972	298	86	86	76	-12
2-methyl propene	Elliott and Watts, 1972	298	81	81	76	-7

Comments:

1-butene, cis-2-butene, trans-2-butene, and 2-methyl propene: The diffusivities of 1-tutene and its other three isomers were measured by one study (Elliott and Watts, 1972) at 298 K, and the differences between the measured and estimated diffusivities are typically ~10%.

Preferred value in N$_2$ (or air/O$_2$) at 298 K:

1-butene, cis-2-butene, trans-2-butene, and 2-methyl propene: (83±10) Torr cm^2 s^{-1}

The preferred diffusivities are based on the measurement by Elliott and Watts (1972). S single preferred value is given to all the four isomers, equal to the average of measured diffusivitie of these four compounds, and the given uncertainty (±12%) reflect the difference between the measurement and estimation.

Last change in the preferred value: 11 July 2014

References:

Elliott, R. W., and Watts, H.: Diffusion of some Hydrocarbons in Air: a Regularity in the Diffusion Coefficients of a Homologous Series, *Can. J. Chem.*, 50, 31-34.

2.3 C_5H_{10} (1-pentene), C_6H_{12} (1-hexene, 2-3-dimethyl-2-butene), C_8H_{16} (1-octene)

Last evaluated: 11 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	$(D_e/D_m$-1) (%)
1-pentene	Elliott and Watts, 1972	298	73	73	67	-8
1-hexene	Altshuller and Cohen, 1960	293	60	62	58	-3
2,3-dimethyl-2-butene	Cummings et al., 1955	288	57	60	57	0
1-octene	Altshuller and Cohen, 1960	313	54	49	56	4

Comments:

1-pentene: The diffusivity of 1-pentene was measured by one study (Elliott and Watts, 1972) at 298 K, and the reported value is 8% larger than the estimated one.

1-hexene and 2,3-dimethyl-2-butane: The diffusivity of 1-hexene was measured by Altshuller and Cohen (1960) at 293 K and that of 2,3-dimethyl-2-butene was measured by Cummings et al. (1955) at 288 K. Both measurements show excellent agreement with the estimations.

1-octene: The diffusivity of 1-octene was measured at 313 K by Altshuller and Cohen (1960), and the measured value is 4% lower than the estimated one.

Preferred value in N_2 (or air/O_2) at 298 K:

1-pentene: (73±6) Torr cm^2 s^{-1}

The preferred diffusivity of 1-pentene, (73±6) Torr cm^2 s^{-1}, is based on the measurement by Elliott and Watts (1972), and the given uncertainty reflects the difference between the measured and estimated values.

1-hexene and 2,3-dimethyl-2-butene: (61±2) Torr cm^2 s^{-1}

A single preferred diffusivity at 298 K, (61±2) Torr cm^2 s^{-1}, is given to both 1-hexene and 2,3-dimethyl-2-butene. It is the average of those extrapolated to 298 K from that measured at 293 K for 1-hexene by Altshuller and Cohen (1960) and at 288 K for 2,3-dimethyl-2-butene by Cummings et al. (1955).

1-octene: (49±2) Torr cm^2 s^{-1}

The preferred diffusivity of 1-octene, is based on the measurement at 313 K by Altshuller and Cohen (1960), extrapolated to 298 K. The given uncertainty reflects the difference between the measured and estimated diffusivities.

Last change in the preferred value: 11 July 2014

References:

Altshuller, A. P., and Cohen, I. R.: Application of Diffusion Cells to Production of Known Concentration of Gaseous Hydrocarbons, *Anal. Chem.*, 32, 802-810, 1960.

Cummings, G. A. M., McLaughlin, E., and Ubbelohde, A. R.: Collision parameters of C6-C9 hydrocarbons in the vapour phase: the hydrogen effect, *J. Chem. Soc.*, 1141-1144, 1955.

Elliott, R. W., and Watts, H.: Diffusion of some Hydrocarbons in Air: a Regularity in the Diffusion Coefficients of a Homologous Series, *Can. J. Chem.*, 50, 31-34.

2.4 C_3H_4 (propadiene), C_4H_6 (1,3-butadiene), C_5H_8 (isoprene), C_6H_{10} (1,5-hexadiene, 2,3-dimethyl-1,2-butadiene)

Last evaluated: 11 July 2014

Species	Reference	T (K)	$D_m(T)$	$D_m(298)$	$D_e(T)$	$(D_e/D_m\text{-}1)$ (%)
propadiene	Elliott and Watts, 1972	298	106	106	93	-12
1,3-butadiene	Elliott and Watts, 1972	298	88	88	78	-11
isoprene	Altshuller and Cohen, 1960	288	69	73	64	-7
1,5-hexadiene	Cummings et al., 1955	288	59	62	58	-1
2,3-dimethyl-1,3-butadiene	Cummings et al., 1955	288	57	60	58	2

Comments:

propadiene, 1,3-butadiene and C_5H_8: The diffusivities of propadiene and 1,3-butadiene were measured by Elliott and Watts (1972) at 298 K and that of isoprene was measured by Altshuller and Cohen (1960) at 288 K. The differences between the measured and estimated values are ~10%.

1,5-hexadiene and 2,3-dimethyl-1,3-butadiene: The diffusivities of 1,5-hexadiene and 2,3-dimethyl-1,3-butadiene were measured at 288 K by Cummings et al. (1955), and the measured diffusivities are in excellent agreement with the estimated values.

Preferred value in N_2 (or air/O_2) at 298 K:

propadiene: (106±13) Torr cm^2 s^{-1}

1,3-butadiene: (88±10) Torr cm^2 s^{-1}

isoprene: (73±6) Torr cm^2 s^{-1}

The preferred diffusivities of propadiene and 1,3-butadiene are based on the measurement of Elliott and Watts (1972) at 298 K, and that of isoprene is based on the measurement of Altshuller and Cohen (1960) at 288 K, extrapolated to 298 K. The uncertainties reflects the corresponding difference between the measurements and estimations.

1,5-hexadiene and 2,3-dimethyl-1,3-butadiene: (61±2) Torr cm^2 s^{-1}

A single preferred diffusivity, (61±2) Torr cm^2 s^{-1}, is given to both 1,5-hexadiene and 2,3-dimethyl-1,3-butadiene. It is the average of those extrapolated to 298 K from those measured at 288 K by Cummings et al. (1955). The given uncertainty reflects the difference between the measured and estimated diffusivities.

References:

Altshuller, A. P., and Cohen, I. R.: Application of Diffusion Cells to Production of Known Concentration of Gaseous Hydrocarbons, *Anal. Chem.*, 32, 802-810, 1960.

Cummings, G. A. M., McLaughlin, E., and Ubbelohde, A. R.: Collision parameters of C6-C9 hydrocarbons in the vapour phase: the hydrogen effect, *J. Chem. Soc.*, 1141-1144, 1955.

Elliott, R. W., and Watts, H.: Diffusion of some Hydrocarbons in Air: a Regularity in the Diffusion Coefficients of a Homologous Series, *Can. J. Chem.*, 50, 31-34.

2.5 C_2H_2 (ethyne), C_3H_4 (propyne), C_4H_6 (1-butyne)

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
ethyne	Elliott and Watts, 1972	298	111	111	123	11
propyne	Elliott and Watts, 1972	298	100	100	93	-7
1-butyne	Elliott and Watts, 1972	298	88	88	78	-12

Comments:

ethyne, propyne, and 1-butyne: The diffusivities of ethyne, propyne, and 1-butyne were measured at 298 K by Elliott and Watts (1972), and the differences between the measured and estimated values are ~10%.

Preferred value in N_2 (or air/O_2) at 298 K:

ethyne: (111 ± 12) Torr cm^2 s^{-1}

propyne: (100 ± 7) Torr cm^2 s^{-1}

1-butyne: (88 ± 10) Torr cm^2 s^{-1}

The preferred diffusivities of ethyne, propyne, and 1-butyne are based on the measurement by Elliott and Watts (1972), and the given uncertainties reflects the corresponding differences between the measured and estimated values.

References:

Elliott, R. W., and Watts, H.: Diffusion of some Hydrocarbons in Air: a Regularity in the Diffusion Coefficients of a Homologous Series, *Can. J. Chem.*, 50, 31-34.

3 Aromatic hydrocarbons

3.1 C$_6$H$_6$ (benzene)

Last evaluated: 12 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	$(D_e/D_m$-1) (%)
benzene	Lee and Wilke, 1954	298	73	73	69	-6
	Altshuller and Cohen, 1960	300	70	70	70	-1
		303	72		71	-2
		334	87		84	-4
	Hudson et al., 1960	311	77	72	74	-4
	Getzinger and Wilke, 1967	308	81	77	73	-10
	Lugg, 1968	298	71	71	69	-3
	Katan, 1969	295	69	70	68	-1
	Arnikar and Ghule, 1969	353	101	75	93	-8
	Nagata and Hasegawa, 1970	364	98	69	98	0
		378	106		105	-1
		393	117		113	-3
		408	124		119	-4
		423	125		127	1

Comments:

The diffusivities of benzene were measured over a broad temperature range (295-423 K), and the differences between the measured and estimated values are <10%. If extrapolated to 298 K, the diffusivities measured at other temperatures (Altshuller and Cohen, 1960; Hudson et al., 1960; Getzinger and Wilke, 1967; Katan, 1969, Arnikar and Ghule, 1969; Nagata and Hasegawa, 1970) agree well with those measured at 298 K (Lee and Wilke, 1954; Lugg, 1968).

Preferred value in N$_2$ (or air/O$_2$) at 298 K: (72±3) Torr cm^2 s^{-1}

The preferred diffusivity at 298 K, is the average of those measured at 298 K (Lee and Wilke, 1954; Lugg, 1968) and those extrapolated to 298 K from those measured at other temperatures (Altshuller and Cohen, 1960; Hudson et al., 1960; Getzinger and Wilke, 1967; Katan, 1969, Arnikar and Ghule, 1969; Nagata and Hasegawa, 1970).

Last change in the preferred value: 12 July 2014

References:

Altshuller, A. P., and Cohen, I. R.: Application of Diffusion Cells to Production of Known Concentration of Gaseous Hydrocarbons, *Anal. Chem.*, 32, 802-810, 1960.

Arnikar, H. J., and Ghule, H. M.: Electrodeless discharge as detector in the rapid determination of binary diffusion coefficient of gases, ***Int. J. Electronics.***, 26, 159-162, 1969.

Getzinger, R. W., and Wilke, C. R.: An experimental study of nonequimolal diffusion in ternary gas mixtures, ***Aiche J.***, 13, 577-580, 1967.

Hudson, G. H., McCoubrey, J. C., and Ubbelohde, A. R.: Vapour diffusion coefficients and collision parameters for cyclic molecules, ***Trans. Faraday Soc.***, 56, 1144-1151, 1960.

Katan, T.: Diffusion Coefficients of Vapors Measured with a Moving Boundary, ***J. Chem. Phys.***, 50, 233-238, 1969.

Lee, C. Y., and Wilke, C. R.: Measurements of vapor diffusion coefficient, ***Ind. Eng. Chem.***, 46, 2381-2387, 1954.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Anal. Chem.***, 40, 1072-1077, 1968.

Nagata, I., and Hasegawa, T.: Gaseous interdiffusion coefficients, ***J. Chem. Eng. Japan***, 3, 143-145, 1970.

3.2 C$_7$H$_8$ (toluene)

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
toluene	Mack, 1925	298	64	64	62	-3
	Gilliland, 1937	299	65	65	62	-5
		312	70		67	-4
		332	79		75	-5
	Fairbanks and Wilke, 1950	301	74	73	63	-15
	Altshuller and Cohen, 1960	298	69	69	62	-10
		318	73		69	-6
	Lugg, 1968	298	65	65	62	-4

Comments:

The diffusivities of toluene were measured over 298-332 K, and the differences between the measured and estimated diffusivities are <15%.

Preferred value in N$_2$ (or air/O$_2$) at 298 K: (67±4) Torr cm^2 s^{-1}

The preferred diffusivity at 298 K, is the average of those measured at 298 K (Mack, 1925; Altshuller and Cohen, 1960; Lugg, 1968) and those extraploted to 298 K from those measured at other temperatures (Gilliland, 1937; Fairbank and Wilke, 1950).

References:

Altshuller, A. P., and Cohen, I. R.: Application of Diffusion Cells to Production of Known Concentration of Gaseous Hydrocarbons, *Anal. Chem.*, 32, 802-810, 1960.

Fairbanks, D. F., and Wilke, C. R.: Diffusion Coefficients in Multicomponent Gas Mixtures, *Ind. Eng. Chem.*, 42, 471-475, 1950.

Gilliland, E. R.: Diffusion Coefficients in Gaseous Systems, *Ind. Eng. Chem.*, 26, 681-685, 1934.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

Mack, E.: Average cross-sectional areas of molecules by gaseous diffusion methods, *J. Am. Chem. Soc.*, 47, 2468-2482, 1925.

3.3 C$_8$H$_{10}$ (ethyl benzene, o-xylene, m-xylene, p-xylene)

Last evaluated: 11 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
ethyl benzene	Lugg, 1968	298	57	57	57	-1
o-xylene	Lugg, 1968	298	55	55	57	3
m-xylene	Lugg, 1968	298	52	52	57	9
p-xylene	Lugg, 1968	298	51	51	57	12

Comments:

ethyl benzene, o-xylene, m-xylene, p-xylene:

The differences between the measured (Lugg, 1968) and estimated diffusivities at 298 K are 1%, 3%, 9%, and 12% for ethyl benzene, o-xylene, m-xylene and p-xylene, respectively.

Preferred value in N$_2$ (or air/O$_2$) at 298 K:

ethyl benzene: (57±1) Torr cm^2 s^{-1}

o-xylene: (55±2) Torr cm^2 s^{-1}

m-xylene: (52±5) Torr cm^2 s^{-1}

p-xylene: (51±6) Torr cm^2 s^{-1}

The measured diffusivities at 298 K by Lugg (1968) are preferred, and the given uncertainties reflects the differences between the measurements and estimations.

Last change in the preferred value: 11 July 2014

References:

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

3.4 C$_9$H$_{12}$ (n-propylbenzene, iso-propylbenzene, 1,2,4-trymethylbenzene, 1,3,5-trimethylbenzene)

Last evaluated: 11 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
n-propyl benzene	Lugg, 1968	298	51	51	53	4
iso-propyl benzene	Lugg, 1968	298	51	51	53	3
1,2,4-trimethyl benzene	Lugg, 1968	298	49	49	53	9
1,3,5-trimethyl benzene	Lugg, 1968	298	50	50	53	5

Comments:

n-propyl benzene, iso-propyl benzene, 1,2,4-trimethyl benzene, 1,3,5-trimethyl benzene:

The measured diffusivities of n-propyl benzene, iso-propyl benzene, 1,2,4-trimethyl benzene, and 1,3,5-trimethyl benzene at 298 K are 4%, 3%, 9%, and 5% lower than the estimated values, respectively.

Preferred value in N$_2$ (or air/O$_2$) at 298 K:

n-propyl benzene: (51±2) Torr cm^2 s^{-1}

iso-propyl benzene: (51±2) Torr cm^2 s^{-1}

1,2,4-trimethyl benzene: (49±4) Torr cm^2 s^{-1}

1,3,5-trimethyl benzene: (50±3) Torr cm^2 s^{-1}

The measured diffusivities at 298 K by Lugg (1968) are preferred, and the given uncertainties reflects the differences between the measurements and estimations.

Last change in the preferred value: 11 July 2014

References:

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

3.5 $C_{10}H_{14}$ (p-cymene, p-tert-butyltolyene) and C_8H_8 (styrene)

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
p-cymene	Lugg, 1968	298	48	48	49	2
p-tert-butyl toluene	Lugg, 1968	298	43	43	49	13
styrene	Lugg, 1968	298	53	53	58	9

Comments:

p-cymene, p-tert-butyl toluene, styrene: The measured diffusivities of p-cymene, p-tert-butyl toluene, and styrene at 298 K (Lugg, 1968) are 2%, 13%, and 9% lower than the estimated values, respectively.

Preferred value in N_2 (or air/O_2) at 298 K:

p-cymene: (48±1) Torr cm^2 s^{-1}

p-tert-butyl toluene: (43±6) Torr cm^2 s^{-1}

styrene: (53±5) Torr cm^2 s^{-1}

The measured diffusivities at 298 K by Lugg (1968) are preferred, and the given uncertainties reflects the differences between the measurements and estimations.

References:

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

3.6 $C_{10}H_8$ (naphthalene), $C_{12}H_{10}$ (diphenyl), $C_{14}H_{10}$ (anthracene)

Last evaluated: 11 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
naphthalene	Mack, 1925	298	46	46	51	10
diphenyl	Mack, 1925	298	55	55	48	-13
	Gilliland, 1937	490	122	51	115	-5
anthracene	Mack, 1925	373	60	40	65	9

Comments:

naphthalene The measured diffusivity of naphthalene at 298 K (Mack, 1925) is 10% lower than the estimated value.

diphenyl: The measured diffusivities at 298 K (Mack, 1925) and at 490 K (Gilliland, 1937) show good agreement with the estimated values. If extrapolated to 298 K, the measurement carried out at 490 K by Gilliland (1937) agrees well with that measured at 298 K (Mack, 1925)

anthracene: The diffusivity measured at 373 K (Mack, 1925) is 9% lower than the estimated value.

Preferred value in N_2 (or air/O_2) at 298 K:

naphthalene: (46±5) Torr cm^2 s^{-1}

The measured diffusivity at 298 K by Mack (1925) is preferred, and the given uncertainties reflects the difference between the measurement and estimation.

diphenyl: (52±7) Torr cm^2 s^{-1}

The preferred diffusivity is the average of that measured at 298 K (Mack, 1925) and that extrapolated to 298 K from the measurement at 490 K (Gilliand, 1937). The given uncertainty (±13%) reflects the difference between the measurement and estimation at 298 K.

anthracene: (40±4) Torr cm^2 s^{-1}

The preferred diffusivity at 298 K, (40±4) Torr cm^2 s^{-1}, is extrapolated to 298 K from the measurement carried out at 373 K by Mack (1925). The given uncertainty reflects the relative difference between the measurement and estimation at 373 K.

Last change in the preferred value: 11 July 2014

References:

Gilliland, E. R.: Diffusion Coefficients in Gaseous Systems, ***Ind. Eng. Chem.***, 26, 681-685, 1934.

Mack, E.: Average cross-sectional areas of molecules by gaseous diffusion methods, ***J. Am. Chem. Soc.***, 47, 2468-2482, 1925.

4 Alcohols

4.1 CH$_4$O (methanol)

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	$(D_e/D_m$-1) (%)
methanol	Altshuller and Cohen, 1960	298	117	117	123	5
	Getzinger and Wilke, 1967	308	145	137	160	10
	Lugg, 1968	298	116	116	123	6
	Mrazek et al., 1968	328	149	126	146	-2
	Katan, 1969	295	121	123	121	0
	Arnikar and Ghule, 1969	355	190	140	167	-12

Comments:

The measured diffusivities of methanol over 295-355 K show good agreement with estimated values. If extrapolated to 298 K, the measurements carried out at 308 K (Getzinger and Wilke, 1967), 328 K (Mrzzek et al., 1968), 295 K (Katzan, 1968) and 355 K (Arnikar and Ghuele, 1969) agree well with those performed at 298 K (Altshuller and Cohen, 1960; Lugg, 1968).

Preferred value in N$_2$ (or air/O$_2$) at 298 K: (126±11) Torr cm^2 s^{-1}

The preferred diffusivity of methanol at 298 K, is the average of those measured at 298 K by Altshuller and Cohen (1960) and Lugg (1968) and those extrapolated to 298 K from those measured at 295 K (Katzan, 1968), 308 K (Getzinger and Wilke, 1967), 328 K (Mrzzek et al., 1968), and 355 K (Arnikar and Ghuele, 1969).

References:

Altshuller, A. P., and Cohen, I. R.: Application of Diffusion Cells to Production of Known Concentration of Gaseous Hydrocarbons, *Anal. Chem.*, 32, 802-810, 1960.

Arnikar, H. J., and Ghule, H. M.: Electrodeless discharge as detector in the rapid determination of binary diffusion coefficient of gases, *Int. J. Electronics.*, 26, 159-162, 1969.

Getzinger, R. W., and Wilke, C. R.: An experimental study of nonequimolal diffusion in ternary gas mixtures, *Aiche J.*, 13, 577-580, 1967.

Katan, T.: Diffusion Coefficients of Vapors Measured with a Moving Boundary, *J. Chem. Phys.*, 50, 233-238, 1969.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

Mrazek, R. V., Wicks, C. E., and Prabhu, K. N. S.: Dependence of the diffusion coefficient on composition in binary gaseous systems, *J. Chem. Eng. Data*, 13, 508-510, 1968.

4.2 C$_2$H$_6$O (ethanol)

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
ethanol	Lee and Wilke, 1954	298	103	103	94	-8
	Arnikar et al., 1967	353	141	105	127	-10
	Getzinger and Wilke, 1967	308	109	103	100	-9
	Lugg, 1968	298	90	90	94	5
	Arnikar and Ghule, 1969	355	135	99	128	-5
	Katan, 1969	295	88	90	93	5

Comments:

The measured diffusivities of ethanol over 295-355 K show good agreement with the estimated values. If extrapolated to 298 K, the measurements performed at 295 K (Katan 1969), 308 K (Getzinger and Wilke, 1967), 355 K (Arnikar and Ghule, 1969), and 353 K (Arnikar et al., 1967) agree well with those at 298-299 K (Lee and Wilkem 1954; Lugg, 1968).

Preferred value in N$_2$ (or air/O$_2$) at 298 K: (98±7) Torr cm^2 s^{-1}

The preferred diffusivity of ethanol at 298 K, is the average of those measured at 298-299 K (Lee and Wilkem 1954; Lugg, 1968) and those extrapolated to 298 K from measurements at 295 K (Katan 1969), 308 K (Getzinger and Wilke, 1967), 355 K (Arnikar and Ghule, 1969), and 353 K (Arnikar et al., 1967).

References:

Arnikar, H. J., and Ghule, H. M.: Electrodeless discharge as detector in the rapid determination of binary diffusion coefficient of gases, Int. J. Electronics., 26, 159-162, 1969.

Arnikar, H. J., Rao, T. S., and Karmarkar, K. H.: Electrodeless Discharge as Detector in Gas Chromatography III. Study of Inter-diffusion of Gases†, Int. J. Electronics., 22, 381-385, 1967.

Getzinger, R. W., and Wilke, C. R.: An experimental study of nonequimolal diffusion in ternary gas mixtures, Aiche J., 13, 577-580, 1967.

Katan, T.: Diffusion Coefficients of Vapors Measured with a Moving Boundary, J. Chem. Phys., 50, 233-238, 1969.

Lee, C. Y., and Wilke, C. R.: Measurements of vapor diffusion coefficient, Ind. Eng. Chem., 46, 2381-2387, 1954.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, Anal. Chem., 40, 1072-1077, 1968.

4.3 C_3H_8O (1-propanol, 2-propanol), C_3H_6O (prop-2-en-1-01)

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
1-propanol	Lugg, 1968	298	75	75	79	5
2-propanol	Gilliland, 1934	299	75	75	79	5
		312	81		85	5
		332	92		95	3
	Lugg, 1968	298	77	77	79	3
	Arnikar and Ghule, 1969	358	111	80	109	-2
	Nagata and Hasegawa, 1970	363	121	86	111	-8
		383	128		122	-4
prop-2-en-1-ol	Lugg, 1968	298	78	78	81	4

Comments:

1-propanol, prop-2-en-1-ol: The measured diffusivities of 1-propanol and prop-2-en-1-ol at 298 K by Lugg (1968) are in good agreement with the estimated values.

2-propanol:

2-propanol: The measured diffusivities of 2-propanol over 298-383 K all agree well with the estimated values. If extrapolated to 298 K, the measurements carried out at other temperatures (Arnikar and Ghule, 1969; Nagata and Hasegawa, 1970) show good agreement with those carried out at 298-299 K (Gilliland, 1934; Lugg, 1968).

Preferred value in N_2 (or air/O_2) at 298 K:

1-propanol: (75±4) Torr cm^2 s^{-1}

prop-2-en-1-ol: (78±3) Torr cm^2 s^{-1}

The measured diffusivities of 1-propabol and prop-2-en-1-ol at 298 K by Lugg (1968) are preferred, and the given uncertainties reflect the corresponding differences between the measured and estimated values.

2-propanol: (79±5) Torr cm^2 s^{-1}

The preferred diffusivity of 2-propanol, is the average of those measured at 298-299 K by Gilliland (1934) and Lugg (1968) and those extrapolated to 298 K from that measured at 358 K by Arnikar and Ghule (1969) and that measured at 363 K by Nagata and Hasegawa (1970).

References:

Arnikar, H. J., and Ghule, H. M.: Electrodeless discharge as detector in the rapid determination of binary diffusion coefficient of gases, *Int. J. Electronics.*, 26, 159-162, 1969.

Gilliland, E. R.: Diffusion Coefficients in Gaseous Systems, *Ind. Eng. Chem.*, 26, 681-685, 1934.

Katan, T.: Diffusion Coefficients of Vapors Measured with a Moving Boundary, *J. Chem. Phys.*, 50, 233-238, 1969.

Lee, C. Y., and Wilke, C. R.: Measurements of vapor diffusion coefficient, *Ind. Eng. Chem.*, 46, 2381-2387, 1954.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

Nagata, I., and Hasegawa, T.: Gaseous interdiffusion coefficients, *J. Chem. Eng. Japan*, 3, 143-145, 1970.

4.4 C$_4$H$_{10}$O (1-butanol, 2-butanol, methyl-1-propanol, methyl-2-proponol)

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
1-butanol	Gilliland, 1934	299	66	66	69	4
		312	70		75	7
		332	79		83	5
	Lugg, 1968	298	65	65	69	5
2-butanol	Gilliland, 1934	299	68	67	69	2
		312	73		75	3
		332	82		83	1
	Lugg, 1968	298	68	68	69	2
methyl-1-propanol	Lugg, 1968	298	67	67	69	3
methyl-2-propanol	Lugg, 1968	298	66	66	69	4

Comments:

1-butanol: The diffusivities of 1-butanol were measured at 299, 312, and 332 K by Gilliland (1934) and at 298 L by Lugg (1968). The diffiusivities at 298-299 K reported by the two studies show excellent agreement, and the estimated diffusivities agree well with the measured value over 298-332 K.

2-butanol: The diffusivities of 2-butanol were measured at 299, 312, and 332 K by Gilliland (1934) and at 298 L by Lugg (1968). The diffiusivities at 298-299 K reported by the two studies show excellent agreement, and the estimated diffusivities agree well with the measured value over 298-332 K.

methyl-1-propanol, methyl-2-propanol: The diffusivities of methyl-1-propanol and methyl-2-propanol were measured by Lugg (1968) at 298 K, and the measured diffusivities are in excellent agreement with estimated values.

Preferred value in N$_2$ (or air/O$_2$) at 298 K:

1-butanol: (66±1) Torr cm^2 s^{-1}

2-butanol: (67±1) Torr cm^2 s^{-1}

The preferred diffusivities of 1-butanol and 2-butanol at 298 K are the avearge of those measured at 298-299 K by Gilliland (1934) and Lugg (1968).

methyl-1-propanol: (67±2) Torr cm^2 s^{-1}

methyl-2-propanol: (66±3) Torr cm^2 s^{-1}

The diffusivities of methyl-1-propanol and methyl-2-propanol measured by Lugg (1968) are preferred, and the given uncertainties reflect the corresponding differences between the measured and estimated values.

Last change in the preferred value: 12 July 2014

References:

Gilliland, E. R.: Diffusion Coefficients in Gaseous Systems, ***Ind. Eng. Chem.***, 26, 681-685, 1934.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Anal. Chem.***, 40, 1072-1077, 1968.

4.5 C$_5$H$_{12}$O (1-pentanol, 2-pentanol)

Last evaluated: 12 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	$(D_e/D_m$-1) (%)
1-pentanol	Lugg, 1968	298	54	54	62	14
2-pentanol	Gilliland, 1934	299	54	54	62	15
		312	58		67	16
		332	65		75	15
	Lugg, 1968	298	55	55	62	12

Comments:

1-pentanol: The measured diffusivity of 1-pentanol at 298 K by Lugg (1968) is 14% lower than the estimated value.

2-pentanol: The differences between the measured diffusivities at 299, 312, and 332 K by Gilliland (1934) and that at 298 K by Lugg (1968) are ~15%. The measured diffusivity at 299 K by Gilliand (1967) show excellent agreement with that measured at 298 K by Lugg (1968).

Preferred value in N$_2$ (or air/O$_2$) at 298 K:

1-pentanol: (54±8) Torr cm^2 s^{-1}

The diffusivity of 1-pentanol measured by Lugg (1968) at 298 K is preferred, and the given uncertainties reflects the difference between the measured and estimated diffusivities at 298 K.

2-pentanol: (54±8) Torr cm^2 s^{-1}

The preferred diffusivity at 298 K is the average of that measured by Gilliand (1934) at 299 K and that measured by Lugg (1968) at 298 K, and the given uncertainty reflects the difference between the measurements and estimations at 298-299 K.

Last change in the preferred value: 12 July 2014

References:

Gilliland, E. R.: Diffusion Coefficients in Gaseous Systems, *Ind. Eng. Chem.*, 26, 681-685, 1934.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968

4.6 C₆H₁₄O (1-hexanol, 2-ethyl-2-pentanol), C₇H₁₆O (1-heptanol), C₈H₁₈O (1-octanol)

4.6 $C_6H_{14}O$ (1-hexanol, 2-ethyl-2-pentanol), $C_7H_{16}O$ (1-heptanol), $C_8H_{18}O$ (1-octanol)

Last evaluated: 12 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
1-hexanol	Lugg, 1968	298	47	47	57	21
2-ethyl-1-butanol	Lugg, 1968	298	50	50	57	14
1-methyl-2-pentanol	Lugg, 1968	298	47	47	57	21
1-heptanol	Lugg, 1968	298	42	42	52	24
1-octanol	Lugg, 1968	298	38	38	49	27

Comments:

1-hexanol, 2-ethyl-1-butanol, 1-methyl-2-pentanol, 1-heptanol, 1-octanol: The differences between the measured (Lugg, 1968) and estimated diffusivities are 21% for 1-hexanol, 14% for 2-ethyl-1-butanol, 21% for 1-methyl-2-pentanol, 24% for 1-heptanol, and 27% for 1-octanol, respectively.

Preferred value in N₂ (or air/O₂) at 298 K:

1-hexanol: (47 ± 10) Torr cm^2 s^{-1}

2-ethyl-1-butanol: (50 ± 7) Torr cm^2 s^{-1}

1-methyl-2-pentanol: (47 ± 10) Torr cm^2 s^{-1}

1-heptanol: (42 ± 10) Torr cm^2 s^{-1}

1-octanol: (38 ± 11) Torr cm^2 s^{-1}

The measured diffusivities of 1-hexanol, 2-ethyl-1-butanol, 1-methyl-2-pentanol, 1-heptanol, and 1-octanol at 298 K by Lugg (1968) are preferred, and the given uncertainties reflects the corresponding differences between the measurements and estimations.

Last change in the preferred value: 12 July 2014

References:

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968

4.7 glycols

Species	Reference	T (K)	Cm(T)	Cm(298)	Ce(T)	(Ce/Cm-1) (%)
ethyl glycol	Lugg, 1968	298	76	76	86	13
propyl glycol	Lugg, 1968	298	67	67	74	11
diethyl glycol	Lugg, 1968	298	55	55	63	14
triethyl glycol	Lugg, 1968	298	45	45	55	23

Comments:

ethyl glycol, propyl glycol, diethyl glycol, triethyl glycol: The differences between the measured (Lugg, 1968) and estimated diffusivities at 298 K are 13% for ethyl glycol, 11% for propyl glycol, 14% for diethyl glycol, and 23% for triethyl glycol.

Preferred value in N_2 (or air/O_2) at 298 K:

ethyl glycol: (76 ± 10) Torr cm^2 s^{-1}

propyl glycol: (67 ± 7) Torr cm^2 s^{-1}

diethyl glycol: (55 ± 8) Torr cm^2 s^{-1}

triethyl glycol: (45 ± 10) Torr cm^2 s^{-1}

The preferred diffusivities of ethyl glycol, propyl glycol, diethyl glycol, and triethyl glycol at 298 K are based on the measurement of Lugg (1968), and the given uncertainties reflects the corresponding differences between the measured and estimated diffusivities.

References:

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968

5 Aldehydes and ketones

5.1 C₃H₆O (acetone)

Last evaluated: 11 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
acetone	Arnikar et al., 1967	353	114	85	109	-4
	Lugg, 1968	298	80	80	79	-1
	Arnikar and Ghule, 1969	355	103	76	111	8
	Nagaka and Hasegawa, 1970	343	106	83	104	-2
		363	117		115	-2
		383	129		126	-2

Comments:

The measured diffusivities over 298-383 K (Arnikar et al., 1967; Lugg, 1968; Arnikar and Ghule, 1969; Nagaka and Hasegawa, 1970) show good agreement with estimated values. If extrapolated to 298 K, the measurements carried out at high temperature (Arnikar et al., 1967; Arnikar and Ghule, 1969; Nagaka and Hasegawa, 1970) agree well with the measurement performed at 298 K by Lugg (1968).

Preferred value in N₂ (or air/O₂) at 298 K: (81 ± 5) Torr cm² s⁻¹

The preferred diffusivity of acetone at 298 K, (81 ± 5) Torr cm² s⁻¹, is the average of that measured at 298 K by Lugg (1968) and those extrapolated to 298 K from the measurements at high temperature (Arnikar et al., 1967; Arnikar and Ghule, 1969; Nagaka and Hasegawa, 1970).

Last change in the preferred value: 11 July 2014

References:

Arnikar, H. J., and Ghule, H. M.: Electrodeless discharge as detector in the rapid determination of binary diffusion coefficient of gases, *Int. J. Electronics.*, 26, 159-162, 1969.

Arnikar, H. J., Rao, T. S., and Karmarkar, K. H.: Electrodeless Discharge as Detector in Gas Chromatography m. Study of Inter-diffusion of Gases, *Int. J. Electronics.*, 22, 381-385, 1967.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

Nagata, I., and Hasegawa, T.: Gaseous interdiffusion coefficients, *J. Chem. Eng. Japan*, 3, 143-145, 1970.

5.2 C_4H_8O (methyl ethyl ketone), $C_5H_{10}O$ (methyl n-propyl ketone), $C_6H_{10}O$ (4-methyl pent-3-en-2-one), $C_9H_{10}O$ (isophorone)

Last evaluated: 11 July 2014

Species	Reference	T (K)	$D_m(T)$	$D_m(298)$	$D_e(T)$	$(D_e/D_m$-1) (%)
methyl ethyl ketone	Lugg, 1968	298	69	69	71	3
methyl n-propyl ketone	Lugg, 1968	298	60	60	63	5
4-methyl pent-3-en-2-one	Lugg, 1968	298	58	58	59	2
isophorone	Lugg, 1968	298	46	46	49	7

Comments:

methyl ethyl ketone, methyl n-propyl ketone, 4-methylpent-3-en-2-one, isophorone:
The diffusivities of methyl ethyl ketone, methyl n-propyl ketone, 4-methylpent-3-en-2-one, and isophorone were measured at 298 K by Lugg (1968). The differences between the measurements and estimation are <10%.

Preferred value in N_2 (or air/O_2) at 298 K:

methyl ethyl ketone: (69±2) Torr cm^2 s^{-1}

methyl n-propyl ketone: (60±3) Torr cm^2 s^{-1}

4-methyl pent-3-en-2-one: (58±1) Torr cm^2 s^{-1}

isophorone: (46±3) Torr cm^2 s^{-1}

The measurements by Lugg (1968) at 298 K are preferred. The given uncertainties reflect the differences between the measurements and estimations.

Last change in the preferred value: 11 July 2014

References:

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

5 Acids

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
formic acid	Lugg, 1968	298	116	116	112	-4
acetic acid	Lugg, 1968	298	94	94	89	-5
propanoic acid	Lugg, 1968	298	72	72	76	5
n-butyric acid	Lugg, 1968	298	59	59	67	14
2-methyl propanoic acid	Lugg, 1968	298	60	60	67	12
3-methyl butanoic acid	Lugg, 1968	298	50	50	60	21
hexanoic acid	Lugg, 1968	298	46	46	56	22
4-methyl pentanoic acid	Lugg, 1968	298	45	45	56	24

Comments:

formic acid, acetic acid, propanoic acid, n-butyric acid, 2-methyl butyric acid, 3-methyl butanoic acid, hexanoic acid, 4-methyl pentanic acid: The diffusivities of formic acid, acetic acid, propanoic acid, n-butyric acid, 2-methyl propanoic acid, 3-methyl butanoic acid, hexanoic acid, and 4-methyl pentanoic acid were measured at 298 K by Lugg (1968).

The differences between the measured and estimated diffusivities are ~5% for formic acid, acetic acid and propanoic acid, ~15% for n-butyric acid and iso-butyric acid, and ~25% for 3-methyl butanoic acid, hexanoic acid, and iso-hexanoic acid.

Preferred value in N_2 (or air/O_2) at 298 K:

formic acid: (116±4) Torr cm^2 s^{-1}

acetic acid: (94±5) Torr cm^2 s^{-1}

propanoic acid: (72±4) Torr cm^2 s^{-1}

n-butyric acid: (59±8) Torr cm^2 s^{-1}

2-methyl propanoic acid: (60±7) Torr cm^2 s^{-1}

3-methyl butanoic acid: (50±10) Torr cm^2 s^{-1}

hexanoic acid: (46±10) Torr cm^2 s^{-1}

4-methyl pentanoic acid: (45±11) Torr cm^2 s^{-1}

The preferred diffusivities of formic acid, acetic acid, propanoic acid, n-butyric acid, 2-methyl propanoic acid, 3-methyl butanoic acid, hexanoic acid, and 4-methyl pentanoic acid are based on the measurements at 298 K by Lugg (1968). The given uncertainties reflect the differences between the measured and estimated diffusivities.

Last change in the preferred value: 11 July 2014

References:

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

6 Ethers

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	$(D_e/D_m$-1) (%)
diethyl ether	Lugg, 1968	298	70	70	69	-1
di-iso-propyl ether	Lugg, 1968	298	52	52	57	10
di-n-butyl ether	Lugg, 1968	298	41	41	49	20
1,4-dioxane	Lugg, 1968	298	70	70	67	-4

Comments:

diethyl ether, di-iso-propyl ether, di-n-butyl ether, and 1,4-dioxane: The diffusivities of diethyl ether, di-iso-propyl ether, di-n-butyl ether, and 1,4-dioxane at 298 K were measured by Lugg (1968). The differences between the measured and estimated diffusivities are 1% for diethyl ether, 10% for di-iso-propyl ether, 20% for di-n-butyl ether, and 4% for 1,4-dioxane, respectively.

Preferred value in N_2 (or air/O_2) at 298 K:

diethyl ether: (70 ± 1) Torr cm^2 s^{-1}

di-iso-propyl ether: (52 ± 5) Torr cm^2 s^{-1}

di-n-butyl ether: (41 ± 8) Torr cm^2 s^{-1}

1,4-dioxane: (70 ± 3) Torr cm^2 s^{-1}

The preffered diffusivities of diethyl ether, di-iso-propyl ether, di-n-butyl ether, and 1,4-dioxane at 298 K are based on the measurement by Lugg (1968). The given uncertainties reflect the corresponding differences between the measured and estimated diffusivities.

References:

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

7 Esters

7.1 $C_2H_4O_2$ (methyl formate), $C_3H_6O_2$ (ethyl formate, methyl acetate)

Last evaluated: 12 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
methyl formate	Lugg, 1968	298	83	83	89	7
ethyl formate	Lugg, 1968	298	74	74	76	2
	Nagata and	344	100	77	97	-3
	Hasegawa, 1970	363	109		107	-2
		383	120		117	-3
		403	128		128	0
methyl acetate	Arnikar et al., 1967	353	107	80	102	-5
	Arnikar and Ghule, 1969	358	128	93	104	-19
	Lugg, 1968	298	74	74	76	2
	Nagata and	364	130	92	107	-18
	Hasegawa, 1970	383	146		117	-20
		403	159		128	-19

Comments:

methyl formate: The diffusivity of methyl formate measured at 298 K by Lugg (1968) agrees well with the estimated value.

ethyl formate: The measured diffusivities of ethyl formate at 298 K by Lugg (1968) and at 344-403 K by Nagata and Hasegawa (1970) show good agreement with the estimated values. If extrapolated to 298 K, the measured diffusivity at 344 K by Nagata and Hasegawa (1970) agrees well with that measured by Lugg (1968).

methyl acetate: The measured diffusivities at 353 K by Arnikar et al. (1967) and at 298 K by Lugg (1968) show good agreement with the estimated values, while the differences between the diffusivities measured at 358 K by Arnikar and Ghule (1969) and at 364-403 K and estimated values are ~20%.

Preferred value in N_2 (or air/O_2) at 298 K:

methyl formate: (83±6) Torr cm^2 s^{-1}

The measured diffusivity at 298 K by Lugg (1968) is preferred, and the given uncertainty reflects the difference between the measurement and estimation.

ethyl formate: (76±2) Torr cm^2 s^{-1}

The preferred diffusivity of ethyl formate, is the average of that measured at 298 K by Lugg (1968) and that extrapolated to 298 K from the measured value at 344 K by Nagata and Hasegawa (1970).

methyl acetate: (85 ± 10) Torr cm^2 s^{-1}

The preferred diffusivity, is the average of that measured at 298 K by Lugg (1968), those extrapolated to 298 K from those measured at 353 K by Arnikar et al. (1967), at 358 K by Arnikar and Ghule (1969), and at 364 K by Nagata and Hasegawa (1970).

Last change in the preferred value: 12 July 2014

References:

Arnikar, H. J., and Ghule, H. M.: Electrodeless discharge as detector in the rapid determination of binary diffusion coefficient of gases, *Int. J. Electronics.*, 26, 159-162, 1969.

Arnikar, H. J., Rao, T. S., and Karmarkar, K. H.: Electrodeless Discharge as Detector in Gas Chromatography m. Study of Inter-diffusion of Gases, *Int. J. Electronics.*, 22, 381-385, 1967.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

Nagata, I., and Hasegawa, T.: Gaseous interdiffusion coefficients, *J. Chem. Eng. Japan*, 3, 143-145, 1970.

7.2 C$_4$H$_8$O$_2$ (prolyl formate, ethyl acetate, methyl propionate)

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
propyl formate	Lugg, 1968	298	63	63	67	6
ethyl acetate	Gilliland, 1934	299	66	66	67	1
		312	71		72	1
		332	81		81	1
	Lugg, 1968	298	65	65	67	2
	Katan, 1969	295	65	66	66	2
	Arnikar and Ghule, 1969	355	104	77	91	-13
methyl propionate	Lugg, 1968	298	66	66	67	2

Comments:

propyl formate, methyl propionate: The diffusivities of propyl formate and methyl propionate measured at 298 K by Lugg (1968) agrees well with the estimated values.

ethyl acetate: The measured diffusivities at 299-332 K by Gilliland (1934), at 298 K by Lugg (1968), and at 295 K by Katan (1969) show excellent agreement with estimated values, while the difference between the measured value at 355 K by Arnikar and Ghule (1969) and the estimated one is 13%. If extrapolated to 298 K, the measurement at 355 K by Arnikar and Ghule (1969) agrees well with all the other measurements at 295-299 K.

Preferred value in N$_2$ (or air/O$_2$) at 298 K:

propyl formate: (63±4) Torr cm^2 s^{-1}

propyl formate: (66±1) Torr cm^2 s^{-1}

The measured diffusivities of propyl formate and methyl propionate at 298 K by Lugg (1968) are preferred, and the given uncertainties reflect the corresponding differences between the measurements and estimations.

propyl formate: (67±6) Torr cm^2 s^{-1}

The preferred diffusivity, is the average of that measured at 298 K by Lugg (1968) and those extrapolated to 298 K from those measured at 299 K by Gilliland (1934), at 298 K by Katan (1969), and at 355 K by Arnikar and Ghule (1969).

References:

Arnikar, H. J., and Ghule, H. M.: Electrodeless discharge as detector in the rapid determination of binary diffusion coefficient of gases, *Int. J. Electronics.*, 26, 159-162, 1969.

Gilliland, E. R.: Diffusion Coefficients in Gaseous Systems, *Ind. Eng. Chem.*, 26, 681-685, 1934.

Katan, T.: Diffusion Coefficients of Vapors Measured with a Moving Boundary, *J. Chem. Phys.*, 50, 233-238, 1969.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

7.3 $C_5H_{10}O_2$ (2-methylpropyl formate, n-propyl acetate, 2-methylethyl acetate, ethyl propionate, methyl n-hutyrate, methyl isobutyrate)

Last evaluated: 12 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
2-methylpropyl formate	Lugg, 1968	298	60	60	60	1
n-propyl acetate	Lugg, 1968	298	58	58	60	3
2-methylethyl acetate	Lugg, 1968	298	59	59	60	3
ethyl propionate	Fairbanks and Wilke, 1950	301	64	64	62	-3
	Lugg, 1968	298	58	58	60	3
methyl n-butyrate	Lugg, 1968	298	57	57	60	6
methyl isobutyrate	Lugg, 1968	298	57	57	60	6

Comments:

2-methylpropyl formate, n-propyl acetate, 2-methylethyl acetate, methyl n-butyrate, methyl isobutyrate: The diffusivities of 2-methylpropyl formate, n-propyl acetate, 2-methylethyl acetate, methyl n-butyrate, and methyl isobutyrate measured by Lugg (1968) show excellent agreement with the estimed values.

ethyl propionate: The diffusivities measured at 301 K by Fairbank and Wilke (1950) and at 298 K by Lugg (1968) are in good agreement, and both measurements agree very well with the estimations.

Preferred value in N_2 (or air/O_2) at 298 K:

2-methylpropyl formate: (60±1) Torr cm^2 s^{-1}

n-propyl acetate: (58±2) Torr cm^2 s^{-1}

2-methylethyl acetate: (59±1) Torr cm^2 s^{-1}

methyl n-butyrate: (57±3) Torr cm^2 s^{-1}

methyl isobutyrate: (57±3) Torr cm^2 s^{-1}

The diffusivities of 2-methylpropyl formate, n-propyl acetate, 2-methylethyl acetate, methyl n-butyrate, and methyl isobutyrate measured by Lugg (1968) are preferred, and the given uncertainties reflect the corresponding differences between the measured and estimated diffusivities.

ethyl propionate: (61±3) Torr cm^2 s^{-1}

The preferred diffusivity, is the average of that measured at 298 K by Lugg (1968) and that extrapolated to 298 K from that measured at 303 K by Fairbank and Wilke (1950).

Last change in the preferred value: 12 July 2014

References:

Fairbanks, D. F., and Wilke, C. R.: Diffusion Coefficients in Multicomponent Gas Mixtures, *Ind. Eng. Chem.*, 42, 471-475, 1950.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

7.4 $C_6H_{12}O_2$ (n-pentyl formate, iso-pentyl formate, n-butyl acetate, 2-methypropyl acetate, ethyl n-butyrate, ethyl isobutyrate, methyl n-pentanoate)

Last evaluated: 12 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
n-pentyl formate	Lugg, 1968	298	50	50	56	11
iso-pentyl formate	Lugg, 1968	298	51	51	56	9
n-butyl acetate	Lugg, 1968	298	51	51	56	10
2-methylpropyl acetate	Lugg, 1968	298	52	52	56	7
ethyl n-butyrate	Lugg, 1968	298	51	51	56	10
ethyl iso-butyrate	Lugg, 1968	298	51	51	56	9
methyl n-pentanoate	Lugg, 1968	298	51	51	56	11

Comments:

n-pentyl formate, iso-pentyl formate, n-butyl acetate, 2-methylpropyl acetate, ethyl n-butyrate, ethyl iso-butyrate, methyl n-pentanoate: The differences between the measured (Lugg, 1968) and estimated diffusivities of n-pentyl formate, iso-pentyl formate, n-butyl acetate, 2-methylpropyl acetate, ethyl n-butyrate, ethyl iso-butyrate, and methyl n-pentanoate are ~10%.

Preferred value in N_2 (or air/O_2) at 298 K:

n-pentyl formate: (50±6) Torr cm^2 s^{-1}

iso-pentyl formate: (51±5) Torr cm^2 s^{-1}

n-butyl acetate: (51±5) Torr cm^2 s^{-1}

2-methylpropyl acetate: (52±4) Torr cm^2 s^{-1}

ethyl n-butyrate: (51±5) Torr cm^2 s^{-1}

ethyl iso-butyrate: (51±5) Torr cm^2 s^{-1}

methyl n-pentanoate: (51±5) Torr cm^2 s^{-1}

The diffusivities of n-pentyl formate, iso-pentyl formate, n-butyl acetate, 2-methylpropyl acetate, ethyl n-butyrate, ethyl iso-butyrate, and methyl n-pentanoate at 298 K measured by Lugg (1968) are preferred, and the given uncertainties reflect the corresponding differences between the measured and estimated diffusivities.

Last change in the preferred value: 12 July 2014

References:

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Anal. Chem.***, 40, 1072-1077, 1968.

7.5 $C_7H_{14}O_2$ (n-pentyl acetate, n-butyl propionate, iso-butyl propionate, n-propyl n-butyrate, n-propyl iso-butyrate, iso-propyl iso-butyrate, ethyl n-pentonoate, methyl hexanonate)

Last evaluated: 12 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
n-pentyl acetate	Lugg, 1968	298	46	46	52	12
n-butyl propionate	Lugg, 1968	298	46	46	52	13
iso-butyl propionate	Lugg, 1968	298	46	46	52	12
n-propyl n-butyrate	Lugg, 1968	298	46	46	52	12
n-propyl iso-butyrate	Lugg, 1968	298	47	47	52	10
iso-propyl iso-butyrate	Lugg, 1968	298	48	48	52	7
ethyl n-pentanoate	Lugg, 1968	298	46	46	52	13
methyl n-hexanonate	Lugg, 1968	298	46	46	52	12

Comments:

n-pentyl acetate, n-butyl propionate, iso-butyl propionate, n-propyl n-butyrate, n-propyl iso-butyrate, iso-propyl iso-butyrate, ethyl n-pentanoate, methyl hexanonate: The differences between the measured (Lugg, 1968) and estimated diffusivities of n-pentyl acetate, n-butyl propionate, iso-butyl propionate, n-propyl n-butyrate, n-propyl iso-butyrate, iso-propyl iso-butyrate, ethyl-n-pentanoate, and methyl n-hexanonate are ~10%.

Preferred value in N_2 (or air/O_2) at 298 K:

n-pentyl acetate: (46±6) Torr cm^2 s^{-1}

n-butyl propionate: (46±6) Torr cm^2 s^{-1}

iso-butyl propionate: (46±6) Torr cm^2 s^{-1}

n-propyl n-butyrate: (46±6) Torr cm^2 s^{-1}

n-propyl iso-butyrate: (47±5) Torr cm^2 s^{-1}

iso-propyl iso-butyrate: (48±4) Torr cm^2 s^{-1}

ethyl n-pentanoate: (46±6) Torr cm^2 s^{-1}

methyl n-hexanonate: (46±6) Torr cm^2 s^{-1}

The diffusivities of n-pentyl acetate, n-butyl propionate, iso-butyl propionate, n-propyl n-butyrate, n-propyl iso-butyrate, iso-propyl iso-butyrate, ethyl-n-pentanoate, and methyl n-hexanonate at 298 K measured by Lugg (1968) are preferred, and the given

uncertainties reflect the corresponding differences between the measured and estimated diffusivities.

References:

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

7.6 $C_8H_{16}O_2$ (n-pentyl acetate, n-butyl propionate, iso-butyl propionate, n-propyl n-butyrate, n-propyl iso-butyrate, iso-propyl iso-butyrate, ethyl n-pentonoate, methyl hexanonate)

Last evaluated: 12 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
n-pentyl propionate	Lugg, 1968	298	42	42	48	13
iso-butyl n-butyrate	Lugg, 1968	298	42	42	48	13
iso-butyl iso-butyrate	Lugg, 1968	298	42	42	48	15
iso-proyl n-pentanoate	Lugg, 1968	298	42	42	48	14

Comments:

n-pentyl propionate, iso-butyl n-butyrate, iso-butyl iso-butyrate, iso-proyl n-pentanoate:

The differences between the measured (Lugg, 1968) and estimated diffusivities of n-pentyl propionate, iso-butyl n-butyrate, iso-butyl iso-butyrate, and iso-proyl n-pentanoateate ~15%.

Preferred value in N_2 (or air/O_2) at 298 K:

n-pentyl propionate: (42±6) Torr cm^2 s^{-1}

iso-butyl n-butyrate: (42±6) Torr cm^2 s^{-1}

iso-butyl iso-butyrate: (42±6) Torr cm^2 s^{-1}

iso-proyl n-pentanoate: (42±6) Torr cm^2 s^{-1}

The diffusivities of n-pentyl propionate, iso-butyl n-butyrate, iso-butyl iso-butyrate, and iso-proyl n-pentanoateate at 298 K measured by Lugg (1968) are preferred, and the given uncertainties reflect the corresponding differences between the measured and estimated diffusivities.

Last change in the preferred value: 12 July 2014

References:

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

7.7 $C_9H_{19}O_2$ (m-pentyl n-butyrate, n-pentyl iso-butyrate, iso-butyl n-pentanoate) and $C_9H_{10}O_2$ (benzyl acetate)

Last evaluated: 12 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
n-pentyl n-butyrate	Lugg, 1968	298	37	37	46	25
n-pentyl iso-butyrate	Lugg, 1968	298	38	38	46	22
iso-butyl n-pentanoate	Lugg, 1968	298	38	38	46	23
benzyl acetate	Lugg, 1968	298	46	46	50	10

Comments:

n-pentyl n-butyrate, n-pentyl iso-butyrate, iso-butyl n-pentanoate, benzyl acetate:

The differencs between the measured (Lugg, 1968) and estimated diffusivities at 298 K are 25% for n-pentyl n-butyrate, 22% for n-pentyl iso-butyrate, 23% for iso-butyl n-pentanoate, and 10% for benzyl acetate.

Preferred value in N_2 (or air/O_2) at 298 K:

n-pentyl n-butyrate: (37 ± 9) Torr cm^2 s^{-1}

n-pentyl iso-butyrate: (38 ± 8) Torr cm^2 s^{-1}

iso-butyl n-pentanoate: (38 ± 8) Torr cm^2 s^{-1}

benzyl acetate: (46 ± 4) Torr cm^2 s^{-1}

The diffusivities of n-pentyl n-butyrate, n-pentyl iso-butyrate, iso-butyl n-pentanoate, and benzyl acetate at 298 K measured by Lugg (1968) are preferred, and the given uncertainties reflect the corresponding differences between the measured and estimated diffusivities.

Last change in the preferred value: 12 July 2014

References:

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

7.8 $C_{20}H_{38}O_4$ (dipentyl sebacate), $C_{12}H_{14}O_4$ (diethyl phthalate), $C_{16}H_{22}O_4$ (di-n-butyl phthalate), $C_{24}H_{38}O_4$ (di-2-ethylhexyl phathalate)

Last evaluated: 12 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
dipentyl sebacate	Monchick and	298	18	18	30	67
	Reiss, 1954	308	19		32	66
diethyl phthalate	Lugg, 1968	298	38	38	42	11
di-n-butyl	Birks and	288	26		34	32
phthalate	Vradley, 1949	293	29		35	19
		298	32	32	36	14
		303	32		37	14
		308	32		38	18
		313	36		39	8
	Lugg, 1968	298	32	32	36	13
di-2-ethylhexyl phthalate	Lugg, 1968	298	26	26	29	13

Comments:

dipentyl sebacate: The diffusivities of dipentyl sebacate were measured at 298 and 308 K by Monchick and Reiss (1954), and the reported diffusivities are ~66% lower than the estimated values.

diethyl phthalate, di-2-ethylhexyl phthalate: The diffusivities of diethyl phthalate and di-2-ethylhexyl phthalate were measured by Lugg (1968) at 298 K. The measured values are 11% lower than the estimated value for diethyl phthalate and 13% for di-2-ethylhexyl phthalate.

di-n-butyl phthalate: The diffusivities of di-n-butyl phthalate were measured over 288-313 K by Birks and Vraley (1949) and at 298 K by Lugg (1968). The two measurements show excellent agreement at 298 K. The differences between the measured and estimated values appears to decrease with increasing temperature.

Preferred value in N_2 (or air/O_2) at 298 K:

dipentyl sebacate: no recommendation

The only available measurement (Monchick and Reiss, 1954) is ~66% lower than the estimated larger than the estimated value. Because the difference between the measured and estimated diffusivities ofr dipentyl sebacate is much larger than those for most other species, no preferred value is recommended.

diethyl phthalate: (38±4) Torr cm^2 s^{-1}

di-2-ethylhexyl phthalate: (26 ± 3) Torr cm^2 s^{-1}

The diffusivities of diethyl phthalate and di-2-ethylhexyl phthalate at 298 K measured by Lugg (1968) are preferred, and the given uncertainties reflect the corresponding differences between the measured and estimated diffusivities.

di-n-butyl phthalate: (32 ± 4) Torr cm^2 s^{-1}

The preferred diffusivity at 298 K is based on the two measured diffusivities of di-n-butyl phthalate at 298 K (Birks and Vraley, 1949; Lugg, 1968). Though the two measurements are in excellent agreement, an uncertainty of ±4 Torr cm^2 s^{-1} is given to reflect the difference between the measured and estimated diffusivities.

Last change in the preferred value: 12 July 2014

References:

Birks, J., and Bradley, R. S.: The Rate of Evaporation of Droplets. II. The Influence of Changes of Temperature and of the Surrounding Gas on the Rate of Evaporation of Drops of Di-n-butyl Phthalate, *Proc. Roy. Soc. A*, 198, 226-239, 1949.

Monchick, L., and Reiss, H.: Studies of Evaporation of Small Drops, *J. Chem. Phys.*, 22, 831-836, 1954.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

8 Multifuntional species

8.1 $C_3H_8O_2$ (2-methoxy ethanol), $C_4H_{10}O_2$ (2-ethoxy ethanol), $C_4H_{10}O_3$ (diethyl glycol), $C_6H_{14}O_4$ (triethyl glycol), $C_6H_{14}O_3$ (dioxitol)

Last evaluated: 11 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
2-methoxy ethanol	Lugg, 1968	298	67	67	74	10
2-ethoxy ethanol	Lugg, 1968	298	60	60	65	9
diethyl glycol	Lugg, 1968	298	55	55	63	14
triethyl glycol	Lugg, 1968	298	45	45	55	23
dioxitol	Lugg, 1968	298	46	46	53	14

Comments:

2-methoxy ethanol, 2-ethoxy ethanol, diethyl glycol, triethyl glycol, and dioxitol: The diffusivities of 2-methoxy ethanol, 2-ethoxy ethanol, diethyl glycol, triethyl glycol, and dioxitol were measured at 298 K by Lugg (1968). The difference between the measured and estimated diffusivities are 10% for 2-methoxy ethanol, 9% for 2-ethoxy ethanol, 14% for diethyl glycol, 23% for triethyl glycol, and 14% for dioxitol, respectively.

Preferred value in N_2 (or air/O_2) at 298 K:

2-methoxy ethanol: (67 ± 7) Torr cm^2 s^{-1}

2-ethoxy ethanol: (60 ± 5) Torr cm^2 s^{-1}

diethyl glycol: (55 ± 8) Torr cm^2 s^{-1}

triethyl glycol: (45 ± 10) Torr cm^2 s^{-1}

dioxitol: (46 ± 7) Torr cm^2 s^{-1}

The measured diffusivities of 2-methoxy ethanol, 2-ethoxy ethanol, diethyl glycol, triethyl glycol, and dioxitol at 298 K by Lugg (1968) are preferred. The given uncertainties reflect the corresponding differences between the measured and estimated diffusivities.

Last change in the preferred value: 11 July 2014

References:

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

8.2 C$_5$H$_4$O$_2$ (furdural), C$_6$H$_{12}$O$_2$ (4-hydroxyl-4-methyl-2-pentanone), C$_6$H$_{12}$O$_3$ (2-ethoxy ethyl acetate), C$_8$H$_8$O$_3$ (methyl salicylate)

Last evaluated: 11 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	$(D_e/D_m$-1) (%)
furfural	Brookfield et al., 1947	298	66	66	64	-3
		323	82		74	-10
4-hydroxy-4-methyl-2-pentanone	Lugg, 1968	298	49	49	56	14
2-ethoxy ethyl acetate	Lugg, 1968	298	46	46	54	16
methyl salicylate	Brookfield et al., 1947	298	62	62	52	-17
		323	108		60	-44

Comments:

furfural: The measured diffusivities of furfural by Brookfield et al. (1947) are 3% larger than the estimated value at 298 K and 10% at 323 K.

4-hydroxyl-4-methyl-2-pentanone, 2-ethoxy ethyl acetate: The measured diffusivities of 4-hydroxyl-4-methyl-2-pentanone and 2-ethoxy ethyl acetate at 298 K by Lugg (298) are 14% and 16% smaller than the estimated values, respectively.

methyl salicylate: The measured diffusivities of furfural by Brookfield et al. (1947) are 17% larger than the estimated value at 298 K and 44% at 323 K.

Preferred value in N$_2$ (or air/O$_2$) at 298 K:

furfural: (66±4) Torr cm^2 s^{-1}

The measurement by Brookfield et al. (1947) is preferred, and the given uncertainty reflects the difference between the measured and estimated diffusivities at 298 K.

4-hydroxyl-4-methyl-2-pentanone: (49±7) Torr cm^2 s^{-1}

2-ethoxy ethyl acetate: (46±8) Torr cm^2 s^{-1}

The measurements at 298 K by Lugg (1968) are preferred, and the given uncertainties reflect the differences between the measured and estimated diffusivities at 298 K.

methyl salicylate: (62±10) Torr cm^2 s^{-1}

The measurement by Brookfield et al. (1947) is preferred, and the given uncertainty reflects the difference between the measured and estimated diffusivities at 298 K.

Last change in the preferred value: 11 July 2014

References:

Brookfield, K. J., Fitzpatrick, H. D. N., Jackson, J. F., Matthews, J. B., and Moelwyn-Hughes, E. A.: The Escape of Molecules from a Plane Surface into a Still Atmosphere, *Proc. Roy. Soc. A*, 190, 59-67, 1947.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

9 N-containing species

9.1 $C_4H_{11}N$ (n-butylamine, iso-butylamine, and diethylamine), $C_2H_8N_2$ (ethyl diamine), C_3H_7NO (dimethyl formamide), $C_6H_{15}N$ (triethylamine), $C_{12}H_{12}N_2$ (benzidine)

Last evaluated: 11 July 2014

Species	Reference	T (K)	$D_m(T)$	$D_m(298)$	$D_e(T)$	(D_e/D_m-1) (%)
n-butylamine	Lugg, 1968	298	66	66	69	4
iso-butylamine	Lugg, 1968	298	68	68	69	1
diethylamine	Lugg, 1968	298	75	75	69	-9
ethyl diamine	Lugg, 1968	298	77	77	85	11
dimethyl formamide	Lugg, 1968	298	74	74	76	3
triethylamine	Lugg, 1968	298	57	57	57	-1
benzidine	Mack, 1925	372	42	29	68	61

Comments:

n-butylamine, iso-butylamine, diethylamine, ethyl diamine, dimethyl formamide and triethylamine: The diffusivities of n-butylamine, iso-butylamine, diethylamine, ethyl diamine, dimethyl formamide and triethylamine at 298 K were measured by Lugg (1968). Differences between the measured and estimated diffusivities are ~10% or smaller.

benzidine: The diffusivity of benzidine was measured at 372 K by Mack (1925). The measured diffusivity was 61% lower than the estimated one.

Preferred value in N_2 (or air/O_2) at 298 K:

n-butylamine: (66±3) Torr cm^2 s^{-1}

iso-butylamine: (68±1) Torr cm^2 s^{-1}

diethylamine: (75±6) Torr cm^2 s^{-1}

ethyl diamine: (77±8) Torr cm^2 s^{-1}

dimethyl formamide: (74±2) Torr cm^2 s^{-1}

 triethylamine: (57±1) Torr cm^2 s^{-1}

The preferred diffusivities of n-butylamine, iso-butylamine, diethylamine, ethyl diamine, dimethyl formamide and triethylamine at 298 K are based on the measurement by Lugg (1968). The given uncertainties reflect the corresponding differences between the measured and estimated diffusivities.

benzidine: no recommondation

Because the measured diffusivity reported by the only study (Mack, 1925) differs largely (by ~60%) from the estimated value, no preferred value is recommended.

Last change in the preferred value: 11 July 2014

References:

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.

Mack, E.: Average cross-sectional areas of molecules by gaseous diffusion methods, *J. Am. Chem. Soc.*, 47, 2468-2482, 1925.

9.2 $C_6H_7N_2$ (aniline), $C_6H_5NO_2$ (nitrobenzene)

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
aniline	Mack, 1925	298	55	55	63	14
	Gilliland, 1934	299	56	56	63	12
		312	60		68	13
		332	68		76	11
	Lugg, 1968	298	56	56	63	13
nitrobenzene	Lee and Wilke, 1954	298	65	65	62	-5
	Lugg, 1968	298	55	55	62	13

Comments:

aniline: The diffusivities of aniline at 298-299 K, measured by Mack (1925), Gilliland (1934) and Lugg (1968) show excellent agreement. The measured diffusivities from 298-332 K are ~10% lower than the estimated ones.

nitrobenzene: Lee and Wilke (1954) and Lugg (1968) measured the diffusivity of nitrobenzene at 298 K. Two measurements are in good agreement, and the differences between the measured and estimated diffusivities are ~10%.

Preferred value in N_2 (or air/O_2) at 298 K:

aniline: (56±6) Torr cm^2 s^{-1}

The preferred diffusivity of aniline at 298 K, (56±6) Torr cm^2 s^{-1}, is based on the measurements by Mack (1925), Gilliland (1934) and Lugg (1968). The given uncertainty reflects the differences between measured and estimated diffusivities.

nitrobenzene: (60±5) Torr cm^2 s^{-1}

The preferred diffusivity of nitrobenzene at 298 K, (60±5) Torr cm^2 s^{-1}, is the average of those reported by Lee and Wilke (1954) and Lugg (1968).

References:

Lee, C. Y., and Wilke, C. R.: Measurements of vapor diffusion coefficient, ***Ind. Eng. Chem.***, 46, 2381-2387, 1954.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, ***Anal. Chem.***, 40, 1072-1077, 1968.

Mack, E.: Average cross-sectional areas of molecules by gaseous diffusion methods, *J. Am. Chem. Soc.*, 47, 2468-2482, 1925.

9.3 HCN, C_3H_3N (acrylonitrile), $C_6H_7NO_2$ (ethyl cyanoacrylate), C_7H_5N (benzonitrile), C_5H_5N (pyridine), $C_5H_{11}N$ (piperidine)

Last evaluated: 11 July 2014

Species	Reference	T (K)	D_m(T)	D_m(298)	D_e(T)	(D_e/D_m-1) (%)
HCN	Klotz and Miller, 1947	273	131	153	143	9
acrylonitrile	Lugg, 1968	298	80	80	87	8
ethyl cyanoacrylate	Lugg, 1968	298	54	54	56	4
benzonitrile	Lugg, 1968	298	54	54	62	15
pyridine	Hudson et al., 1960	318	81	72	82	1
piperidine	Hudson et al., 1960	315	72	66	75	4

Comments:

HCN: The diffusivity of HCN was measured only by one study (Klotz and Miller, 1947) at 273 K, and the measured diffusivity is 9% lower than the estimated value.

acrylonitrile, ethyl cyanoacrylate, benzonitrile: The diffusivities of acrylonitrile, ethyl cyanoacrylate and benzonitrile were measured at 298 K by Lugg (1968), which are 8%, 4%, and 15% lower than the estimated values.

pyridine and piperidine: The diffusivities of pyridine and piperidine were measured by one study (Hudson et al., 1960) at 318 and 315 K, respectively. Both measured values show excellent agreement with the estimated ones.

Preferred value in N_2 (or air/O_2) at 298 K:

HCN: (153 ± 14) Torr cm^2 s^{-1}

The preferred diffusivity of HCN at 298 K, (153 ± 14) Torr cm^2 s^{-1}, is based on the measurement at 273 by Klotz and Miller (1947), extrapolated to 298 K. The given uncertainty reflects the difference between the measurement and estimation.

acrylonitrile: (80 ± 7) Torr cm^2 s^{-1}

ethyl cyanoacrylate: (54 ± 2) Torr cm^2 s^{-1}

benzonitrile: (54 ± 8) Torr cm^2 s^{-1}

The preferred diffusivities of acrylonitrile, ethyl cyanoacrylate and benzonitrile at 298 K are based on the measurements by Lugg (1968). The given uncertainties reflect the differences between the measurement and estimation.

pyridine: (72 ± 1) Torr cm^2 s^{-1}

piperidine: (66 ± 3) Torr cm^2 s^{-1}

The preferred diffusivities of pyridine and piperidine are based on the measurement by Hudson et al. (1960), extrapolated to 298 K.

Last change in the preferred value: 11 July 2014

References:

Hudson, G. H., McCoubrey, J. C., and Ubbelohde, A. R.: Vapour diffusion coefficients and collision parameters for cyclic molecules, *Trans. Faraday Soc.*, 56, 1144-1151, 1960.

Klotz, I. M., and Miller, D. K.: Diffusion Coefficients and Molecular Radii of Hydrogen Cyanide, Cyanogen Chloride, Phosgene and Chloropicrin1, *J. Am. Chem. Soc.*, 69, 2557-2558, 1947.

Lugg, G. A.: Diffusion coefficients of some organic and other vapors in air, *Anal. Chem.*, 40, 1072-1077, 1968.