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Improved AIOMFAC model parameterisation of the temperature dependence of activity coefficients for aqueous organic mixtures

G. Ganbavale[1], A. Zuend[1,2,3], C. Marcolli[1,4], and T. Peter[1]

[1]Institute for Atmospheric and Climate Science, ETH Zurich, Zurich, Switzerland
[2]Department of Chemical Engineering, California Institute of Technology, Pasadena, California, USA
[3]Department of Atmospheric and Oceanic Sciences, McGill University, Montreal, Quebec, Canada
[4]Marcolli Chemistry and Physics Consulting GmbH, Zurich, Switzerland

Correspondence to: A. Zuend (andreas.zuend@mcgill.ca)

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Abstract

This study presents a new, improved parameterisation of the temperature dependence of activity coefficients in the AIOMFAC (Aerosol Inorganic–Organic Mixtures Functional groups Activity Coefficients) model applicable for aqueous as well as water-free organic solutions. For electrolyte-free organic and organic–water mixtures the AIOMFAC model uses a group-contribution approach based on UNIFAC (UNIversal quasi-chemical Functional-group Activity Coefficients). This group-contribution approach explicitly accounts for interactions among organic functional groups and between organic functional groups and water. The previous AIOMFAC version uses a simple parameterisation of the temperature dependence of activity coefficients, aimed to be applicable in the temperature range from ∼ 275 to ∼ 400 K. With the goal to improve the description of a wide variety of organic compounds found in atmospheric aerosols, we extend the AIOMFAC parameterisation for the functional groups carboxyl, hydroxyl, ketone, aldehyde, ether, ester, alkyl, aromatic carbon-alcohol, and aromatic hydrocarbon to atmospherically relevant low temperatures with the introduction of a new temperature dependence parameterisation. The improved temperature dependence parameterisation is derived from classical thermodynamic theory by describing effects from changes in molar enthalpy and heat capacity of a multicomponent system. Thermodynamic equilibrium data of aqueous organic and water-free organic mixtures from the literature are carefully assessed and complemented with new measurements to establish a comprehensive database, covering a wide temperature range (∼ 190 to ∼ 440 K) for many of the functional group combinations considered. Different experimental data types and their processing for the estimation of AIOMFAC model parameters are discussed. The new AIOMFAC parameterisation for the temperature dependence of activity coefficients from low to high temperatures shows an overall improvement of 25 % in comparison to the previous model version. The new parameterisation of AIOMFAC agrees well with a large number of experimental datasets and enables the calculation of activity coef-

ficients of a wide variety of different aqueous/water-free organic solutions down to the low temperatures present in the upper troposphere.

1 Introduction

Atmospheric aerosols are complex mixtures of inorganic and organic components. A large variety of organic compounds account for a significant fraction of the tropospheric aerosol composition. Airborne and ground-based measurements suggest that the aerosols in the free troposphere are composed of $\sim 30\%$ up to about $\sim 80\%$ of carbonaceous material mostly in the form of organics (Murphy et al., 2006; Jacobson et al., 2000; Hallquist et al., 2009). Aerosol loading, size distribution, composition, morphology and physical states of particles affect the Earth's radiative budget through the direct effects of aerosols on climate and the indirect effects, in which aerosols act as cloud condensation (CCN) or ice nuclei (IN), affecting cloud particle number concentrations, precipitation, cloud albedo, and life time (Lohmann et al., 2005). Organic aerosols are expected to stay in a liquid, viscous semi-solid, or amorphous solid state, since the very large number of organic compounds depresses the temperature at which organic crystal formation takes place (Marcolli et al., 2004; Virtanen et al., 2010; Koop et al., 2011).

Non-ideal interactions between different organic and inorganic species in the particle phase influence water uptake and release (hygroscopicity), may induce liquid–liquid phase separation (LLPS) (e.g., Marcolli and Krieger, 2006; Zuend et al., 2010; Song et al., 2012), influence gas-particle partitioning of semivolatile compounds (e.g., Zuend et al., 2010; Zuend and Seinfeld, 2012), and alter efflorescence and deliquescence relative humidities (e.g., Krieger et al., 2012). Thermodynamic phase equilibrium calculations allow to determine whether the aerosol phase is a liquid (or viscous amorphous phase), a crystalline solid, or a mixture of solid and liquid phases and to what degree semivolatile species partition to the condensed phases (Pankow, 2003; Zuend et al., 2010; Zuend and Seinfeld, 2012; Shiraiwa et al., 2013). Phase equilibria calculations

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can be carried out by using composition dependent activity coefficients which account for the non-ideality of the liquid/amorphous phase (Gmehling, 1995; Raatikainen and Laaksonen, 2005; Zuend et al., 2010). The mole fraction based activity coefficient, $\gamma_s^{(x)}$ and activity $a_s^{(x)}$ of a compound s are related by $a_s^{(x)} = \gamma_s^{(x)} x_s$, where x_s is the mole fraction of s in the liquid (homogeneous, amorphous) mixture.

Thermodynamic models for mixtures of organics and water in condensed phases are usually based on the UNIQUAC (UNIversal QUAsi Chemical) model (Abrams and Prausnitz, 1975) or its group contribution version UNIFAC (UNIquac Functional group Activity Coefficients) (Fredenslund et al., 1975). The original UNIFAC model was developed for vapour–liquid equilibria (VLE) calculations within a temperature range from ∼ 275 to ∼ 400 K. Using the UNIFAC model outside of its intended temperature range may result in poor predictions of real phase behaviour (Lohmann et al., 2001). For very dilute mixtures, UNIFAC thermodynamic model calculations for component activity coefficients at infinite dilution are sometimes not in agreement with the experimental data. This can be understood since most VLE measurements were performed for liquid mole fractions between 0.02 to 0.98 and, hence, do not provide specific information for the highly dilute regions (Compernolle and Müller, 2014). Inaccurate results were obtained for other types of thermodynamic data, e.g., molar enthalpies of mixing (h^E) or solid–liquid equilibrium (SLE) data, following the Gibbs–Helmholtz relation, this leads to inaccurate description of activity coefficients as a function of temperature (Lohmann et al., 2001; Gmehling, 2003, 2009). With the original UNIFAC model, due to data insufficiency, inaccurate predictions were often obtained for asymmetric systems (systems containing molecules of different sizes and shapes) (Lohmann et al., 2001; Gmehling, 2003). Since then, the original UNIFAC model has been improved and in addition, modified UNIFAC versions such as modified UNIFAC (Dortmund) and modified UNIFAC (Lyngby) have been developed (Larsen et al., 1987; Hansen et al., 1991; Gmehling et al., 1998, 2002; Jakob et al., 2006), which amended some of the original weaknesses. For mixtures containing multifunctional components, both UNIFAC and modified UNIFAC (Dortmund) sometimes show poor results since the functional group

interaction parameters were mainly determined based on experimental data of mixtures of simple, monofunctional components (Weidlich and Gmehling, 1987; Gmehling et al., 2012).

One of the important differences between the UNIFAC model by Hansen et al. (1991), which we call here "standard UNIFAC", and the modified UNIFAC (Dortmund), is the use of a more elaborate parameterisation for the temperature dependence of activity coefficients in the modified UNIFAC (Dortmund) model. However, the modified UNIFAC models still may often not provide reliable predictions of activity coefficients at low temperatures relevant in the troposphere. Calculations of water activity (a_w) of atmospherically relevant aqueous organic solutions have shown that the performance of standard UNIFAC may be poor when the organic fraction consists of multifunctional molecules typically carrying several strong polar functional groups with enhanced hydrogen-bonding potential (Saxena and Hildemann, 1997; Peng et al., 2001). Marcolli and Peter (2005) have therefore proposed improved sets of interaction parameters for standard UNIFAC for alcohols and polyols. Peng et al. (2001) reparameterised the interaction of the water (group) with the carboxyl group and the hydroxyl group based on measured water activities of aqueous systems containing dicarboxylic acids and substituted dicarboxylic and tricarboxylic acids.

For atmospheric applications, an accurate description of aqueous organic mixtures at atmospherically relevant temperatures is required. At low temperatures a_w is a crucial parameter for homogeneous ice nucleation (Koop et al., 2000). Extrapolations of a_w of different aqueous organic solutions measured in the temperature range from the ice melting curve to 313 K suggest that if the temperature dependence of the activity coefficients is neglected, errors on the order of 10 to 15 % result for a_w at the homogeneous freezing temperature (Zobrist et al., 2008). The uncertainty in predicted homogeneous ice nucleation temperatures is stated as ±0.025 in a_w at melting points and ±0.05 in a_w at ice freezing temperatures (Koop et al., 2000; Koop, 2004). A small uncertainty in a_w of about 0.025 can change the corresponding homogeneous nucleation rate coefficients by 6 orders of magnitude and may significantly affect predictions of the onset of

ice crystal formation in cloud microphysical models (Knopf and Rigg, 2011; Alpert et al., 2011). This shows the need for an improved UNIFAC (and AIOMFAC) parameterisation at low temperatures.

2 AIOMFAC model

The AIOMFAC model (Aerosol Inorganic–Organic Mixtures Functional groups Activity Coefficients) by Zuend et al. (2008, 2011) is a thermodynamic group-contribution model specifically developed to meet the requirements of typical tropospheric aerosol compositions. The model enables calculations of activity coefficients covering inorganic (water, electrolytes), organic, and organic–inorganic interactions in multicomponent solutions over a wide concentration range. AIOMFAC is based on the group-contribution model LIFAC by Yan et al. (1999) and, therefore, includes the standard UNIFAC model, yet also includes the modified parameter sets from Peng et al. (2001) and those from Marcolli and Peter (2005). In its short-range interaction part, the AIOMFAC model shares the simple temperature dependence expressions of the original UNIFAC model and involves only one main group interaction term involving two adjustable parameters, $a_{m,n}$ and $a_{n,m}$ per binary interaction (of groups m and n). Throughout this article, we will refer to this (original) AIOMFAC model as "AIOMFAC-P1". The aim of this study is to improve the performance of AIOMFAC at low temperatures for multicomponent organic + water systems. We will refer to the new AIOMFAC version, with an improved temperature dependence parameterisation with two additional main group interaction terms, as AIOMFAC-P3, indicating a 3-term parameterisation in the short-range (mod. UNIFAC) part. The focus is on a list of major organic functional groups that have been identified in tropospheric aerosols, namely hydroxyl, carboxyl, ketone, ether, ester, aldehyde, alkyl, and aromatic functionalities.

The thermodynamic group-contribution model AIOMFAC allows thermodynamically consistent calculations of activity coefficients at temperatures close to 298 K and covers multicomponent solutions containing water, inorganic ions, and organic compounds.

For electrolyte-free systems of organic compounds and water, the applicable temperature range is ~ 275 to ~ 400 K, as for the original UNIFAC model. As mentioned above, the concept of AIOMFAC is based on the LIFAC model (Yan et al., 1999), which merges a Pitzer-like approach with a slightly modified version of the original UNIFAC model to calculate activity coefficients.

The non-ideality of a thermodynamic system is characterized by the excess Gibbs energy $G^{ex}(p,T,n_j)$, which in AIOMFAC is expressed as the sum of long range (LR), middle range (MR) and short range (SR) contributions:

$$G^{ex}(p,T,n_j) = G^{ex}_{LR} + G^{ex}_{MR} + G^{ex}_{SR}. \tag{1}$$

Here, p is the total pressure, T the absolute temperature, and n_j ($j = 1,\ldots,k$) the molar amounts of the k components in a system. Mole fraction based activity coefficients $\gamma_j^{(x)}$ with n_j moles in a mixture are derived from expressions for the different parts of G^{ex} using the relation

$$\ln\gamma_j^{(x)} = \left[\frac{\partial G^{ex}/(RT)}{\partial n_j}\right]_{p,T,n_{j'\neq j}} \tag{2}$$

where R is the universal gas constant. Activity coefficients are calculated from the three model parts related to Eq. (1):

$$\ln\gamma_j^{(x)} = \ln\gamma_j^{(x),LR} + \ln\gamma_j^{(x),MR} + \ln\gamma_j^{(x),SR}. \tag{3}$$

Electrolyte solutions, which may range from dilute to highly supersaturated concentrations are, aside from their SR contribution, considered in the Pitzer-like part, which combines LR and MR interactions. The LR interactions are described by an extended Debye–Hückel term and represents contributions by Coulomb electrostatic forces between permanently charged ions, moderated by the presence of the dielectric solvent

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medium (e.g., a homogeneous mixture of water + organic compounds act as the solvent medium). The MR part represents the effects of interactions involving ions and permanent or induced dipoles and contains most of the adjustable parameters to describe concentrated aqueous electrolyte solutions and organic–inorganic mixtures. The original AIOMFAC model by Zuend et al. (2008) has been extended and re-parameterised to include organic–inorganic interactions of most of the functional groups typically present in atmospheric organic compounds (carboxyl, hydroxyl, ketone, aldehyde, ether, ester, alkyl, aromatic carbon-alcohol, and aromatic hydrocarbon) (Zuend et al., 2011). In addition, Zuend and Seinfeld (2012) introduced the functional groups hydroperoxide, peroxyacid, and peroxide, including estimated interaction parameters with the inorganic ions of the model. For further details of the thermodynamic description of the LR and MR interactions within the Pitzer-like part of AIOMFAC we refer to Zuend et al. (2008, 2011). The interactions among non-charged species (organic molecules and water) are calculated in the SR part of AIOMFAC, see Sect. 2.2.

2.1 Group-contribution method

A group-contribution concept similar to the one in UNIFAC has been adopted for the AIOMFAC model. According to the group-contribution concept, it is assumed that the system (and its organic constituents) are composed of combinations of functional groups instead of whole molecule entities. The advantage of applying the group-contribution method is that a very large number of organic compounds can be defined using the various combinations of a limited number of functional groups. In accordance to the UNIFAC model, the functional groups are further classified into so-called main groups and subgroups for their application in different model parts (Fredenslund et al., 1975; Marcolli and Peter, 2005; Zuend et al., 2008, 2011). The main groups cover subgroups of the same functionality that only differ by the number of hydrogen atoms. The subgroup classification of a variety of organic compounds can be found in Table 1.

2.2 Short-range contribution

As in the UNIFAC model, in the SR part of AIOMFAC, activity coefficients of a mixture component j are in general expressed as the sum of contributions of a combinatorial part (denoted by superscript C), which accounts for the size and shape of the molecule, and the residual part (denoted by superscript R), which reflects the residual contribution from intermolecular (inter-group) interactions (Fredenslund et al., 1975; Marcolli and Peter, 2005; Zuend et al., 2008).

$$\ln \gamma_j^{SR,(x)} = \ln \gamma_j^{C} + \ln \gamma_j^{R} \tag{4}$$

The expression for the combinatorial part of UNIFAC is (Fredenslund et al., 1975; Zuend et al., 2008):

$$\ln \gamma_j^{C} = \ln \frac{\Phi_j}{x_j} + \frac{z}{2} q_j \ln \frac{\Theta_j}{\Phi_j} + l_j - \frac{\Phi_j}{x_j} \sum_{j'} x_{j'} l_{j'} \tag{5}$$

where

$$\Phi_j = \frac{r_j x_j}{\sum\limits_{j'} r_{j'} x_{j'}}; \quad \Theta_j = \frac{q_j x_j}{\sum\limits_{j'} q_{j'} x_{j'}} \tag{6}$$

and

$$r_j = \sum_t v_t^{(j)} R_t; \quad q_j = \sum_t v_t^{(j)} Q_t; \tag{7}$$

$$l_j = \frac{z}{2}(r_j - q_j) - (r_j - 1). \tag{8}$$

In these equations, x_j is the mole fraction of component j and $v_t^{(j)}$ denotes the number of subgroups of type t present in a formula unit of component j. The relative van

der Waals subgroup volume and surface area are given by R_t and Q_t respectively. The lattice coordinate number z is typically assumed to be a constant set to $z = 10$ (Fredenslund et al., 1975). Relative subgroup volume and surface area parameters published by Hansen et al. (1991) are used for the neutral species.

Enthalpic interaction contributions are considered in the residual part of UNIFAC. The residual part (γ_j^R) of the activity coefficient of component j is given by:

$$\ln \gamma_j^R = \sum_t v_t^{(j)} \left[\ln \Gamma_t - \ln \Gamma_t^{(j)} \right], \tag{9}$$

where Γ_t is the group residual activity coefficient in the mixture, while $\Gamma_t^{(j)}$ represents the one in a reference liquid containing only compound j. $v_t^{(j)}$ is the number of subgroups of type t in molecule j. The residual activity coefficient of subgroup t is:

$$\ln \Gamma_t = Q_t \left[1 - \ln \left(\sum_m \Theta_m \Psi_{m,t} \right) - \sum_m \left(\frac{\Theta_m \Psi_{t,m}}{\sum_n \Theta_n \Psi_{n,m}} \right) \right], \tag{10}$$

where

$$\Theta_m = \frac{Q_m X_m}{\sum_n Q_n X_n}. \tag{11}$$

In these expressions Θ_m is the relative surface area fraction of subgroup m, X_m is the mole fraction of m in the mixture of subgroups (note: X_m is different from the mole fraction x_j that would refer to the mixture of components, not mixture of subgroups). The standard UNIFAC temperature-dependent interaction between the subgroups m and n is given by Fredenslund et al. (1975):

$$\ln \Psi_{n,m} = - \left[\frac{U_{n,m} - U_{n,n}}{RT} \right] \tag{12}$$

where $U_{n,m}$ is a measure of change in the molar Gibbs free energy due to interaction between subgroups m and n. Eq. (12) is typically represented in the more compact form of Eq. (13).

$$\ln \Psi_{n,m} = - \left[\frac{a_{n,m}}{T} \right] \qquad (13)$$

Due to the formulation of Eq. (12), with equivalent differences for the interactions between subgroups m and n (with the difference $U_{m,n} - U_{m,m}$), the main group interaction parameters $a_{n,m}$ are unsymmetrical i.e., $a_{n,m} \neq a_{m,n}$. Note that all interaction parameters are only resolved on the main group level, i.e., all subgroups of a certain main group interacting with a subgroup of a different main group will share the same interaction parameter. Hence, we refer to the set of $a_{n,m}$ as main group interaction parameters. In standard UNIFAC, the $a_{n,m}$ interaction parameters of organic solutions were estimated using a large database of experimental vapour–liquid equilibrium (VLE) and a few liquid–liquid equilibrium (LLE) datasets. This approach leads to satisfying predictions for vapour–liquid equilibria, but reliable simultaneous description of VLE, LLE, solid–liquid equilibria (SLE), and molar enthalpies of mixing (h^E) can often not be obtained (Lohmann et al., 2001). In order to overcome these deficiencies of the standard UNIFAC, modified UNIFAC (Dortmund) uses three main group interaction parameters in the residual part to improve predictions of activity coefficients over a wider range of temperatures and different types of phase equilibria (Gmehling et al., 1993; Lohmann et al., 2001; Jakob et al., 2006):

$$\ln \Psi_{n,m} = - \left[\frac{a_{n,m} + b_{n,m}T + c_{n,m}T^2}{T} \right]. \qquad (14)$$

In modified UNIFAC (Dortmund) the relative van der Waals volume (R_t) and surface (Q_t) coefficients for the structural groups are not calculated from molecular parameters as in the standard UNIFAC approach; rather, they are fit together with the interaction parameters ($a_{n,m}$, $b_{n,m}$, $c_{n,m}$) to experimental data.

The AIOMFAC model is aimed for a wide range of applications, including the calculation of solid–liquid equilibria and other thermodynamic phase equilibria. The temperature dependence of these equilibria is related to the molecular interaction of the components in the liquid phase. Hence, the temperature dependence of chemical reaction equilibria and phase equilibra are described by the same thermodynamic functions and we can express them with parameterisations for the temperature dependence of reaction equilibria. According to Clarke and Glew (1966), if the equilibrium constant K_p of a chemical reaction or exchange process is a function of temperature, the changes in the standard thermodynamic functions, i.e., change in molar Gibbs free energy $\Delta g°$, change in molar enthalpy $\Delta h°$ and change in molar heat capacity $\Delta c_p°$ are directly related to K_p (by definition) and are well-behaved functions of T. The relationship for the equilibrium constant K_p and temperature T, when excluding higher order derivatives of the molar heat capacity change with temperature, are given by (Clarke and Glew, 1966):

$$R \ln K_p = -\frac{\Delta g°_{T_\ominus}}{T_\ominus} + \Delta h°_{T_\ominus} \left[\frac{1}{T_\ominus} - \frac{1}{T} \right] + \Delta c°_{p,T_\ominus} \left[\frac{T_\ominus}{T} - 1 + \ln \frac{T}{T_\ominus} \right], \tag{15}$$

where $T_\ominus$ is a reference temperature at which the changes in $\Delta g°$, $\Delta h°$ and $\Delta c_p°$ are determined or known. In order to better describe activity coefficients at low (and high) temperatures while preserving compatibility with the already estimated values of the interaction parameters $a_{n,m}$ at room temperature, we introduce a similar but slightly modified expression for $\Psi'_{n,m}$. We define the temperature dependent interaction potential in AIOMFAC as

$$\ln \Psi'_{n,m} = -\frac{a_{n,m}}{T} + b_{n,m} \left[\frac{1}{T_\ominus} - \frac{1}{T} \right] + c_{n,m} \left[\frac{T_\ominus}{T} - 1 + \ln \frac{T}{T_\ominus} \right] \tag{16}$$

with the reference temperature $T_\ominus = 298.15$ K. The first term on the right hand side is exactly the same as in standard UNIFAC, but slightly different from the equivalent term in Eq. (15), due to the use of actual temperature T instead of reference temperature

$T_\ominus$ for consistency with standard UNIFAC/AIOMFAC. This term in Eq. (16) therefore includes both changes in $\Delta g^\circ_{T_\ominus}$ as well as a part of the changes related to $\Delta h^\circ_{T_\ominus}$ (note: this is obvious when considering a hypothetical, very high reference temperature for the second term on the right hand side of Eq. 16). The second term includes the change in enthalpy and in addition acts as a correction term for parameters $a_{n,m}$ at temperatures different from the reference temperature. The third term accounts for the contribution related to the heat capacity change of a main group interaction, whose importance increases for temperatures far away from the reference temperature.

We use a database of experimental thermodynamic equilibrium data for organic and organic–water systems (see Sects. 3 and 4), covering a wide temperature and concentration range, to determine simultanously the AIOMFAC group interaction parameters $b_{n,m}$ and $c_{n,m}$ for pertaining organic funcational groups. To preserve compatibility with the AIOMFAC model version of Zuend et al. (2011), and its fitted organic–inorganic interaction parameters at room temperature, all group-interaction parameters $a_{m,n}$ are kept the same, which implies that the performance of AIOMFAC at 298.15 K will not be altered by the improved three-parameter temperature-dependence parameterisation. With a goal to describe a wide variety of organic compounds at relevant atmospheric temperatures, we focus on the aqueous systems of oxidized organics at lower temperatures. The temperature dependence formulation given by Eq. (16) will at this point only be parameterised for interactions between the UNIFAC main groups alkyl (CH_n), specific variants of alkyl groups in alcohols $(CH_n^{[alc]})$, $(CH_n^{[alc-tail]})$, and $(CH_n^{[OH]})$, hydroxyl (OH), carboxyl (COOH), ketone (CH_nCO), aldehyde (CHO), ether (CH_nO), ester (CCOO), alkenyl (C=C), aromatic carbon (ACH_n), aromatic carbon-alcohol (ACOH) (a phenol group), and water (H_2O). For all other group interactions not considered, $b_{n,m}$ and $c_{n,m}$ are set to zero so that Eq. (16) reduces to Eq. (13). The rules for the use of specific alkyl groups are described below. With this approach, an improved description of activities for organic systems at low temperatures can be achieved, while maintaining compatibility with standard UNIFAC, hence, preserving the applicability of AIOMFAC to a wider range of functional groups.

The UNIFAC functional groups in AIOMFAC include some modifications with respect to standard UNIFAC to better describe the specific properties of organic aerosol constituents, which typically are molecules composed of several (polar) functional groups. Therefore a more detailed description of alcohol/polyol group interaction parameters published by Marcolli and Peter (2005) was implemented, where the relative positions of the OH functional group, as well as those of neighboring alkyl groups are taken into account (Zuend et al., 2011). According to this approach, water-alkyl and water-hydroxyl group interaction parameters for alcohols/polyols are treated specifically, while keeping the alkyl-hydroxyl interaction parameter unchanged in order to maintain the performance of AIOMFAC in case of water free alkane/alcohol systems compatible with standard UNIFAC. Except for $CH_n^{[OH]}$ groups directly bonded to an OH group, standard UNIFAC CH_n groups are used for alkyl groups in multifunctional molecules that contain hydroxyl groups combined with different other functional groups. Another difference with respect to standard UNIFAC is that we use the parameters of Peng et al. (2001) for the interaction of the COOH group with the OH group and the H_2O group. The use of these modified UNIFAC group interaction parameters leads to improvements for certain aqueous systems of alcohols, dicarboxylic and hydroxycarboxylic acids, while being compatible with the use of standard UNIFAC parameters for other group interactions, as described in more detail in Zuend et al. (2011).

3 Experimental data

A reliable estimation of group interaction parameters and temperature dependence relies on a comprehensive database covering a wide variety of compounds consisting of the targeted functional groups with consideration of a large temperature range. In order to establish such a database, an extensive literature search was carried out. The DETHERM databank (Gesellschaft für Chemische Technik und Biotechnologie e.V., www.dechema.de), which offers the world's largest collection of thermodynamic

mixture data was used to check the completeness of the literature search and to directly purchase data for which the original publication was not easily accessible.

Figure 1 provides an overview of the database collected in this study. The matrix lists the number of datasets at temperatures substantially different from 298 K available for each main group pair interaction. The green bars indicate the maximum number of overall datasets including all datatypes available for each main group interaction pair. For each interaction pair, the highest temperature (red shaded boxes) and lowest temperature (blue shaded boxes), for which datapoints are available, is indicated. The database overall consists of 677 datasets covering different data types, for monofunctional and multifunctional organic molecules in aqueous and water-free mixtures of binary and ternary systems. Table 1 lists the datasets and the data types used for determining the main group interaction parameters ($b_{n,m}$ and $c_{n,m}$) in the SR part of the AIOMFAC model. The table lists the mixture components, main groups, chemical formula (subgroups), data type, number of data points, temperature range, assigned initial weighting used in the model parameter fit, and the data source. Tables reporting new water activity measurements are provided in the Appendix (Tables A1 to A8). Different data types and their processing for use with the model parameterisation are described in the following.

3.1 Solid–liquid equilibrium data

Most low temperature data available for the model parameterisation are binary SLE data with water and an organic component. SLE data can be obtained by measuring the melting point depression of solutes as a function of solution composition. Consequently, at maximum two data points for each temperature level can be acquired for binary systems, corresponding to the points on the melting curves of the two components. However, most datasets collected provide only data for one component forming a solid in equilibrium with the remaining liquid solution. In many of these cases, hexagonal water ice is the solid phase. Since the temperature dependence of water activity (a_w) of aqueous solutions in equilibrium with ice is well known, an accurate determination

of the activity coefficients ($\gamma_w^{(x)} = \frac{a_w}{x_w}$) of water as a function of solution composition and temperature using SLE data is possible. At SLE, the activity of water in a solution with organic mole fraction x_{org} at thermodynamic equilibrium with ice, $a_w^{SLE}(T, p)$, is given by (Koop et al., 2000):

$$a_w^{SLE}(T, p) = \exp\left[\frac{\mu_w^S(T, p) - \mu_w^{\circ, L}(T, p)}{RT}\right], \tag{17}$$

where $\mu_w^S(T)$ and $\mu_w^{\circ, L}(T)$ are the pressure and temperature dependent chemical potentials of ice (superscript S) and pure liquid water (superscript $\circ, L$), respectively. At ambient pressures, neglecting the pressure dependence of the liquids and solids is well justified.

$$\mu_w^S(T) - \mu_w^{\circ, L}(T) = 210\,368 + 131.438\,T - 3.32373 \times 10^6\,T^{-1} - 41\,729.1\ln(T). \tag{18}$$

The parameterisation in Eq. (18) represents the thermodynamically consistent function for use with Eq. (17) valid at low (ambient) pressure in the temperature range $150 < T < 273\,\mathrm{K}$ (Koop et al., 2000).

The activity of a dissolved organic component in equilibrium with its pure crystalline solid can be calculated using the following relationship (Prausnitz et al., 1986; Domán-ska et al., 2009):

$$\ln x_i \gamma_i^{SLE} = -\frac{\Delta h_{m,i}}{RT}\left(1 - \frac{T}{T_{m,i}}\right) - \frac{\Delta h_{tr,i}}{RT}\left(1 - \frac{T}{T_{tr,i}}\right) + \frac{\Delta c_{p,m,i}}{R}\left[\left(1 - \frac{T}{T_{m,i}}\right) + \ln\frac{T}{T_{m,i}}\right]. \tag{19}$$

where $\Delta h_{m,i}$ is the molar enthalpy of fusion (melting, subscript m), $\Delta h_{tr,i}$ is the molar enthalpy of a certain solid–solid phase transition, $\Delta c_{p,m,i}$ is the molar heat capacity change upon fusion at constant pressure, T_{tr} is the solid–solid phase transition temperature and $T_{m,i}$ the melting temperature of pure component i. The second term is only of

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significance when there is a solid–solid phase transition (change of polymorphic form) between T and $T_{m,i}$. Equation (19) uses the simplification that the melting temperature and the triple point temperature of an organic compound are relatively close at atmospheric pressure. For obtaining activity coefficients from experimental data at given temperatures and mole fractions (x_{org}, T), Eq. (19) can be solved for the SLE organic activity and/or activity coefficients. Pure component physicochemical properties such as $\Delta h_{m,i}$ and $\Delta c_{p,m,i}$ are obtained from tabulated experimental data (Dean, 1999) and (Domalski and Hearing, 1996).

3.2 Water activity measurements

Water activity measurements were conducted for aqueous organic solutions with an Aqualab dew point water activity meter (Model 3TE, Decagon Devices, USA), which enables water activity measurements within the temperature range from 289–313 K for several concentrations at each temperature level. Water activity data for measured binary aqueous organic bulk solutions are tabulated in Tables A1–A8. Additional measurements of aqueous multifunctional organic solutions are provided in Ganbavale et al. (2014). Measured water activities were then used directly for the AIOMFAC-P3 parameter determination.

3.3 Liquid–liquid equilibria data

The equilibrium state between coexisting liquid phases is known as liquid–liquid equilibrium (LLE). Liquid–liquid equilibria are useful as a source of data for systems containing relatively hydrophobic organic compounds and water, with a miscibility gap that depends on temperature and mixture composition. In general, multicomponent systems may form more than two phases (in binary systems at maximum two liquid phases may coexist). For salt-free aqueous organic systems with two coexisting liquid phases, usually one phase is an aqueous (water-rich) phase while the other is an organic-rich phase. Most available experimental LLE data has been measured relatively close

to room temperature and is useful for a better description of the phase behaviour. However, for the purpose of our new parameterisation of AIOMFAC with regard to low temperatures far from room temperature, the LLE data tend to be less useful than, e.g., SLE data. We use the tie-line data from LLE measurements, which represents

5 the composition of the two liquid phases in equilibrium at a certain temperature. Initial mixture composition of experimental tie-lines are used as input for computation of LLE phase separation in order to compare the AIOMFAC model with the experimental data. A direct calculation and comparison of activities in coexisting phases is possible at experimental LLE compositions. This data type can be implemented in the model fit by

10 minimizing the relative differences between the activities of the components in the two liquid phases. We use the method introduced by Zuend et al. (2011) for the comparison of calculated relative activity deviations between the activities of components j present in the two phases. An initial mixture composition with mole fraction x_j^{init} of component j on a unstable/metastable point on a tie-line is generated by:

15
$$x_j^{\text{init}} = \frac{1}{2} \left(x_j^{\alpha} + x_j^{\beta} \right) \tag{20}$$

where x_j^{α} and x_j^{β} are the experimental compositions of the two liquid phases α and β at equilibrium. This allows a direct comparison of the measured and calculated phase compositions. According to the reference state definitions of AIOMFAC, different in-

20 dependent components j should have the same activities in coexisting phases. i.e. $a_j^{(x),\alpha} = a_j^{(x),\beta}$.

Forward computations of LLE were also performed using the method of Zuend and Seinfeld (2013), particularly for the graphical comparison of measured and predicted tie-line LLE data. For more details about the LLE computations with AIOMFAC we

25 refer to Zuend et al. (2010) and Zuend and Seinfeld (2013); the specific method used for fitting LLE data based on relative activity deviations is described in more detail in Zuend et al. (2011).

3.4 Vapour–liquid equilibria

VLE data represent the temperature and pressure conditions where a liquid (mixture) and its vapour(s) (gas phase) are in equilibrium with each other. The VLE data is usually obtained by performing measurements either at isobaric or isothermal conditions. VLE data considered in the model include binary water + organic systems and binary data for water-free organic (1) + organic (2) systems. Since isobaric measurements are usually conducted at 1 atm (= 101.325 kPa) pressure by measuring the boiling point temperature, they typically provide data at relatively high temperatures. In order to be used for the model parameterisation, the composition of the liquid in terms of mole fraction x_j of each component j, the composition of the gas phase in terms of mole fraction y_j and the total pressure p of the gas phase have to be stated or need to be derived from the data source. VLE data provide the composition dependence of activity coefficients. Assuming that the gas phase can be treated as an ideal gas mixture, activity coefficients of the components in the solution can be calculated by modified Raoult's law:

$$\gamma_j^{(x)} = \frac{p_j}{p_j^0 x_j}, p_j = y_j p, \tag{21}$$

where p_j is the partial pressure of component j, and $p_j^0(T)$ is the pure liquid component saturation vapour pressure calculated at the measurement temperatures using the Antoine equation with coefficients from the Landolt–Börnstein database (Dykyj et al., 2000), from Yaws et al. (2005) or, in some cases, the $p_j^0(T)$ are directly available from the reference of the experimental VLE data. Except for monocarboxylic acids such as formic, acetic, and propionic acid, which exhibit significant gas phase association (dimers, trimers), assuming an ideal gas mixture for the total pressure and temperature ranges of the data is acceptable. Other exceptions include certain diols and triols, e.g., glycerol, which show moderate non-ideality in the gas phase, requiring fugacity corrections. For mono-alcohols, fugacity corrections of the gas phase did not lead to

substantial changes in activity coefficients, due to the form of Eq. (21) (where the ratio of partial pressure and saturation vapour pressure, both similarly affected by association effects, cancel most of the non-ideality effects), and were typically ignored. To account for the gas phase dimerisation of carboxylic acids we obtain the monomer partial pressures using the dimerisation equilibrium coefficients from Tsonopoulos and Prausnitz (1970). The procedure for calculating experimental activity coefficients using this dimerization correction is described in more detail in Zuend et al. (2011).

4 Objective function and model parameter estimation

Organic–organic and organic–water main group interactions are parameterised in the SR part of AIOMFAC. The model parameter determination procedure involves simultaneous fitting of the various group interaction parameters to available thermodynamic phase equilibria data (see the database overview in Fig. 1). In order to ensure inter-comparability of different thermodynamic quantities and with due consideration of the various aspects of uncertainty in measurements and the group-contribution concept of the model, we use the following general objective function (F_{obj}), subject to minimization (Zuend et al., 2011):

$$F_{obj} = \sum_{d} \sum_{u} w_{d,u} \left[\frac{Q_{d,u}^{calc} - Q_{d,u}^{ref}}{\left| Q_{d,u}^{ref} \right| + Q_{d,u}^{tol}} \right]^2 . \tag{22}$$

Here, $w_{d,u}$ is the weighting value of a data point and the sums cover all data points u in all datasets d considered. $Q_{d,u}^{ref}$ is a reference quantity, directly determined from experiments (e.g., measured water activity value at a certain T and x_w) or derived from measurements by means of thermodynamic relations, e.g., SLE water activity on the ice melting curve at a specific temperature. $Q_{d,u}^{calc}$ represents the corresponding quantity calculated with the model at the given conditions. $Q_{d,u}^{tol}$ is a tolerance quantity (> 0)

which represents the measurement uncertainty or model sensitivity and has the same units as $Q_{d,u}^{\text{ref}}$. During the iterative fitting of the model parameters, we use the AIOMFAC model (with the so far fitted parameter set at that iteration step) to calculate the model activity sensitivity with respect to an assumed representative uncertainty in absolute mixture composition, a mole fraction tolerance set to: $x^{\text{tol}} = 0.01$. We refer to Zuend et al. (2011) (their Sect. 3.3) for a detailed description of how the model sensitivity is calculated. We use the AIOMFAC model to calculate the effect of a tiny change in composition on the activity coefficients of the different mixture components by means of a total molar derivative. Technically, this is done by scaling and summation of the partial derivatives of the activity coefficients at a given solution composition by means of finite differences in molar composition (Eq. 10 of Zuend et al., 2011).

4.1 Dataset weighting and temperature range

Both experimental uncertainties and model deficiencies need to be considered while determining the main group interaction parameters. The measured experimental quantities have some level of random and systematic errors, which may also depend on mixture composition, rendering some data points more reliable than others. This is considered during the parameter estimation procedure by giving appropriate weighting to the datasets and by data point-specific tolerance quantities computed in parallel from the model sensitivities as the iterative model fit progresses. With the aim of reducing a disproportionate influence of datasets with a large number of data points, as well as preventing an immoderate high weighting of datasets with a small number of data points, Zuend et al. (2011) propose a simplified procedure of assigning individual weighting to datasets on the basis of data type and number of data points N_d in a dataset:

$$w_{d,u} = \begin{cases} w_d^{\text{init}} & \text{if } N_d \leq \eta \\ w_d^{\text{init}} \times \frac{\eta}{N_d} & \text{if } N_d > \eta \end{cases} \tag{23}$$

where w_d^{init} is an initial weighting of dataset d on the basis of its temperature range, data type, and, in certain cases, additional expert judgement of its reliability. η is a characteristic number of data points per dataset. The weighting of individual data points that are part of large datasets can be reduced by multiplication with η/N_d. In this work, we keep $\eta = 10$ as in Zuend et al. (2011). Initial weightings assigned to datasets for the model fit are given in Table 1.

With the goal of fitting the AIOMFAC model parameters for a better description of activities at (low/high) temperatures far from room temperature, a set of rules was applied to assign initial weightings based on data type and the temperature range covered. Low temperature a_w data were assigned an initial weighting $w_d^{\text{init}} = 5.0$ while the SLE organic activity (SLE(org)) datasets (i.e., SLE data where an organic compound forms the solid in equilibrium with the liquid solution) are given an initial weighting of $w_d^{\text{init}} = 0.2$ because of the lower reliability of deriving solute activities using Eq. (19) compared to calculating water activities with Eq. (17). Relying on the water activity parameterisation of homogeneous freezing temperatures in aqueous solutions (Koop and Zobrist, 2009), freezing point depressions were also used as data source for parameter fitting. The a_w from DSC measurements at homogeneous freezing temperatures (T_{hom}) are assigned $w_d^{\text{init}} = 1.0$ (considering some uncertainties associated with the T_{hom} determination from DSC measurements). The weighting of all types of datasets close to room temperature (289–307 K) are set to zero to keep AIOMFAC unchanged around room temperature and guarantee consistency with functional groups that were not included in the new three-parameter temperature-dependence parameterisation. The LLE and VLE datasets are assigned an initial weighting of $w_d^{\text{init}} = 1.0$. However, datasets showing large scatter or inconsistencies with other comparable data (direct comparison of measurements or comparable via the thermodynamic relations underpinning AIOMFAC) were given lower or even zero weightings. To obtain parameters representing the best simultaneous description of all phase equilibria, thermodynamically inconsistent data have been excluded from the parameter fitting process (but only after test runs and a careful data quality review).

For determining the set of main group interaction parameters, i.e., the set of $b_{m,n}$ and $c_{m,n}$ values, where m, n represent all combinations of different main groups, we use a set of selective criteria by considering the temperature range of available experimental data. These criteria are separately applied to each group interaction pair as follows: the $b_{m,n}$ values are determined only if: $\Delta T_{\text{low}} = |T_{\text{low}} - T_\ominus|$ or $\Delta T_{\text{high}} = |T_{\text{high}} - T_\ominus| > 40\,\text{K}$ and $\Delta T = |T_{\text{low}} - T_{\text{high}}| > 40\,\text{K}$, where $T_\ominus = 298.15\,\text{K}$ is the reference temperature. Similarly, the $c_{m,n}$ parameters for the main groups are determined only if $\Delta T_{\text{low}} > 80\,\text{K}$ or $\Delta T_{\text{high}} > 80\,\text{K}$ and if $\Delta T > 80\,\text{K}$. In addition, we set numeric bounds on the values of the fitted parameters, described below. The three terms on the right hand side of Eq. (16) contain parameters of different thermodynamical meaning (see Eq. 15) and different magnitude. The terms containing $a_{m,n}$ and $b_{m,n}$ are associated with changes of molar enthalpy over a certain temperature difference, while $c_{m,n}$ is related to changes in the molar heat capacity at constant pressure (hence, accounting for the change of the change of enthalpy with temperature). These thermodynamic quantities tend to be of different magnitude (molar heat capacity changes are roughly two to three orders of magnitude smaller in value than changes in molar enthalpy). Hence, the expected values and set numeric bounds on the parameters $b_{m,n}$ and $c_{m,n}$ are quite different for these reasons. Symmetric parameter bounds for permissible values of $b_{m,n}$ are set to $\pm\max[a_{m,n}, 200]$, while the numerical limits on $c_{m,n}$ are set to $\pm\max[4 \times 10^{-3} \times \max(a_{m,n}, 200)]$.

With the implementation of these parameter bounds and based on the reduced set of experimental data fulfilling the selection criteria, 150 new short-range interaction parameters were determined simultaneously for 14 functional main groups. As described in Zuend et al. (2011), due to the high dimensionality, and nonlinear coupling of the fit parameters, the minimization problem is a challenging task for any global optimization method. For the parameter optimization, it is sufficient to find a "good" local minimum, which may not be the global minimum. As a part of data quality control and to avoid that a few datasets dominate the parameter optimization due to potential numerical issues or other reasons, such as inconsistent datasets and outliers, a large number of

trial parameter optimization runs were carried out. To solve the parameter optimization problem, we use the formulation introduced by Zuend et al. (2011) by using a combination of algorithms to solve the parameter optimization problem. First, a Best-of-Random Differential Evolution (BoRDE) algorithm (Lin et al., 2011) is used to explore the parameter space and to broadly locate a minimum of F_{obj}. Second, the global trust region method BOBYQA of Powell (2009) is applied to further refine the solution. Finally, the Downhill-Simplex algorithm by Nelder and Mead (1965) is used to fully converge to the minimum. More details are given in Zuend et al. (2011).

During trial runs, the contributions of the individual datasets to the objective function value Eq. (22) were used to identify potential inconsistencies among datasets, errors in data calculations and conversion or the implementation in the model. This allowed us to establish a high level of data quality, correct mistakes (e.g. typing errors) and compare thermodynamic data from different types of experiments and references for general consistency. Table 2 provides the final values of the determined organic main group interaction parameters. For comparison and completeness, the values of $a_{m,n}$ parameters, which were preserved in the new UNIFAC parameterisation are listed as well. All main group interaction parameters $b_{m,n}$ and $c_{m,n}$, for which the database does not satisfy our criteria concerning temperature range and data availability, are set to zero.

5 Results and discussion

The new temperature dependence parameterisation is applied to aqueous organic and water-free organic solutions covering a wide concentration and temperature range. In this section, we compare and discuss the model performance of the new AIOMFAC-P3 version, with AIOMFAC-P1 (original AIOMFAC version) for a selection of aqueous organic mixtures and water-free organic mixtures. The new AIOMFAC-P3 parameterisation for the temperature dependence of activity coefficients shows an overall improvement of 25 % in terms of F_{obj} in comparison to AIOMFAC-P1. As stated ear-

lier, AIOMFAC-P1 uses the temperature-dependence expression of standard UNIFAC and represents the AIOMFAC performance using only $a_{m,n}$ interaction paramters. The AIOMFAC-P3 model version uses all the three parameters i.e., $a_{m,n}$, $b_{m,n}$ and $c_{m,n}$, where applicable, with our new expression for the temperature dependence of group interactions.

It should be noted that the model was not just fitted to the selection of datasets shown; rather the figures show a few examples, and the AIOMFAC-P3 model is, of course, based on the simultaneous optimisation of all fit parameters to the complete database. For each individual system, a specific fit of either AIOMFAC-P1 or -P3 (to that dataset only) would represent those data better, but that is not the goal of a versatile group-contribution model.

5.1 Aqueous organic mixtures

Figure 2 shows the comparison of aqueous 1,2-ethanediol solutions using the AIOMFAC-P1 and AIOMFAC-P3 models. Panels (a–c) represent the AIOMFAC-P1 performance while panels (d–f) represent the corresponding AIOMFAC-P3 results. The low-temperature SLE data (a and d) are well represented by both AIOMFAC-P1 and AIOMFAC-P3. The high-temperature VLE data are much better represented by AIOMFAC-P3 in comparison to AIOMFAC-P1. Panels (c) and (f) show predicted water activities covering the full concentration space from pure water to pure organic for 12 different temperature levels between 150 K and 480 K. Over all concentrations, AIOMFAC-P3 (f) indicates a small temperature dependence. In comparison to the AIOMFAC-P1, the resulting temperature dependence from low to high x_{org} is relatively small in the AIOMFAC-P3 case.

Figure 3 compares the model performance of AIOMFAC-P1 and AIOMFAC-P3 for SLE and VLE experimental data of aqueous acetic acid systems. The SLE data is well represented by both AIOMFAC-P1 and AIOMFAC-P3 (Fig. 3a and d). At higher temperatures, covered by VLE data, the AIOMFAC-P3 prediction is clearly in better agreement with the experimental data than the AIOMFAC-P1 calculation. However, both model pa-

rameterisations tend to underestimate the activity coefficients of water and acetic acid, particularly at high and low mole fractions of water. Overall for this system, the extended description of the temperature dependence of activity coefficients in AIOMFAC-P3 allows a relatively good representation of observations at low and high temperatures,

5 while AIOMFAC-P1 shows quite large deviations at higher temperatures. The temperature dependence predictions for the temperature range 150–480 K are given in panels (c, f). AIOMFAC-P1 predicts less pronounced temperature dependence at higher temperatures, 360–480 K, while AIOMFAC-P3 predicts an overall larger temperature dependence of water activity over the whole temperature range. This steeper slope of

10 changes in water activity with temperature seems to be necessary to reproduce both VLE and SLE data for this system and other systems containing compounds with common functional groups.

Figure 4 shows measured SLE data for the malonic acid + water system and its comparison with the predictions from AIOMFAC-P1 and AIOMFAC-P3. In the panels a and

15 c, water is the component in equilibrium with ice (hence the data describes the ice melting curve at different T and mixture composition), while panels b and e show analogous data for the malonic acid melting curve. The temperature ranges are slightly different, with the highest temperature in the plots referring to the melting temperature of the pure component or the SLE at the highest concentration of the organic com-

20 ponent, respectively. The predicted a_w shows slight deviations from the experimental data towards lower water activities for both AIOMFAC-P1 and AIOMFAC-P3 (a, d). The predicted a_{org} (in a range closer to and above room temperature) is well represented in both AIOMFAC-P1 and AIOMFAC-P3 (b, e). No VLE data is available for aqueous malonic acid at higher temperatures and hence could not be compared. AIOMFAC-P3

25 predicts a larger temperature dependence in comparison to AIOMFAC-P1, the latter shows a relatively small temperature dependence of water activity at higher temperatures (c, f).

Figure 5 shows an example of a binary system consisting of water and 2-butanone with a miscibility gap present over a large temperature and composition range. Both

model parameterisations show deviations from the SLE data (a, d). However, the AIOMFAC-P3 parameterisation clearly reduces the deviations from the experimental data in comparison to AIOMFAC-P1, the latter showing deviations up to > 0.3 in a_w at low water contents. On the other hand, at the higher temperatures covered by VLE data, both AIOMFAC-P1 (Fig. 5b) and AIOMFAC-P3 (Fig. 5e) are in good agreement with the experimental data. A miscibility gap is also predicted by both AIOMFAC parameterisations, although the width and temperature range of the predicted phase separations do differ between the model results. According to the AIOMFAC-P3 prediction, a phase separation occurs in the temperature range 150 to ~ 390 K. The composition space where a liquid–liquid phase separation occurs is indicated in such diagrams by drawing a horizontal line (parallel to the abscissa) from one of the local minima of a_w to the point where it intersects with the a_w curve at a different x_{org} value. For example, for the a_w curve at $T = 150$ K, liquid–liquid phase separation is predicted at $a_w = 0.98$ in the composition range between x_{org}(2-butanone) = 0.04 and x_{org}(2-butanone) = 0.62. A miscibility gap is also found in the experiments and is the reason why in panels (a, b, d, e) there are no data points in the mole fraction range $0.35 < x$ (H$_2$O) < 0.85.

Figure 6 shows the model-measurement comparison for aqueous 2-butoxyethanol. AIOMFAC-P1 and AIOMFAC-P3 show similar performance. Both models are not in good agreement with the experimental data. Contrary to the experimental data, both AIOMFAC-P1 and AIOMFAC-P3 predict $a_w > 1$ in a certain composition range and both models predict a liquid–liquid phase separation over a wide range of temperatures, explaining the reason for deviations in predicted water activity shown in Fig. 6a and d (see also local minima in a_w curves of panels c, f). Note that the model predictions in these figures do not include phase separation computations on purpose, since the experimental data are for a homogenous single phase (no phase separation found experimentally) so are the model calculations here. Also, at higher temperatures the activity coefficients of both water and 2-butoxyethanol show deviation from experimental data (b, e). AIOMFAC-P3 shows a larger temperature dependence over the entire temperature range in comparison to AIOMFAC-P1 (c, f).

5.2 Binary organic mixtures

Figure 7 shows the model-measurement comparison for SLE data of the water-free mixture of cyclohexanol + adipic acid. The AIOMFAC-P3 prediction is in better agreement with the experimental data than AIOMFAC-P1, which shows a positive deviation at lower mole fractions of component 1 (cyclohexanol). In this binary system, the AIOMFAC-P3 parameterisation leads to a relatively large temperature dependence of the activity of cyclohexanol, a_{org} (1), (panel d). In addition, with that parameterisation a phase separation occurs at lower x_{org} (2) values for temperatures below $\sim 180\,K$. However, no phase separation is expected at higher temperatures, more relevant in the troposphere. AIOMFAC-P1 on the other hand shows a much smaller temperature dependence and does not predict a phase separation.

Measurements for water-free binary organic mixtures of ethanol + acetone are shown in Fig. 8. The AIOMFAC-P3 predictions of the activities of acetone are in a very good agreement with the experimental SLE-derived data (Fig. 8d), while AIOMFAC-P1 shows larger deviations from the experimental data at these low temperatures (a). At high temperatures, the VLE data for both AIOMFAC-P1 and AIOMFAC-P3 show similar results (b, e), with slightly larger deviations of $\gamma_{org_2}^{(x)}$ (activity coefficient of acetone) in AIOMFAC-P1. At temperatures higher than $300\,K$ both AIOMFAC-P1 and AIOMFAC-P3 show a much smaller temperature dependence than for the range below room temperature.

Figure 9 shows a similar example, for ethanol + 3-heptanone mixtures. The prediction from AIOMFAC-P3 is in relatively good agreement with the experimental SLE data, showing less deviations in 3-heptanone activities than the results from the AIOMFAC-P1 calculations. Achieving better agreement with the new (AIOMFAC-P3) parameterisation requires a larger temperature dependence of the organic activities, particularly towards lower temperatures.

Figure 10 shows the binary ethanol + diethyl ether system, where experimental data are available for a temperature range spanning more than $200\,K$: from $149\,K$ up to

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378 K. Of course, additional data from other systems of our database are also affecting the main group interaction parameters that are necessary to describe this system with AIOMFAC-P3. Both models describe the diethyl ether activity derived from SLE at low temperatures quite well (a and d). AIOMFAC-P3 shows slight overprediction of the diethyl ether activity, while AIOMFAC-P1 tends to underpredict the experimental data. In contrast, at higher temperatures ($\sim$ 350 to 380 K) covered by experimental VLE data (b and e), the predicted $\gamma_{\mathrm{org}_2}^{(x)}$ both by AIOMFAC-P1 and AIOMFAC-P3 are not in good agreement with the VLE experimental data. The main reason for the observed deviations is due to inaccurately predicted activity coefficients at infinite dilution (i.e., when one of the compounds is present only as a tiny mole fraction in the solution) of the two organic compounds at these temperatures. At infinite dilution conditions the activity coefficients are dominated by subgroup volume and surface area properties in the UNIFAC/AIOMFAC model, so that the activity coefficient values are largely unaffected by the new main group interaction parameterisation of AIOMFAC-P3 in comparison to AIOMFAC-P1. As is visible from Fig. 10c and f, particularly at x(diethyl ether) > 0.4, the temperature dependence of ethanol activities predicted by AIOMFAC-P3 is larger than the original one in AIOMFAC-P1. The example of this system shows that it is not always possible to achieve good model predictions for the full temperature range with the new treatment of temperature dependence in AIOMFAC. For further improvements, other model parts, such as the lattice constant (z), which is not really a constant, may need to be considered for the introduction of additional, physically meaningful temperature dependent parameterisations.

5.3 Scope and limitations of the new parameterisation

The thermodynamic model AIOMFAC has been developed based on modified versions of UNIFAC and LIFAC, with the aim to establish a versatile activity coefficient model for atmospheric applications. The new parameterisation of the model aims at improving AIOMFAC predictions particularly at lower temperatures of atmospheric relevance. Deviations between the experimental data and model predictions from the new AIOMFAC-

P3 version are associated with either the inaccuracy of the measurements, the lack of data to better cover and parameterise the model for a wide composition and temperature range, or limitations of the AIOMFAC expressions and the group contribution method. Own measurements were performed for selected aqueous organic systems at low temperatures and at temperatures around room temperature, which were used together with experimental data from the literature for parameterising the model over a wider temperature range. The complexity of organics in terms of their physical and chemical properties such as size, shape and combinations of groups in multifunctional molecules are important factors that influence the quality of AIOMFAC predictions.

Most of the SLE data at low temperature are limited to simple organic molecules, which thus make up the majority of the model parameterisation database. Due to this, the accuracy of AIOMFAC predictions is expected to decrease with increasing complexity of multifunctional organic compounds. However, the new AIOMFAC parameterisation provides a tool to predict activity coefficients with better overall accuracy than the previous version and offers the versatility of a group-contribution method for the prediction of activity coefficients in complex mixtures containing many tens to thousands of individual components.

6 Conclusions

An improved temperature dependence parameterisation of aqueous organic and water-free organic mixtures is presented for the thermodynamic group contribution model AIOMFAC. A comprehensive database of experimental thermodynamic equilibria data is established by collecting and carefully validating different data types covering a wide temperature and concentration range. In addition, new measurements that have been performed for selected aqueous organic systems, at room temperature and below, were also included in the database. The database is used to determine new AIOMFAC group interaction parameters for organic main groups of atmospheric relevance: carboxyl, hydroxyl, ketone, aldehyde, ether, ester, alkyl, aromatic carbon-alcohol, and aromatic

hydrocarbons. The parameter fitting procedure involved the simultaneous determination of 150 interaction parameters for the 14 main groups. Thus, the new temperature dependence parameterisation allows to calculate activity coefficients and their temperature dependence for a wide variety of organic and water-free mixtures. In general, the new AIOMFAC parameterisation achieves good agreement with a large number of experimental datasets. In the case of some organic systems, lack of experimental data to constrain the activity coefficients is a major limitation. Further improvements of the AIOMFAC model description of these systems and by that, the interactions of the functional groups involved, will require additional measurements over a wide temperature and concentration range. The improved AIOMFAC model can be used to better account for the temperature dependence of activity coefficients relevant in predictions related to atmospheric ice nucleation and gas-particle partitioning in multicomponent systems.

Appendix A

Bulk water activities, a_w, were measured for aqueous organic solutions using an AquaLab water activity meter (Model 3TE, Decagon devices, USA). The instrument applies the chilled mirror technology to determine the dewpoint temperature of air equilibrated with the aqueous solution being measured which is then translated to water activity. The instrument's infrared thermometry indicates the sample temperature and, which is then considered in the determination of water activity. So, accurate measurements are not dependent on precise thermal equilibrium at a set temperature level. The internal temperature control allows to perform measurements under stable temperature from 289–313 K. The standard sample block with a specified error of ±0.003 in a_w was used for most experiments. For the more volatile polyols (2,5-hexanediol, 1,2,6-hexanetriol, and glycerol) the volatile sample block available using a hygroscopic polymer sensor to detect the equilibrium relative humidity of air in the headspace above the sample was used to perform measurements.

The stated error for the volatile sample block is ±0.015 a_w. Instrument offset is frequently corrected and the performance of the sample block was controlled and readjusted with reference samples. All measurements were performed at 289–313 K. The substances were purchased from Sigma-Aldrich in the best available purity. The following solutes were investigated: glycerol (Sigma, > 99 %), 2,5-hexanediol (Fluka, > 97 %), 1,2,6-hexanetriol (Fluka, > 95 %), 1,2,7,8-octanetetrol (Fluka, > 97 %), 2,2,6,6-Tetrakis(hydroxymethyl)cyclohexanol (Aldrich, 97 %), DL-4-Hydroxy-3-methoxy mandelic acid (Sigma, > 95 %), raffinose (Sigma, > 98 %), The substances were used without further purification. The water/polyol mixtures were prepared by mass percent with MilliQ water using an analytical balance. Each solution was measured at least three times at each temperature. Water activity data for these aqueous solution are tabulated in Appendix Tables A1–A8.

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Table 1. Components, main groups, temperature range, number of data points (N_d), initial weighting (w_d^{init}) and references of "water + organic and organic + organic" datasets used for the short-range parameterization of organic main group ↔ water and organic ↔ organic main group interactions.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
– water + alcohol/polyol –							
ethanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$	220–269	SLE	7	5.00	Ross (1954)
ethanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$	265–273	SLE	31	5.00	Knight (1962)
ethanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$	211–273	SLE	62	1.00	Pickering (1893)
ethanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$	307–318	VLE	11	1.00	Gmehling and Onken (1977)
ethanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$	341–353	VLE	11	1.00	Gmehling and Onken (1977)
ethanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$	350–363	VLE	11	1.00	Gmehling and Onken (1977)
ethanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$	351–372	VLE	34	1.00	Gmehling and Onken (1977)
1-propanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH_2^{[OH]})(OH)$	263–273	SLE	3	5.00	Ross (1954)
1-propanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH_2^{[OH]})(OH)$	264–270	SLE	7	5.00	Chapoy et al. (2008)
1-propanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH_2^{[OH]})(OH)$	264–270	SLE	12	5.00	Pickering (1893)
1-propanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH_2^{[OH]})(OH)$	264–270	SLE	14	5.00	Pickering (1893)
1-propanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH_2^{[OH]})(OH)$	330–339	VLE	8	1.00	Gmehling and Onken (1977)
1-propanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH_2^{[OH]})(OH)$	345–355	VLE	8	1.00	Gmehling and Onken (1977)
1-propanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH_2^{[OH]})(OH)$	355–365	VLE	8	1.00	Gmehling and Onken (1977)
1-propanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH_2^{[OH]})(OH)$	361–372	VLE	8	1.00	Gmehling and Onken (1977)
2-propanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})(OH)$	266–273	SLE	29	5.00	Knight (1962)
2-propanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})(OH)$	271–273	SLE	9	5.00	Okamoto et al. (1978)
2-propanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})(OH)$	272–273	SLE	17	5.00	Webb and Lindsley (1934)
2-propanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})(OH)$	353–372	VLE	24	1.00	Gmehling and Onken (1977)
2-propanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})(OH)$	341–357	VLE	19	1.00	Gmehling and Onken (2003a)
2-propanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})(OH)$	325–340	VLE	19	1.00	Gmehling and Onken (2003a)
2-propanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})(OH)$	328	VLE	8	1.00	Gmehling and Onken (1977)
2-propanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})(OH)$	318	VLE	8	1.00	Gmehling and Onken (1977)
2-propanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})(OH)$	308	VLE	8	1.00	Gmehling and Onken (1977)
1-butanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2(CH_2^{[OH]})(OH)$	271–273	SLE	22	5.00	Knight (1962)
1-butanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2(CH_2^{[OH]})(OH)$	200–273	SLE	10	5.00	Lohmann et al. (1997)
1-butanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2(CH_2^{[OH]})(OH)$	366–384	VLE	12	1.00	Gmehling and Onken (1977)
1-butanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2(CH_2^{[OH]})(OH)$	365–382	VLE	8	1.00	Gmehling and Onken (2003a)
1-butanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2(CH_2^{[OH]})(OH)$	323	VLE	4	1.00	Gmehling et al. (1988)
1-butanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2(CH_2^{[OH]})(OH)$	343	VLE	4	1.00	Gmehling et al. (1988)
1-butanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2(CH_2^{[OH]})(OH)$	363	VLE	4	1.00	Gmehling et al. (1988)
2-butanol	$CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$	215–259	SLE	10	5.00	Lohmann et al. (1997)
2-butanol	$CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$	240–273	SLE	2	5.00	Lohmann et al. (1997)
2-butanol	$CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$	268–273	SLE	28	2.00	Knight (1962)
2-butanol	$CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$	330–335	VLE	11	1.00	Gmehling and Onken (2003a)
2-butanol	$CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$	345–351	VLE	11	1.00	Gmehling and Onken (2003a)
2-butanol	$CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$	355–360	VLE	11	1.00	Gmehling and Onken (2003a)
2-butanol	$CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$	360–367	VLE	20	1.00	Gmehling and Onken (2003a)
2-butanol	$CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$	361–367	VLE	11	1.00	Gmehling and Onken (2003a)
isobutanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})_2(CH^{[alc-tail]})(CH_2^{[OH]})(OH)$	225–273	SLE	10	5.00	Lohmann et al. (1997)
tert-butanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_3(C^{[OH]})(OH)$	266–273	SLE	34	5.00	Knight (1962)
tert-butanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_3(C^{[OH]})(OH)$	353–364	VLE	15	1.00	Gmehling et al. (1981)

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Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
tert-butanol	$CH_3^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_3(C^{[OH]})(OH)$	331–339	VLE	15	1.00	Gmehling and Onken (1977)
tert-butanol	$CH_3^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_3(C^{[OH]})(OH)$	308–317	VLE	17	1.00	Gmehling and Onken (1977)
tert-butanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_3(C^{[OH]})(OH)$	353	VLE	9	1.00	Gmehling and Onken (2003a)
tert-butanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_3(C^{[OH]})(OH)$	343	VLE	9	1.00	Gmehling and Onken (2003a)
tert-butanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_3(C^{[OH]})(OH)$	303	VLE	16	1.00	Gmehling and Onken (2003a)
glycerol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})(OH)_3$	189–231	$a_w(T_{hom})^a$	10	1.00	Kanno et al. (2004)
glycerol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})(OH)_3$	225–271	SLE	7	5.00	Ross (1954)
glycerol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})(OH)_3$	232–271	SLE	10	5.00	Olsen et al. (1930)
glycerol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})(OH)_3$	258–272	SLE	5	5.00	Lerici et al. (2006)
glycerol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})(OH)_3$	255–291	SLE(org)^d	11	0.20	Pushin and Glagoleva (1922)
glycerol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})(OH)_3$	289	a_w (bulk)	15	0.0	this work
glycerol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})(OH)_3$	298	a_w (bulk)	15	0.0	this work
glycerol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})(OH)_3$	313	a_w (bulk)	15	1.0	this work
glycerol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})(OH)_3$	347–421	VLE	8	0.001	Soujanya et al. (2010)
glycerol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})(OH)_3$	353–447	VLE	9	0.001	Soujanya et al. (2010)
glycerol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})(OH)_3$	358–454	VLE	10	0.001	Soujanya et al. (2010)
glycerol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})(OH)_3$	364–484	VLE	9	0.001	Soujanya et al. (2010)
glycerol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})(OH)_3$	373–410	VLE	7	0.001	Soujanya et al. (2010)
1,2-ethanediol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(OH)_2$	220–270	SLE	6	5.00	Dykyj et al. (1956)
1,2-ethanediol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(OH)_2$	271–273	SLE	10	5.00	Okamoto et al. (1978)
1,2-ethanediol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(OH)_2$	225–267	SLE	7	5.00	Ott et al. (1972)
1,2-ethanediol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(OH)_2$	224–273	SLE	7	2.00	Ott et al. (1972)
1,2-ethanediol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(OH)_2$	223–270	SLE	6	5.00	Clendenning (1946)
1,2-ethanediol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(OH)_2$	230–260	SLE(org)^d	11	0.20	Ott et al. (1972)
1,2-ethanediol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(OH)_2$	298.15	a_w (bulk)	14	0.0	Marcolli and Peter (2005)
1,2-ethanediol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(OH)_2$	323	VLE	19	1.00	Gmehling et al. (1988)
1,2-ethanediol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(OH)_2$	333	VLE	20	1.00	Gmehling et al. (1988)
1,2-ethanediol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(OH)_2$	338	VLE	10	1.00	Gmehling et al. (1988)
1,2-ethanediol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(OH)_2$	343	VLE	15	0.20	Gmehling and Onken (2003a)
1,2-ethanediol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(OH)_2$	363	VLE	12	1.00	Gmehling et al. (1988)
1,2-ethanediol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(OH)_2$	359–437	VLE	9	1.00	Gmehling and Onken (2003a)
1,2-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_2^{[OH]})(CH^{[OH]})(OH)_2$	207–270	SLE	7	5.00	Ross (1954)
1,2 propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_2^{[OH]})(CH^{[OH]})(OH)_2$	216–271	SLE	12	5.00	Boese et al. (1953)
1,2-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_2^{[OH]})(CH^{[OH]})(OH)_2$	298	a_w (bulk)	13	0.0	Marcolli and Peter (2005)
1,2-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_2^{[OH]})(CH^{[OH]})(OH)_2$	288	VLE	5	1.00	Gmehling et al. (1988)
1,2-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_2^{[OH]})(CH^{[OH]})(OH)_2$	298	VLE	5	0.0	Gmehling et al. (1988)
1,2-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_2^{[OH]})(CH^{[OH]})(OH)_2$	303	VLE	5	1.00	Gmehling et al. (1988)
1,2-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_2^{[OH]})(CH^{[OH]})(OH)_2$	308	VLE	5	1.00	Gmehling et al. (1988)
1,2-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_2^{[OH]})(CH^{[OH]})(OH)_2$	318	VLE	5	1.00	Gmehling et al. (1988)
1,2-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_2^{[OH]})(CH^{[OH]})(OH)_2$	323	VLE	5	1.00	Gmehling et al. (1988)
1,2-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_2^{[OH]})(CH^{[OH]})(OH)_2$	353	VLE	8	1.00	Gmehling and Onken (2003a)
1,2-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_2^{[OH]})(CH^{[OH]})(OH)_2$	373	VLE	6	0.10	Gmehling and Onken (2003a)
1,2-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_2^{[OH]})(CH^{[OH]})(OH)_2$	383	VLE	11	1.00	Gmehling and Onken (2003a)
1,2-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_2^{[OH]})(CH^{[OH]})(OH)_2$	395	VLE	9	1.00	Gmehling and Onken (2003a)
1,3-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})(CH_2^{[OH]})_2(OH)_2$	200–231	$a_w(T_{hom})^a$	4	1.00	Ganbavale et al. (2014)
1,3-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})(CH_2^{[OH]})_2(OH)_2$	256–270	SLE	5	5.00	Ganbavale et al. (2014)
1,3-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})(CH_2^{[OH]})_2(OH)_2$	249–270	SLE	5	5.00	Ross (1954)
1,3-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})(CH_2^{[OH]})_2(OH)_2$	298	a_w (bulk)	13	0.00	Marcolli and Peter (2005)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
1,3-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})(CH_2^{[OH]})_2(OH)_2$	343–442	VLE	19	0.1	Sanz et al. (2001)
1,3-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})(CH_2^{[OH]})_2(OH)_2$	341–428	VLE	12	1.00	Mun and Lee (1999)
1,3-propanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})(CH_2^{[OH]})_2(OH)_2$	353–441	VLE	18	0.20	Mun and Lee (1999)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	196–230	$a_w(T_{hom})^a$	4	1.00	Zobrist et al. (2008)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	258–270	SLE	4	5.00	Zobrist et al. (2008)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	270	$a_w(p^{tot})^e$	8	1.00	Ganbavale et al. (2014)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	273	$a_w(p^{tot})$	6	1.00	Ganbavale et al. (2014)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	275	$a_w(p^{tot})$	8	1.00	Ganbavale et al. (2014)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	278	$a_w(p^{tot})$	11	1.00	Ganbavale et al. (2014)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	280	$a_w(p^{tot})$	11	1.00	Ganbavale et al. (2014)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	283	$a_w(p^{tot})$	11	1.00	Ganbavale et al. (2014)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	285	$a_w(p^{tot})$	11	1.00	Ganbavale et al. (2014)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	288	$a_w(p^{tot})$	11	0.00	Ganbavale et al. (2014)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	290	$a_w(p^{tot})$	11	0.00	Ganbavale et al. (2014)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	298	a_w (bulk)	16	0.00	Marcolli and Peter (2005)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	289	a_w (bulk)	9	0.00	Ganbavale et al. (2014)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	298	a_w (bulk)	9	0.00	Ganbavale et al. (2014)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	313	a_w (bulk)	9	1.00	Ganbavale et al. (2014)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	333	VLE	10	1.00	Gmehling and Onken (2003b)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	338	VLE	10	1.00	Gmehling and Onken (2003b)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	343	VLE	10	1.00	Gmehling and Onken (2003b)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	348	VLE	10	1.00	Gmehling and Onken (2003b)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	353	VLE	9	1.00	Gmehling and Onken (2003b)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	358	VLE	10	1.00	Gmehling and Onken (2003b)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	363	VLE	10	1.00	Gmehling and Onken (2003b)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	368	VLE	10	1.00	Gmehling and Onken (2003b)
1,4-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH_2^{[OH]})_2(OH)_2$	367–409	VLE	13	1.00	Gmehling et al. (1988)
2,3-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})_2(OH)_2$	232–270	SLE	6	5.00	Clendenning (1946)
2,3-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})_2(OH)_2$	298	a_w (bulk)	13	0.00	Marcolli and Peter (2005)
2,3-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})_2(OH)_2$	375–420	VLE	8	1.00	Gmehling et al. (1988)
2,3-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})_2(OH)_2$	373–379	VLE	7	1.00	Gmehling et al. (1988)
2,3-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})_2(OH)_2$	367–411	VLE	8	1.00	Gmehling et al. (1988)
2,3-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})_2(OH)_2$	356–399	VLE	8	1.00	Gmehling et al. (1988)
2,3-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})_2(OH)_2$	340–380	VLE	8	1.00	Gmehling et al. (1988)
2,3-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})_2(OH)_2$	408–410	VLE	8	1.00	Gmehling et al. (1988)
2,3-butanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH^{[OH]})_2(OH)_2$	426–431	VLE	7	1.00	Gmehling et al. (1988)
1,5-pentanediol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc-tail]})_3(CH_2^{[OH]})_2(OH)_2$	200–232	$a_w(T_{hom})^a$	5	1.00	Ganbavale et al. (2014)
1,5-pentanediol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc-tail]})_3(CH_2^{[OH]})_2(OH)_2$	260–272	SLE	5	5.00	Ganbavale et al. (2014)
1,5-pentanediol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc-tail]})_3(CH_2^{[OH]})_2(OH)_2$	298	SLE	14	0.00	Marcolli and Peter (2005)
1,2-hexanediol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_3(CH_2^{[OH]})(CH^{[OH]})(OH)_2$	223–232	$a_w(T_{hom})^a$	4	1.00	Ganbavale et al. (2014).
1,2-hexanediol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_3(CH_2^{[OH]})(CH^{[OH]})(OH)_2$	272–271	SLE	4	5.00	Ganbavale et al. (2014).
1,2-hexanediol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_3(CH_2^{[OH]})(CH^{[OH]})(OH)_2$	298	a_w (bulk)	12	0.00	Marcolli and Peter (2005)
2,5-hexanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH_2^{[alc]})_2(CH^{[OH]})_2(OH)_2$	204–230	$a_w(T_{hom})^a$	3	1.00	Zobrist et al. (2008)
2,5-hexanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH_2^{[alc]})_2(CH^{[OH]})_2(OH)_2$	264–271	SLE	3	5.00	Zobrist et al. (2008)
2,5-hexanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH_2^{[alc]})_2(CH^{[OH]})_2(OH)_2$	289	a_w (bulk)	9	0.00	this work
2,5-hexanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH_2^{[alc]})_2(CH^{[OH]})_2(OH)_2$	298	a_w (bulk)	9	0.00	this work
2,5-hexanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_2(CH_2^{[alc]})_2(CH^{[OH]})_2(OH)_2$	313	a_w (bulk)	9	1.00	this work

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Extended parameterization of the AIOMFAC model

G. Ganbavale et al.

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Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
1,2,6-hexanetriol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_3(CH_2^{[OH]})_2(CH^{[OH]})$ $(OH)_3$	202–231	$a_w(T_{hom})^a$	4	1.00	Zobrist et al. (2008)
1,2,6-hexanetriol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_3(CH_2^{[OH]})_2(CH^{[OH]})$ $(OH)_3$	251–272	SLE	6	5.00	Ross (1954)
1,2,6-hexanetriol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_3(CH_2^{[OH]})_2(CH^{[OH]})$ $(OH)_3$	263–271	SLE	4	5.00	Zobrist et al. (2008)
1,2,6-hexanetriol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_3(CH_2^{[OH]})_2(CH^{[OH]})$ $(OH)_3$	289	a_w (bulk)	9	0.00	this work
1,2,6-hexanetriol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_3(CH_2^{[OH]})_2(CH^{[OH]})$ $(OH)_3$	298	a_w (bulk)	9	0.00	this work
1,2,6-hexanetriol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_3(CH_2^{[OH]})_2(CH^{[OH]})$ $(OH)_3$	313	a_w (bulk)	9	1.00	this work
1,2,7,8-octanetrol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_4(CH_2^{[OH]})_2(CH^{[OH]})_2$ $(OH)_4$	203–232	$a_w(T_{hom})^a$	4	1.00	Zobrist et al. (2008)
1,2,7,8-octanetrol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_4(CH_2^{[OH]})_2(CH^{[OH]})_2$ $(OH)_4$	266–273	SLE	4	5.00	Zobrist et al. (2008)
1,2,7,8-octanetrol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_4(CH_2^{[OH]})_2(CH^{[OH]})_2$ $(OH)_4$	289	a_w (bulk)	8	0.00	this work
1,2,7,8-octanetrol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_4(CH_2^{[OH]})_2(CH^{[OH]})_2$ $(OH)_4$	298	a_w (bulk)	8	0.00	this work
1,2,7,8-octanetrol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_4(CH_2^{[OH]})_2(CH^{[OH]})_2$ $(OH)_4$	313	a_w (bulk)	9	1.00	this work
2,2,6,6-tetrakis (hydroxymethyl)cyclohexanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH^{[alc]})_2(CH_2^{[OH]})_4$ $(CH^{[OH]})(C^{[alc]})(OH)_5$	208–232	$a_w(T_{hom})^a$	4	1.00	Zobrist et al. (2008)
2,2,6,6-tetrakis (hydroxymethyl)cyclohexanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH^{[alc]})_2(CH_2^{[OH]})_4$ $(CH^{[OH]})(C^{[alc]})(OH)_5$	265–272	SLE	5	5.00	Zobrist et al. (2008)
2,2,6,6-tetrakis (hydroxymethyl)cyclohexanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH^{[alc]})_2(CH_2^{[OH]})_4$ $(CH^{[OH]})(C^{[alc]})(OH)_5$	289	a_w (bulk)	8	0.00	this work
2,2,6,6-tetrakis (hydroxymethyl)cyclohexanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH^{[alc]})_2(CH_2^{[OH]})_4$ $(CH^{[OH]})(C^{[alc]})(OH)_5$	298	a_w (bulk)	8	0.50	this work
2,2,6,6-tetrakis (hydroxymethyl)cyclohexanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc]})_2(CH^{[alc]})_2(CH_2^{[OH]})_4$ $(CH^{[OH]})(C^{[alc]})(OH)_5$	313	a_w (bulk)	8	1.00	this work
sorbitol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})_4(OH)_6$	208–233	$a_w(T_{hom})^a$	5	1.00	Ganbavale et al. (2014).
sorbitol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})_4(OH)_6$	256–272	SLE	6	5.00	Ganbavale et al. (2014).
sorbitol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})_4(OH)_6$	298	a_w (bulk)	7	0.00	Ganbavale et al. (2014).
sorbitol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})_4(OH)_6$	298	a_w (bulk)	8	0.00	Bower and Robinson (1963)
sorbitol	$CH_n^{[OH]}$, OH	$(CH_2^{[OH]})_2(CH^{[OH]})_4(OH)_6$	298	a_w (bulk)	8	0.00	Peng et al. (2001)
– **water + carboxylic/dicarboxylic acid systems** –							
acetic acid	CH_n, COOH	$(CH_3)(COOH)$	249–272	SLE	12	5.00	Faucon (1910)
acetic acid	CH_n, COOH	$(CH_3)(COOH)$	250–289	SLE	26	5.00	Pickering (1893)
acetic acid	CH_n, COOH	$(CH_3)(COOH)$	249–290	SLE(org)^d	11	0.20	Faucon (1910)
acetic acid	CH_n, COOH	$(CH_3)(COOH)$	251–273	SLE(org)^d	20	0.20	Pickering (1893)
acetic acid	CH_n, COOH	$(CH_3)(COOH)$	298	VLE	8	0.00	Campbell et al. (1963)
acetic acid	CH_n, COOH	$(CH_3)(COOH)$	374–389	VLE	10	0.20	Sebastiani and Lacquaniti (1967)
acetic acid	CH_n, COOH	$(CH_3)(COOH)$	373–390	VLE	16	0.20	Ito and Yoshida (1963)
acetic acid	CH_n, COOH	$(CH_3)(COOH)$	340–351	VLE	15	0.20	Ito and Yoshida (1963)
acetic acid	CH_n, COOH	$(CH_3)(COOH)$	318–326	VLE	14	0.20	Ito and Yoshida (1963)
acetic acid	CH_n, COOH	$(CH_3)(COOH)$	343	VLE	11	0.20	Arich and Tagliavini (1958)
acetic acid	CH_n, COOH	$(CH_3)(COOH)$	353	VLE	11	0.20	Arich and Tagliavini (1958)
acetic acid	CH_n, COOH	$(CH_3)(COOH)$	363	VLE	11	0.20	Arich and Tagliavini (1958)
acetic acid	CH_n, COOH	$(CH_3)(COOH)$	322–329	VLE	8	0.20	Keyes (1933)
acetic acid	CH_n, COOH	$(CH_3)(COOH)$	337–342	VLE	8	0.20	Keyes (1933)
acetic acid	CH_n, COOH	$(CH_3)(COOH)$	350–355	VLE	8	0.20	Keyes (1933)
acetic acid	CH_n, COOH	$(CH_3)(COOH)$	373–386	VLE	9	0.20	Narayana et al. (1985)
propanoic acid	CH_n, COOH	$(CH_3)(CH_2)(COOH)$	245–273	SLE	19	5.00	Faucon (1910)
propanoic acid	CH_n, COOH	$(CH_3)(CH_2)(COOH)$	244–254	SLE(org)^d	8	0.20	Faucon (1910)
propanoic acid	CH_n, COOH	$(CH_3)(CH_2)(COOH)$	373–405	VLE	8	0.20	Ito and Yoshida (1963)
propanoic acid	CH_n, COOH	$(CH_3)(CH_2)(COOH)$	340–368	VLE	9	0.20	Ito and Yoshida (1963)
propanoic acid	CH_n, COOH	$(CH_3)(CH_2)(COOH)$	318–345	VLE	7	0.01	Ito and Yoshida (1963)
propanoic acid	CH_n, COOH	$(CH_3)(CH_2)(COOH)$	372–401	VLE	18	0.20	Dakshinamurty et al. (1961)
propanoic acid	CH_n, COOH	$(CH_3)(CH_2)(COOH)$	325–354	VLE	24	0.2	Gmehling and Onken (1977)
propanoic acid	CH_n, COOH	$(CH_3)(CH_2)(COOH)$	339–373	VLE	25	0.2	Gmehling and Onken (1977)
propanoic acid	CH_n, COOH	$(CH_3)(CH_2)(COOH)$	356–392	VLE	23	0.20	Gmehling and Onken (1977)
propanoic acid	CH_n, COOH	$(CH_3)(CH_2)(COOH)$	373–411	VLE	24	0.20	Gmehling and Onken (1977)
propanoic acid	CH_n, COOH	$(CH_3)(CH_2)(COOH)$	373–411	VLE	12	0.01	Gmehling and Onken (2003a)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
butanoic acid	CH_n, COOH	$(CH_3)(CH_2)_2(COOH)$	261–273	SLE	19	5.00	Faucon (1910)
butanoic acid	CH_n, COOH	$(CH_3)(CH_2)_2(COOH)$	261–269	SLE(org)[d]	8	0.20	Faucon (1910)
butanoic acid	CH_n, COOH	$(CH_3)(CH_2)_2(COOH)$	303	VLE	7	0.00	Wright and Akhtar (1970)
butanoic acid	CH_n, COOH	$(CH_3)(CH_2)_2(COOH)$	373–394	VLE	8	1.00	Gmehling and Onken (1977)
oxalic acid	COOH	$(COOH)_2$	272–273	SLE	4	5.00	Braban et al. (2003)
oxalic acid	COOH	$(COOH)_2$	277–308	SLE(org)[d]	11	0.00	Braban et al. (2003)
oxalic acid	COOH	$(COOH)_2$	278–338	SLE(org)[d]	13	0.00	Apelblat and Manzurola (1987)
oxalic acid	COOH	$(COOH)_2$	298	a_w	14	0.00	Peng et al. (2001)
oxalic acid	COOH	$(COOH)_2$	284–352	SLE(org)[d]	8	0.00	Omar and Ulrich (2006)
malic acid	CH_n, $CH_n^{[OH]}$, COOH, OH	$(CH_2)_2(CH^{[OH]})(COOH)_2$ (OH)	278–338	SLE(org)[d]	13	0.2	Apelblat and Manzurola (1987)
malic acid	CH_n, $CH_n^{[OH]}$, COOH, OH	$(CH_2)(CH^{[OH]})(COOH)_2$ (OH)	262–273	SLE	16	2.00	Beyer et al. (2008)
malic acid	CH_n, $CH_n^{[OH]}$, COOH, OH	$(CH_2)(CH^{[OH]})(COOH)_2$ (OH)	298	a_w	6	0.00	Maffia and Meirelles (2001)
malonic acid	CH_n, COOH	$(CH_2)(COOH)_2$	262–273	SLE	22	5.00	Braban et al. (2003)
malonic acid	CH_n, COOH	$(CH_2)(COOH)_2$	278–338	SLE(org)[d]	13	0.2	Apelblat and Manzurola (1987)
malonic acid	CH_n, COOH	$(CH_2)(COOH)_2$	298	a_w	6	0.00	Peng et al. (2001)
malonic acid	CH_n, COOH	$(CH_2)(COOH)_2$	298	a_w	6	0.00	Maffia and Meirelles (2001)
malonic acid	CH_n, COOH	$(CH_2)(COOH)_2$	298	a_w	7	0.00	Peng et al. (2001)
succinic acid	CH_n, COOH	$(CH_2)_2(COOH)_2$	273	SLE	9	5.00	Beyer et al. (2008)
succinic acid	CH_n, COOH	$(CH_2)_2(COOH)_2$	296–447	SLE(org)[d]	10	0.20	Lin et al. (2007)
succinic acid	CH_n, COOH	$(CH_2)_2(COOH)_2$	278–338	SLE(org)[d]	13	0.20	Apelblat and Manzurola (1987)
succinic acid	CH_n, COOH	$(CH_2)_2(COOH)_2$	298	a_w	5	0.00	Maffia and Meirelles (2001)
succinic acid	CH_n, COOH	$(CH_2)_2(COOH)_2$	298	a_w	9	0.00	Peng et al. (2001)
glutaric acid	CH_n, COOH	$(CH_2)_3(COOH)_2$	271–273	SLE	5	5.00	Beyer et al. (2008)
glutaric acid	CH_n, COOH	$(CH_2)_3(COOH)_2$	279–336	SLE(org)[d]	24	0.10	Apelblat and Manzurola (1989)
glutaric acid	CH_n, COOH	$(CH_2)_3(COOH)_2$	277–298	SLE(org)[d]	23	0.10	Beyer et al. (2008)
glutaric acid	CH_n, COOH	$(CH_2)_3(COOH)_2$	298	a_w	34	0.00	Peng et al. (2001)
glutaric acid	CH_n, COOH	$(CH_2)_3(COOH)_2$	291	a_w	57	0.00	Zardini et al. (2008)
citric acid	CH_n, $C^{[OH]}$, COOH, OH	$(CH_2)_2(C^{[OH]})(COOH)_3$ (OH)	278–338	SLE(org)[d]	13	0.0	Apelblat and Manzurola (1987)
citric acid	CH_n, $C^{[OH]}$, COOH, OH	$(CH_2)_2(C^{[OH]})(COOH)_3$ (OH)	291	a_w	90	0.00	Zardini et al. (2008)
citric acid	CH_n, $C^{[OH]}$, COOH, OH	$(CH_2)_2(C^{[OH]})(COOH)_3(OH)$	298	a_w	25	0.00	Peng et al. (2001)
adipic acid	CH_n, COOH	$(CH_2)_4(COOH)_2$	278–338	SLE(org)[d]	13	0.20	Apelblat and Manzurola (1987)
pimelic acid	CH_n, COOH	$(CH_2)_5(COOH)_2$	279–342	SLE(org)[d]	21	0.20	Apelblat and Manzurola (1989)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	191–230	$a_w(T_{hom})$[a]	6	1.00	Zobrist et al. (2008)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	255–271	SLE	6	5.00	Zobrist et al. (2008)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	233	$a_w(EDB)$[f]	3	0.20	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	236	$a_w(EDB)$[f]	2	0.20	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	244	$a_w(EDB)$[f]	6	0.50	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	253	$a_w(EDB)$[f]	3	0.50	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	253	$a_w(p^{tot})$	5	1.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	255	$a_w(p^{tot})$	3	0.50	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	258	$a_w(p^{tot})$	3	0.50	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	260	$a_w(p^{tot})$	4	1.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	263	$a_w(EDB)$[f]	2	1.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	263	$a_w(EDB)$[f]	5	1.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	265	$a_w(p^{tot})$	3	1.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	268	$a_w(p^{tot})$	3	1.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	268	$a_w(EDB)$[f]	8	1.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	270	$a_w(p^{tot})$	3	1.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	273	$a_w(p^{tot})$	3	1.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	273	$a_w(EDB)$[f]	10	1.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	275	$a_w(p^{tot})$	3	1.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	278	$a_w(p^{tot})$	5	1.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	[c]	279	a_w (bulk)	9	1.00	Ganbavale et al. (2014)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	c	280	$a_w(p^{tot})$	5	1.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	c	283	$a_w(p^{tot})$	5	1.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	c	285	$a_w(p^{tot})$	5	1.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	c	288	$a_w(p^{tot})$	5	1.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	c	289	$a_w(EDB)^f$	10	0.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	c	289	a_w (bulk)	10	0.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	c	290	$a_w(p^{tot})$	5	0.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	c	298	a_w (bulk)	10	0.00	Ganbavale et al. (2014)
M5[b]	CH_n, $CH_n^{[OH]}$, COOH, OH, C=C	c	313	a_w (bulk)	10	0.00	Ganbavale et al. (2014)
– water + ketone systems –							
acetone	CH_n, CH_nCO	$(CH_3)(CH_3CO)$	221–273	SLE	17	5.00	Jakob (1994)
acetone	CH_n, CH_nCO	$(CH_3)(CH_3CO)$	298	VLE	13	0.00	Gmehling et al. (1988)
acetone	CH_n, CH_nCO	$(CH_3)(CH_3CO)$	308	VLE	13	1.00	Gmehling et al. (1988)
acetone	CH_n, CH_nCO	$(CH_3)(CH_3CO)$	318	VLE	13	1.00	Gmehling et al. (1988)
acetone	CH_n, CH_nCO	$(CH_3)(CH_3CO)$	323	VLE	13	1.00	Gmehling et al. (1988)
acetone	CH_n, CH_nCO	$(CH_3)(CH_3CO)$	328	VLE	13	1.00	Gmehling et al. (1988)
acetone	CH_n, CH_nCO	$(CH_3)(CH_3CO)$	373	VLE	20	1.00	Griswold and Wong (1952)
acetone	CH_n, CH_nCO	$(CH_3)(CH_3CO)$	295–321	VLE	10	1.00	Othmer and Benenati (1945)
acetone	CH_n, CH_nCO	$(CH_3)(CH_3CO)$	309–340	VLE	12	1.00	Othmer and Benenati (1945)
acetone	CH_n, CH_nCO	$(CH_3)(CH_3CO)$	318–345	VLE	13	1.00	Othmer and Benenati (1945)
acetone	CH_n, CH_nCO	$(CH_3)(CH_3CO)$	331–363	VLE	10	1.00	Othmer and Benenati (1945)
acetone	CH_n, CH_nCO	$(CH_3)(CH_3CO)$	330–361	VLE	13	1.00	Othmer et al. (1952)
acetone	CH_n, CH_nCO	$(CH_3)(CH_3CO)$	371–396	VLE	12	1.00	Othmer et al. (1952)
2-butanone	CH_n, CH_nCO	$(CH_3)(CH_2)(CH_3CO)$	198–273	SLE	19	5.00	Lohmann et al. (1997)
2-butanone	CH_n, CH_nCO	$(CH_3)(CH_2)(CH_3CO)$	293	VLE	5	1.00	Gmehling et al. (1988)
2-butanone	CH_n, CH_nCO	$(CH_3)(CH_2)(CH_3CO)$	308	VLE	4	1.00	Gmehling et al. (1988)
2-butanone	CH_n, CH_nCO	$(CH_3)(CH_2)(CH_3CO)$	323	VLE	4	1.00	Gmehling et al. (1988)
2-butanone	CH_n, CH_nCO	$(CH_3)(CH_2)(CH_3CO)$	323	VLE	15	1.00	Gaube et al. (1996)
2-butanone	CH_n, CH_nCO	$(CH_3)(CH_2)(CH_3CO)$	333	VLE	20	1.00	Zou and Prausnitz (1987)
2-butanone	CH_n, CH_nCO	$(CH_3)(CH_2)(CH_3CO)$	343	VLE	22	1.00	Zou and Prausnitz (1987)
2-butanone	CH_n, CH_nCO	$(CH_3)(CH_2)(CH_3CO)$	313–326	VLE	8	1.00	Gmehling et al. (1981)
2-butanone	CH_n, CH_nCO	$(CH_3)(CH_2)(CH_3CO)$	330–338	VLE	8	1.00	Gmehling et al. (1981)
2-butanone	CH_n, CH_nCO	$(CH_3)(CH_2)(CH_3CO)$	340–348	VLE	8	1.00	Gmehling et al. (1981)
2-butanone	CH_n, CH_nCO	$(CH_3)(CH_2)(CH_3CO)$	347–363	VLE	8	1.00	Gmehling et al. (1981)
2-butanone	CH_n, CH_nCO	$(CH_3)(CH_2)(CH_3CO)$	385–406	VLE	19	1.00	Othmer et al. (1952)
2-pentanone	CH_n, CH_nCO	$(CH_3)(CH_2)_2(CH_3CO)$	273–363	solubil.	20	1.00	Stephenson (1992)
3-pentanone	CH_n, CH_nCO	$(CH_3)_2(CH_2)(CH_2CO)$	273–353	solubil.	18	1.00	Stephenson (1992)
3-pentanone	CH_n, CH_nCO	$(CH_3)_2(CH_2)(CH_2CO)$	323	VLE	12	1.00	Gmehling and Onken (2003b)
3-pentanone	CH_n, CH_nCO	$(CH_3)_2(CH_2)(CH_2CO)$	338	VLE	12	0.50	Gmehling and Onken (2003b)
3-pentanone	CH_n, CH_nCO	$(CH_3)_2(CH_2)(CH_2CO)$	353	VLE	12	0.50	Gmehling and Onken (2003b)
3-pentanone	CH_n, CH_nCO	$(CH_3)_2(CH_2)(CH_2CO)$	368	VLE	12	0.50	Gmehling and Onken (2003b)
3-pentanone	CH_n, CH_nCO	$(CH_3)_2(CH_2)(CH_2CO)$	383	VLE	12	1.00	Gmehling and Onken (2003b)
– water + ether systems –							
diethyl ether	CH_n, CH_nO	$(CH_3)_2(CH_2)(CH_2O)$	269–272	SLE(org)[d]	7	5.00	Lalande (1934)
diethyl ether	CH_n, CH_nO	$(CH_3)_2(CH_2)(CH_2O)$	269–303	solubli.	14	0.20	Hill (1923)
diethyl ether	CH_n, CH_nO	$(CH_3)_2(CH_2)(CH_2O)$	307–367	VLE	10	0.05	Borisova et al. (1983)
2-methoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_2)(CH_2^{[OH]})(CH_3O)(OH)$	343	VLE	16	0.50	Chiavone-Filho et al. (1993)
2-methoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_2)(CH_2^{[OH]})(CH_3O)(OH)$	363	VLE	16	0.50	Chiavone-Filho et al. (1993)
2-methoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_2)(CH_2^{[OH]})(CH_3O)(OH)$	373–394	VLE	12	0.50	Gmehling and Onken (2003a)
2-ethoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)(CH_2^{[OH]})(CH_2O)(OH)$	343	VLE	20	0.50	Chiavone-Filho et al. (1993)
2-ethoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)(CH_2^{[OH]})(CH_2O)(OH)$	363	VLE	18	0.50	Chiavone-Filho et al. (1993)
2-ethoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)(CH_2^{[OH]})(CH_2O)(OH)$	373–407	VLE	34	0.50	Hirata and Hoshino (1982)
2-ethoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)(CH_2^{[OH]})(CH_2O)(OH)$	372–406	VLE	17	0.50	Gmehling and Onken (2003b)
2-butoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)_3(CH_2^{[OH]})(CH_2O)(OH)$	252–273	SLE	23	0.50	Koga et al. (1994)
2-butoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)_3(CH_2^{[OH]})(CH_2O)(OH)$	261–273	SLE	23	5.00	Koga et al. (1994)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
2-butoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)_3(CH_2^{[OH]})(CH_2O)$ (OH)	298	VLE	8	0.00	Scatchard and Wilson (1964)
2-butoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)_3(CH_2^{[OH]})(CH_2O)$ (OH)	318	VLE	8	0.05	Scatchard and Wilson (1964)
2-butoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)_3(CH_2^{[OH]})(CH_2O)$ (OH)	338	VLE	7	0.05	Scatchard and Wilson (1964)
2-butoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)_3(CH_2^{[OH]})(CH_2O)$ (OH)	358	VLE	7	0.50	Scatchard and Wilson (1964)
2-butoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)_3(CH_2^{[OH]})(CH_2O)$ (OH)	358	VLE	19	0.50	Chiavone-Filho et al. (1993)
2-butoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)_3(CH_2^{[OH]})(CH_2O)$ (OH)	363	VLE	22	0.50	Escobedo-Alvarado and Sandler (1999)
2-butoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)_3(CH_2^{[OH]})(CH_2O)$ (OH)	368	VLE	19	0.50	Chiavone-Filho et al. (1993)
2-butoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)_3(CH_2^{[OH]})(CH_2O)$ (OH)	371	VLE	20	0.50	Escobedo-Alvarado and Sandler (1999)
2-butoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)_3(CH_2^{[OH]})(CH_2O)$ (OH)	383	VLE	21	0.50	Schneider and Wilhelm (1959)
2-butoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)_3(CH_2^{[OH]})(CH_2O)$ (OH)	372–423	VLE	8	0.50	Newman et al. (1949)
2-isopropoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)_2(CH)(CH_2^{[OH]})(CH_2O)$ (OH)	358	SLE	16	0.50	Chiavone-Filho et al. (1993)
2-isopropoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)_2(CH)(CH_2^{[OH]})(CH_2O)$ (OH)	368	SLE	16	0.50	Chiavone-Filho et al. (1993)
1-methoxy-2-propanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)(CH^{[OH]})(CH_3O)$ (OH)	353	VLE	13	0.50	Chiavone-Filho et al. (1993)
1-methoxy-2-propanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)(CH^{[OH]})(CH_3O)$ (OH)	363	VLE	13	0.50	Chiavone-Filho et al. (1993)
– water + ester systems –							
methyl acetate	CH_n, CCOO	$(CH_3)(CH_3COO)$	233–273	SLE	7	5.00	Ahlers (1998)
methyl acetate	CH_n, CCOO	$(CH_3)(CH_3COO)$	298	VLE	5	0.00	Gmehling and Onken (1977)
methyl acetate	CH_n, CCOO	$(CH_3)(CH_3COO)$	308	VLE	5	1.00	Gmehling and Onken (1977)
methyl acetate	CH_n, CCOO	$(CH_3)(CH_3COO)$	323	VLE	8	0.02	Gmehling and Onken (1977)
methyl acetate	CH_n, CCOO	$(CH_3)(CH_3COO)$	323	VLE	30	1.00	Loehe et al. (1983)
methyl acetate	CH_n, CCOO	$(CH_3)(CH_3COO)$	333	VLE	8	1.00	Gmehling and Onken (1977)
methyl acetate	CH_n, CCOO	$(CH_3)(CH_3COO)$	343	VLE	8	1.00	Gmehling and Onken (1977)
methyl acetate	CH_n, CCOO	$(CH_3)(CH_3COO)$	353	VLE	8	1.00	Gmehling and Onken (1977)
methyl acetate	CH_n, CCOO	$(CH_3)(CH_3COO)$	330–369	VLE	12	1.00	Álvarez et al. (2011)
ethyl acetate	CH_n, CCOO	$(CH_3)(CH_2)(CH_3COO)$	273–344	solubil.	16	1.00	Stephenson and Stuart (1986)
ethyl acetate	CH_n, CCOO	$(CH_3)(CH_2)(CH_3COO)$	323	VLE	9	1.00	Gmehling et al. (1988)
ethyl acetate	CH_n, CCOO	$(CH_3)(CH_2)(CH_3COO)$	333	VLE	8	1.00	Gmehling et al. (1988)
ethyl acetate	CH_n, CCOO	$(CH_3)(CH_2)(CH_3COO)$	343	VLE	9	1.00	Gmehling et al. (1988)
ethyl acetate	CH_n, CCOO	$(CH_3)(CH_2)(CH_3COO)$	353	VLE	9	1.00	Gmehling et al. (1988)
ethyl acetate	CH_n, CCOO	$(CH_3)(CH_2)(CH_3COO)$	345–367	VLE	9	1.00	Gmehling et al. (1988)
ethyl acetate	CH_n, CCOO	$(CH_3)(CH_2)(CH_3COO)$	344–349	VLE	11	0.20	Gmehling et al. (1988)
1-propyl acetate	CH_n, CCOO	$(CH_3)(CH_2)_2(CH_3COO)$	273–353	solubil.	18	1.00	Stephenson and Stuart (1986)
1-propyl acetate	CH_n, CCOO	$(CH_3)(CH_2)_2(CH_3COO)$	324–338	VLE	7	1.00	Gmehling et al. (1988)
1-propyl acetate	CH_n, CCOO	$(CH_3)(CH_2)_2(CH_3COO)$	340–354	VLE	7	1.00	Gmehling et al. (1988)
1-propyl acetate	CH_n, CCOO	$(CH_3)(CH_2)_2(CH_3COO)$	350–365	VLE	7	1.00	Gmehling et al. (1988)
1-propyl acetate	CH_n, CCOO	$(CH_3)(CH_2)_2(CH_3COO)$	356–371	VLE	7	1.00	Gmehling et al. (1988)
1-propyl acetate	CH_n, CCOO	$(CH_3)(CH_2)_2(CH_3COO)$	338	VLE	7	1.00	Gmehling et al. (1988)
1-propyl acetate	CH_n, CCOO	$(CH_3)(CH_2)_2(CH_3COO)$	353	VLE	7	1.00	Gmehling et al. (1988)
1-butyl acetate	CH_n, CCOO	$(CH_3)(CH_2)_3(CH_3COO)$	273–364	solubil.	20	0.50	Stephenson and Stuart (1986)
1-butyl acetate	CH_n, CCOO	$(CH_3)(CH_2)_3(CH_3COO)$	364–397	VLE	31	0.20	Cho et al. (1983)
isobutyl acetate	CH_n, CCOO	$(CH_3)_2(CH_2)(CH)(CH_3COO)$	273–353	solubil.	18	0.50	Stephenson and Stuart (1986)
2-butyl acetate	CH_n, CCOO	$(CH_3)_2(CH_2)(CH)(CH_3COO)$	273–364	solubil.	20	0.50	Stephenson and Stuart (1986)
1-pentyl acetate	CH_n, CCOO	$(CH_3)(CH_2)_4(CH_3COO)$	273–353	solubil.	16	0.20	Stephenson and Stuart (1986)
1-hexyl acetate	CH_n, CCOO	$(CH_3)(CH_2)_5(CH_3COO)$	273–363	solubil.	20	0.20	Stephenson and Stuart (1986)
1-hexyl acetate	CH_n, CCOO	$(CH_3)(CH_2)_5(CH_3COO)$	371–349	VLE	6	0.001	Bomshtein et al. (1983)
– water + multifunctional aromatic compounds systems –							
benzene	ACH_n	$(ACH)_6$	293–353	solubil.	8	1.00	Udovenko (1963)
benzene	ACH_n	$(ACH)_6$	274–339	solubil.	10	1.00	Alexander (1959)
benzene	ACH_n	$(ACH)_6$	273–229	solubil.	8	1.00	May et al. (1983)
benzene	ACH_n	$(ACH)_6$	342–371	VLE	20	0.01	Gmehling and Onken (2003b)
phenol	ACH_n, ACOH	$(ACH)_5(ACOH)$	284–314	SLE(org)[d]	23	0.20	Paterno and Ampola (1897)
phenol	ACH_n, ACOH	$(ACH)_5(ACOH)$	293–308	SLE(org)[d]	16	0.00	Jaoui et al. (2002)
phenol	ACH_n, ACOH	$(ACH)_5(ACOH)$	318	VLE	22	1.00	Gmehling et al. (1981)
phenol	ACH_n, ACOH	$(ACH)_5(ACOH)$	340–400	VLE	21	1.0	Kliment et al. (1964)
phenol	ACH_n, ACOH	$(ACH)_5(ACOH)$	373–442	VLE	15	1.0	Schreinemakers (1900)
phenol	ACH_n, ACOH	$(ACH)_5(ACOH)$	373–455	VLE	14	1.0	Gmehling and Onken (2003b)
phenol	ACH_n, ACOH	$(ACH)_5(ACOH)$	373–444	VLE	11	1.00	Tochigi et al. (1997)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
tert-butyl acetate	CH_n, CCOO	$(CH_3)_3(C)(CH_3COO)$	273–354	soluibil.	18	0.50	Stephenson and Stuart (1986)
– water + aldehyde systems –							
acetaldehyde	CH_n, CHO	$(CH_3)(CHO)$	283	VLE	5	1.00	d'Avila and Silva (1970)
acetaldehyde	CH_n, CHO	$(CH_3)(CHO)$	288	VLE	5	0.00	d'Avila and Silva (1970)
acetaldehyde	CH_n, CHO	$(CH_3)(CHO)$	293	VLE	5	0.00	d'Avila and Silva (1970)
acetaldehyde	CH_n, CHO	$(CH_3)(CHO)$	298	VLE	5	0.00	d'Avila and Silva (1970)
acetaldehyde	CH_n, CHO	$(CH_3)(CHO)$	303	VLE	5	0.00	d'Avila and Silva (1970)
acetaldehyde	CH_n, CHO	$(CH_3)(CHO)$	306–367	VLE	5	1.00	Coles and Popper (1950)
propionaldehyde	CH_n, CHO	$(CH_3)(CH_2)(CHO)$	288–313	solubil.	12	1.00	Ferino et al. (1983)
propionaldehyde	CH_n, CHO	$(CH_3)(CH_2)(CHO)$	321–342	VLE	6	1.00	Mozzhukhin et al. (1967)
butyraldehyde	CH_n, CHO	$(CH_3)(CH_2)_2(CHO)$	278–313	solubil.	16	1.00	Ferino et al. (1983)
butyraldehyde	CH_n, CHO	$(CH_3)(CH_2)_2(CHO)$	323	VLE	13	0.20	Tapper et al. (1985)
butyraldehyde	CH_n, CHO	$(CH_3)(CH_2)_2(CHO)$	338	VLE	12	0.20	Tapper et al. (1985)
– water + multifunctional systems –							
glucose	$CH_n^{[OH]}$, OH, CHO[ether]	$(CH_2^{[OH]})(CH^{[OH]})_4 (CHO[ether])(OH)_5$	217–233	$a_w(T_{hom})^a$	9	1.00	Miyata and Kanno (2005)
glucose	$CH_n^{[OH]}$, OH, CHO[ether]	$(CH_2^{[OH]})(CH^{[OH]})_4 (CHO[ether])(OH)_5$	204–231	$a_w(T_{hom})^a$	5	1.00	Zobrist et al. (2008)
glucose	$CH_n^{[OH]}$, OH, CHO[ether]	$(CH_2^{[OH]})(CH^{[OH]})_4 (CHO[ether])(OH)_5$	243–273	SLE	8	5.00	Young (1957)
glucose	$CH_n^{[OH]}$, OH, CHO[ether]	$(CH_2^{[OH]})(CH^{[OH]})_4 (CHO[ether])(OH)_5$	260–273	SLE	5	5.00	Zobrist et al. (2008)
glucose	$CH_n^{[OH]}$, OH, CHO[ether]	$(CH_2^{[OH]})(CH^{[OH]})_4 (CHO[ether])(OH)_5$	298	a_w (bulk)	20	0.00	Ruegg and Blanc (1981)
glucose	$CH_n^{[OH]}$, OH, CHO[ether]	$(CH_2^{[OH]})(CH^{[OH]})_4 (CHO[ether])(OH)_5$	298	a_w (bulk)	26	0.00	Bonner and Breazeale (1965)
glucose	$CH_n^{[OH]}$, OH, CHO[ether]	$(CH_2^{[OH]})(CH^{[OH]})_4 (CHO[ether])(OH)_5$	298	a_w (bulk)	8	0.00	Peng et al. (2001)
sucrose	$CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH_2^{[OH]})_3(CH^{[OH]})_5 (CHO[ether])_3(OH)_8$	211–235	$a_w(T_{hom})^a$	16	1.00	Kanno et al. (2007)
sucrose	$CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH_2^{[OH]})_3(CH^{[OH]})_5 (CHO[ether])_3(OH)_8$	217–232	$a_w(T_{hom})^a$	6	1.00	Ganbavale et al. (2014)
sucrose	$CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH_2^{[OH]})_3(CH^{[OH]})_5 (CHO[ether])_3(OH)_8$	237–273	SLE	10	5.00	Ablett et al. (1992)
sucrose	$CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH_2^{[OH]})_3(CH^{[OH]})_5 (CHO[ether])_3(OH)_8$	247–273	SLE	9	5.00	Williams and Carnahan (1990)
sucrose	$CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH_2^{[OH]})_3(CH^{[OH]})_5 (CHO[ether])_3(OH)_8$	259–271	SLE	9	5.00	Blond et al. (1997)
sucrose	$CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH_2^{[OH]})_3(CH^{[OH]})_5 (CHO[ether])_3(OH)_8$	261–272	SLE	8	5.00	Zobrist et al. (2008)
sucrose	$CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH_2^{[OH]})_3(CH^{[OH]})_5 (CHO[ether])_3(OH)_8$	262–273	SLE	16	5.00	Kanno et al. (2007)
sucrose	$CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH_2^{[OH]})_3(CH^{[OH]})_5 (CHO[ether])_3(OH)_8$	264–272	SLE	5	5.00	Sei and Gonda (2006)
sucrose	$CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH_2^{[OH]})_3(CH^{[OH]})_5 (CHO[ether])_3(OH)_8$	269–273	SLE	6	5.00	Lerici et al. (2006)
sucrose	$CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH_2^{[OH]})_3(CH^{[OH]})_5 (CHO[ether])_3(OH)_8$	289	a_w (bulk)	8	0.00	this work
sucrose	$CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH_2^{[OH]})_3(CH^{[OH]})_5 (CHO[ether])_3(OH)_8$	298	a_w (bulk)	8	0.00	this work
sucrose	$CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH_2^{[OH]})_3(CH^{[OH]})_5 (CHO[ether])_3(OH)_8$	313	a_w (bulk)	8	1.00	this work
raffinose	CH_n, $CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH)(CH_2^{[OH]})_3(CH^{[OH]})_8 (CH_2O)(CHO[ether])_4(OH)_{11}$	214–233	$a_w(T_{hom})^a$	4	1.00	Zobrist et al. (2008)
raffinose	CH_n, $CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH)(CH_2^{[OH]})_3(CH^{[OH]})_8 (CH_2O)(CHO[ether])_4(OH)_{11}$	266–273	SLE	4	5.00	Zobrist et al. (2008)
raffinose	CH_n, $CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH)(CH_2^{[OH]})_3(CH^{[OH]})_8 (CH_2O)(CHO[ether])_4(OH)_{11}$	289	a_w (bulk)	4	0.00	this work
raffinose	CH_n, $CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH)(CH_2^{[OH]})_3(CH^{[OH]})_8 (CH_2O)(CHO[ether])_4(OH)_{11}$	298	a_w (bulk)	5	1.00	this work
raffinose	CH_n, $CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH)(CH_2^{[OH]})_3(CH^{[OH]})_8 (CH_2O)(CHO[ether])_4(OH)_{11}$	313	a_w (bulk)	4	1.00	this work
levoglucosan	CH_n, $CH_n^{[OH]}$, OH, CHO[ether]	$(CH)(CH^{[OH]})_3(CH_2O) (CHO[ether]) (OH)_3$	192–233	$a_w(T_{hom})^a$	8	1.00	Zobrist et al. (2008)
levoglucosan	CH_n, $CH_n^{[OH]}$, OH, CHO[ether]	$(CH)(CH^{[OH]})_3(CH_2O) (CHO[ether]) (OH)_3$	187–230	$a_w(T_{hom})^a$	6	1.00	Lienhard et al. (2012)
levoglucosan	CH_n, $CH_n^{[OH]}$, OH, CHO[ether]	$(CH)(CH^{[OH]})_3(CH_2O) (CHO[ether]) (OH)_3$	255–272	SLE	7	5.00	Zobrist et al. (2008)
levoglucosan	CH_n, $CH_n^{[OH]}$, OH, CHO[ether]	$(CH)(CH^{[OH]})_3(CH_2O) (CHO[ether]) (OH)_3$	254–272	SLE	7	5.00	Lienhard et al. (2012)
levoglucosan	CH_n, $CH_n^{[OH]}$, OH, CHO[ether]	$(CH)(CH^{[OH]})_3(CH_2O) (CHO[ether]) (OH)_3$	291	a_w (bulk)	8	0.00	Lienhard et al. (2012)
levoglucosan	CH_n, $CH_n^{[OH]}$, OH, CHO[ether]	$(CH)(CH^{[OH]})_3(CH_2O) (CHO[ether]) (OH)_3$	296	a_w (bulk)	6	0.00	Chan et al. (2005)
levoglucosan	CH_n, $CH_n^{[OH]}$, OH, CHO[ether]	$(CH)(CH^{[OH]})_3(CH_2O) (CHO[ether]) (OH)_3$	298	a_w (bulk)	7	0.00	Lienhard et al. (2012)
glycolic acid	$CH_n^{[OH]}$, OH, COOH	$(CH_2^{[OH]})(OH)(COOH)$	206–230	$a_w(T_{hom})^a$	4	1.00	Ganbavale et al. (2014)
glycolic acid	$CH_n^{[OH]}$, OH, COOH	$(CH_2^{[OH]})(OH)(COOH)$	259–271	SLE	4	5.00	Ganbavale et al. (2014)
glycolic acid	$CH_n^{[OH]}$, OH, COOH	$(CH_2^{[OH]})(OH)(COOH)$	298	a_w (bulk)	8	0.00	Ganbavale et al. (2014)
pyruvic acid	COOH, CH_nCO	$(CH_3CO)(COOH)$	211–232	$a_w(T_{hom})^a$	3	1.00	Ganbavale et al. (2014)
pyruvic acid	COOH, CH_nCO	$(CH_3CO)(COOH)$	254–271	SLE	4	5.00	Ganbavale et al. (2014)
pyruvic acid	COOH, CH_nCO	$(CH_3CO)(COOH)$	298	a_w (bulk)	9	0.00	Ganbavale et al. (2014)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
2-methoxyacetic acid	CH$_n$, COOH, CH$_n$O	(CH$_2$)(CH$_3$O)(COOH)	194–232	$a_w(T_{hom})$[a]	5	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH$_n$, COOH, CH$_n$O	(CH$_2$)(CH$_3$O)(COOH)	251–271	SLE	3	2.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH$_n$, COOH, CH$_n$O	(CH$_2$)(CH$_3$O)(COOH)	268	$a_w(p^{tot})$	4	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH$_n$, COOH, CH$_n$O	(CH$_2$)(CH$_3$O)(COOH)	270	$a_w(p^{tot})$	4	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH$_n$, COOH, CH$_n$O	(CH$_2$)(CH$_3$O)(COOH)	273	$a_w(p^{tot})$	4	0.50	Ganbavale et al. (2014)
2-methoxyacetic acid	CH$_n$, COOH, CH$_n$O	(CH$_2$)(CH$_3$O)(COOH)	275	$a_w(p^{tot})$	5	0.50	Ganbavale et al. (2014)
2-methoxyacetic acid	CH$_n$, COOH, CH$_n$O	(CH$_2$)(CH$_3$O)(COOH)	278	$a_w(p^{tot})$	10	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH$_n$, COOH, CH$_n$O	(CH$_2$)(CH$_3$O)(COOH)	279	a_w (bulk)	10	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH$_n$, COOH, CH$_n$O	(CH$_2$)(CH$_3$O)(COOH)	280	$a_w(p^{tot})$	10	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH$_n$, COOH, CH$_n$O	(CH$_2$)(CH$_3$O)(COOH)	283	$a_w(p^{tot})$	10	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH$_n$, COOH, CH$_n$O	(CH$_2$)(CH$_3$O)(COOH)	285	$a_w(p^{tot})$	10	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH$_n$, COOH, CH$_n$O	(CH$_2$)(CH$_3$O)(COOH)	288	$a_w(p^{tot})$	10	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH$_n$, COOH, CH$_n$O	(CH$_2$)(CH$_3$O)(COOH)	289	a_w (bulk)	10	0.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH$_n$, COOH, CH$_n$O	(CH$_2$)(CH$_3$O)(COOH)	290	a_w (bulk)	10	0.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH$_n$, COOH, CH$_n$O	(CH$_2$)(CH$_3$O)(COOH)	298	a_w (bulk)	9	0.00	Ganbavale et al. (2014)
2-ethoxyethyl acetate	CH$_n$, CH$_n$O, CCOO	(CH$_3$)(CH$_2$)(CH$_2$O)$_2$ (CH$_3$COO)	208–233	$a_w(T_{hom})$[a]	3	1.00	Ganbavale et al. (2014)
2-ethoxyethyl acetate	CH$_n$, CH$_n$O, CCOO	(CH$_3$)(CH$_2$)(CH$_2$O)$_2$ (CH$_3$COO)	271–272	SLE	3	2.00	Ganbavale et al. (2014)
2-ethoxyethyl acetate	CH$_n$, CH$_n$O, CCOO	(CH$_3$)(CH$_2$)(CH$_2$O)$_2$ (CH$_3$COO)	276–368	solubli.	12	1.00	Carvoli and Delogu (1986)
resorcinol	ACH$_n$, ACOH	(ACH)$_4$(ACOH)$_2$	223–232	$a_w(T_{hom})$[a]	4	1.00	Ganbavale et al. (2014)
resorcinol	ACH$_n$, ACOH	(ACH)$_4$(ACOH)$_2$	267–272	SLE	4	2.00	Ganbavale et al. (2014)
resorcinol	ACH$_n$, ACOH	(ACH)$_4$(ACOH)$_2$	298	a_w (bulk)	7	0.00	Ganbavale et al. (2014)
2-hydroxybenzoic acid	ACH$_n$, ACOH, COOH	(ACH)$_4$(AC)(ACOH)(COOH)	298–348	SLE(org)[d]	11	0.20	Shalmashi and Eliassi (2008)
2-hydroxybenzoic acid	ACH$_n$, ACOH, COOH	(ACH)$_4$(AC)(ACOH)(COOH)	283–339	SLE(org)[d]	13	0.20	Apelblat and Manzurola (1989)
2-(2-ethoxyethoxy)ethanol	CH$_n$, CH$_n$O, OH	(CH$_3$)(CH$_2$)$_2$(CH$_2$O)$_2$ (OH)	211–233	$a_w(T_{hom})$[a]	3	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH$_n$, CH$_n$O, OH	(CH$_3$)(CH$_2$)$_2$(CH$_2$O)$_2$ (OH)	260–272	SLE	4	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH$_n$, CH$_n$O, OH	(CH$_3$)(CH$_2$)$_2$(CH$_2$O)$_2$ (OH)	265	$a_w(p^{tot})$	5	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH$_n$, CH$_n$O, OH	(CH$_3$)(CH$_2$)$_2$(CH$_2$O)$_2$ (OH)	268	$a_w(p^{tot})$	5	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH$_n$, CH$_n$O, OH	(CH$_3$)(CH$_2$)$_2$(CH$_2$O)$_2$ (OH)	270	$a_w(p^{tot})$	5	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH$_n$, CH$_n$O, OH	(CH$_3$)(CH$_2$)$_2$(CH$_2$O)$_2$ (OH)	273	$a_w(p^{tot})$	5	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH$_n$, CH$_n$O, OH	(CH$_3$)(CH$_2$)$_2$(CH$_2$O)$_2$ (OH)	275	$a_w(p^{tot})$	6	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH$_n$, CH$_n$O, OH	(CH$_3$)(CH$_2$)$_2$(CH$_2$O)$_2$ (OH)	278	$a_w(p^{tot})$	9	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH$_n$, CH$_n$O, OH	(CH$_3$)(CH$_2$)$_2$(CH$_2$O)$_2$ (OH)	279	a_w (bulk)	12	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH$_n$, CH$_n$O, OH	(CH$_3$)(CH$_2$)$_2$(CH$_2$O)$_2$ (OH)	280	$a_w(p^{tot})$	9	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH$_n$, CH$_n$O, OH	(CH$_3$)(CH$_2$)$_2$(CH$_2$O)$_2$ (OH)	283	$a_w(p^{tot})$	9	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH$_n$, CH$_n$O, OH	(CH$_3$)(CH$_2$)$_2$(CH$_2$O)$_2$ (OH)	285	$a_w(p^{tot})$	9	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH$_n$, CH$_n$O, OH	(CH$_3$)(CH$_2$)$_2$(CH$_2$O)$_2$ (OH)	288	$a_w(p^{tot})$	9	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH$_n$, CH$_n$O, OH	(CH$_3$)(CH$_2$)$_2$(CH$_2$O)$_2$ (OH)	289	a_w (bulk)	12	0.00	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH$_n$, CH$_n$O, OH	(CH$_3$)(CH$_2$)$_2$(CH$_2$O)$_2$ (OH)	290	a_w (bulk)	9	0.00	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH$_n$, CH$_n$O, OH	(CH$_3$)(CH$_2$)$_2$(CH$_2$O)$_2$ (OH)	298	a_w (bulk)	12	0.00	Ganbavale et al. (2014)
vanillylmandelic acid	ACH$_n$, ACOH, CH$_n^{[OH]}$, COOH, CH$_n$O, OH	(ACH)$_3$(AC)$_2$(ACOH)(CH$_3$O) (CH$^{[OH]}$)(OH)(COOH)	214–232	$a_w(T_{hom})$[a]	4	1.00	Zobrist et al. (2008)
vanillylmandelic acid	ACH$_n$, ACOH, CH$_n^{[OH]}$, COOH, CH$_n$O, OH	(ACH)$_3$(AC$_2$)(ACOH)(CH$_3$O) (CH$^{[OH]}$)(OH)(COOH)	267–272	SLE	4	5.00	Zobrist et al. (2008)
vanillylmandelic acid	ACH$_n$, ACOH, CH$_n^{[OH]}$, COOH, CH$_n$O, OH	(ACH)$_3$(AC$_2$)(ACOH)(CH$_3$O) (CH$^{[OH]}$)(OH)(COOH)	289	a_w (bulk)	6	0.00	this work
vanillylmandelic acid	ACH$_n$, ACOH, CH$_n^{[OH]}$, COOH, CH$_n$O, OH	(ACH)$_3$(AC$_2$)(ACOH)(CH$_3$O) (CH$^{[OH]}$)(OH)(COOH)	298	a_w (bulk)	6	0.00	this work
vanillylmandelic acid	ACH$_n$, ACOH, CH$_n^{[OH]}$, COOH, CH$_n$O, OH	(ACH)$_3$(AC$_2$)(ACOH)(CH$_3$O) (CH$^{[OH]}$)(OH)(COOH)	313	a_w (bulk)	6	1.00	this work
− **water + alcohol + alcohol systems** −							
1-butanol, 1-propanol	CH$_n^{[alc-tail]}$, CH$_n^{[OH]}$, OH	(CH$_3^{[alc-tail]}$)(CH$_2^{[alc-tail]}$)$_2$ (CH$_2^{[OH]}$)(OH), (CH$_3^{[alc-tail]}$)(CH$_2^{[alc-tail]}$) (CH$_2^{[OH]}$)(OH)	298	LLE	20	0.00	Gomis-Yagües et al. (1998)
1-butanol, 1-propanol	CH$_n^{[alc-tail]}$, CH$_n^{[OH]}$, OH	(CH$_3^{[alc-tail]}$)(CH$_2^{[alc-tail]}$)$_2$ (CH$_2^{[OH]}$)(OH), (CH$_3^{[alc-tail]}$)(CH$_2^{[alc-tail]}$) (CH$_2^{[OH]}$)(OH)	323	LLE	10	1.00	Gomis-Yagües et al. (1998)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
1-butanol, 1-propanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2 (CH_2^{[OH]})(OH)$, $(CH_3^{[alc-tail]})(CH_2^{[alc-tail]}) (CH_2^{[OH]})(OH)$	358	LLE	6	1.00	Gomis-Yagües et al. (1998)
1-butanol, 1-propanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2 (CH_2^{[OH]})(OH)$, $(CH_3^{[alc-tail]})(CH_2^{[alc-tail]}) (CH_2^{[OH]})(OH)$	368	LLE	8	1.00	Gomis-Yagües et al. (1998)
1-pentanol, ethanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_3 (CH_2^{[OH]})(OH)$, $(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$	298	LLE	12	0.00	Fernández-Torres et al. (1999)
1-pentanol, ethanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_3 (CH_2^{[OH]})(OH)$, $(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$	323	LLE	12	1.00	Fernández-Torres et al. (1999)
1-pentanol, ethanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH,	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_3 (CH_2^{[OH]})(OH)$, $(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$	358	LLE	8	1.00	Fernández-Torres et al. (1999)
1-pentanol, ethanol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_3 (CH_2^{[OH]})(OH)$, $(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$	368	LLE	12	1.00	Fernández-Torres et al. (1999)
– water + alcohol + acid systems –							
1-butanol, acetic acid	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2 (CH_2^{[OH]})(OH)$, $(CH_3)(COOH)$	298	LLE	10	0.00	Ruiz Bevia et al. (1984)
1-butanol, acetic acid	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2 (CH_2^{[OH]})(OH)$, $(CH_3)(COOH)$	303	LLE	12	0.00	Esquível and Bernardo-Gil (1990)
1-butanol, acetic acid	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2 (CH_2^{[OH]})(OH)$, $(CH_3)(COOH)$	323	LLE	14	1.00	Esquível and Bernardo-Gil (1990)
2-butanol, acetic acid	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})$ $(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$, $(CH_3)(COOH)$	303	LLE	10	0.00	Esquível and Bernardo-Gil (1990)
2-butanol, acetic acid	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})$ $(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$, $(CH_3)(COOH)$	323	LLE	14	1.00	Esquível and Bernardo-Gil (1990)
1-butanol, propanoic acid	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2 (CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)(COOH)$	298	LLE	8	0.00	Kim and Park (2005)
1-butanol, propanoic acid	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2 (CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)(COOH)$	303	LLE	14	0.00	Sólimo et al. (1997)
2-butanol, citric acid	CH_n, $CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})$ $(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$, $(CH_2)_2(C^{[OH]})(COOH)_3(OH)$	298	LLE	8	0.00	Lintomen et al. (2001)
2-pentanol, acetic acid	CH_n, $CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})$ $(CH_2^{[alc-tail]})_2(CH^{[OH]})(OH)$, $(CH_3)(COOH)$	288	LLE	20	0.20	Al-Muhtaseb and Fahim (1996)
2-pentanol, acetic acid	CH_n, $CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})$ $(CH_2^{[alc-tail]})_2(CH^{[OH]})(OH)$, $(CH_3)(COOH)$	298	LLE	20	0.00	Al-Muhtaseb and Fahim (1996)
2-pentanol, acetic acid	CH_n, $CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})$ $(CH_2^{[alc-tail]})_2(CH^{[OH]})(OH)$, $(CH_3)(COOH)$	303	LLE	8	0.00	Al-Muhtaseb and Fahim (1996)
2-pentanol, acetic acid	CH_n, $CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})$ $(CH_2^{[alc-tail]})_2(CH^{[OH]})(OH)$, $(CH_3)(COOH)$	308	LLE	10	1.00	Al-Muhtaseb and Fahim (1996)
2-pentanol, acetic acid	CH_n, $CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc]})(CH_3^{[alc-tail]}) (CH_2^{[alc-tail]})_2$ $(CH^{[OH]})(OH)$, $(CH_3)(COOH)$	318	LLE	8	1.00	Al-Muhtaseb and Fahim (1996)
2-pentanol, acetic acid	CH_n, $CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})$ $(CH_2^{[alc-tail]})_2(CH^{[OH]})(OH)$, $(CH_3)(COOH)$	323	LLE	14	1.00	Al-Muhtaseb and Fahim (1996)
1-hexanol, acetic acid	CH_n, $CH_n^{[OH]}$, $CH_n^{[alc-tail]}$, OH,COOH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_4 (CH_2^{[OH]})(OH)$, $(CH_3)(COOH)$	293	LLE	8	0.00	Senol (2004)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
– **water + alcohol + ketone systems** –							
tert-butanol, 4-methyl-2-pentanone	CH_n, $CH_n^{[alc]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3)_3(C^{[OH]})(OH)$, $(CH_3)_2(CH_2)(CH)(CH_3CO)$	288	LLE	14	0.10	Fang et al. (2008)
tert-butanol, 4-methyl-2-pentanone	CH_n, $CH_n^{[alc]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3)_3(C^{[OH]})(OH)$, $(CH_3)_2(CH_2)(CH)(CH_3CO)$	304	LLE	16	0.00	Fang et al. (2008)
tert-butanol, 4-methyl-2-pentanone	CH_n, $CH_n^{[alc]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3)_3(C^{[OH]})(OH)$, $(CH_3)_2(CH_2)(CH)(CH_3CO)$	318	LLE	18	0.10	Fang et al. (2008)
tert-butanol, 4-methyl-2-pentanone	CH_n, $CH_n^{[alc]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3)_3(C^{[OH]})(OH)$, $(CH_3)_2(CH_2)(CH)(CH_3CO)$	333	LLE	16	0.10	Fang et al. (2008)
1-pentanol, acetone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_3(CH_2^{[OH]})(OH)$, $(CH_3)(CH_3CO)$	298	LLE	16	0.00	Tiryaki et al. (1994)
1-pentanol, acetone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_3(CH_2^{[OH]})(OH)$, $(CH_3)(CH_3CO)$	303	LLE	16	0.00	Tiryaki et al. (1994)
1-pentanol, acetone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_3(CH_2^{[OH]})(OH)$, $(CH_3)(CH_3CO)$	308	LLE	16	0.00	Tiryaki et al. (1994)
2-octanol, acetone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[alc]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_3^{[alc]})(CH_2^{[alc-tail]})_5(CH^{[OH]})(OH)$, $(CH_3)(CH_3CO)$	298	LLE	18	0.00	Tiryaki et al. (1994)
2-octanol, acetone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[alc]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_3^{[alc]})(CH_2^{[alc-tail]})_5(CH^{[OH]})(OH)$, $(CH_3)(CH_3CO)$	303	LLE	18	0.00	Tiryaki et al. (1994)
2-octanol, acetone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[alc]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_3^{[alc]})(CH_2^{[alc-tail]})_5(CH^{[OH]})(OH)$, $(CH_3)(CH_3CO)$	308	LLE	16	1.00	Tiryaki et al. (1994)
– **water + alcohol + ether systems** –							
ethanol, 2-ethoxy-2-methyl-propane	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_4(C)(CH_2O)$	288	LLE	14	0.20	Fandary et al. (1999)
ethanol, 2-ethoxy-2-methyl-propane	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_4(C)(CH_2O)$	298	LLE	14	0.00	Fandary et al. (1999)
exthanol, 2-ethoxy-2-methyl-propane	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_4(C)(CH_2O)$	303	LLE	14	0.00	Fandary et al. (1999)
ethanol, 2-ethoxy-2-methyl-propane	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_4(C)(CH_2O)$	308	LLE	14	0.00	Fandary et al. (1999)
– **water + alcohol + ester systems** –							
ethanol, ethyl acetate	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CCOO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})$ (OH), (CH_3) $(CH_2)(CH_3COO)$	313	LLE	10	1.00	Mertl (1972)
ethanol, ethyl acetate	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CCOO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)$ (CH_3COO)	328	LLE	10	1.00	Mertl (1972)
ethanol, ethyl acetate	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CCOO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)$ (CH_3COO)	343	LLE	10	1.00	Mertl (1972)
– **water + alcohol + aromatic systems** –							
1-butanol, phenol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, ACH_n, ACOH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2(CH_2^{[OH]})(OH)$, $(ACH)_5(ACOH)$	298	LLE	12	0.00	De Oliveira and Aznar (2010)
2-butanol, phenol	$CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, ACH_n, ACOH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$, $(ACH)_5(ACOH)$	298	LLE	12	0.00	De Oliveira and Aznar (2010)
2-butanol, phenol	$CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, ACH_n, ACOH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$, $(ACH)_5(ACOH)$	313	LLE	12	1.00	De Oliveira and Aznar (2010)
– **water + alcohol + aldehyde systems** –							
ethanol, butyraldehyde	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CHO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, (CH_3) $(CH_2)_2(CHO)$	298	LLE	10	0.00	Letcher et al. (1996)
2-propanol, butyraldehyde	CH_n, $CH_n^{[alc]}$, $CH_n^{[OH]}$, OH, CHO	$(CH_3^{[alc]})_2(CH^{[OH]})$ (OH), $(CH_3)(CH_2)_2(CHO)$	298	LLE	10	0.00	Letcher et al. (1996)
2-butanol, butyraldehyde	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[alc]}$, $CH_n^{[OH]}$, OH, CHO	$(CH_3^{[alc]})(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$, $(CH_3)(CH_2)_2$ (CHO)	298	LLE	10	0.00	Letcher et al. (1996)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
– **water + acid + ketone systems** –							
acetic acid, 2-butanone	CH_n, COOH, CH_nCO	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3CO)$	298	LLE	8	0.00	Correa et al. (1987)
acetic acid, 2-butanone	CH_n, COOH, CH_nCO	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3CO)$	308	LLE	8	1.00	Correa et al. (1987)
acetic acid, 2-butanone	CH_n, COOH, CH_nCO	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3CO)$	318	LLE	8	1.00	Correa et al. (1987)
propanoic acid, 2-butanone	CH_n, COOH, CH_nCO	$(CH_3)(CH_2)(COOH)$, $(CH_3)(CH_2)(CH_3CO)$	298	LLE	8	0.00	Arce et al. (1995)
propanoic acid, 2-butanone	CH_n, COOH, CH_nCO	$(CH_3)(CH_2)(COOH)$, $(CH_3)(CH_2)(CH_3CO)$	308	LLE	12	1.00	Arce et al. (1995)
propanoic acid, 2-butanone	CH_n, COOH, CH_nCO	$(CH_3)(CH_2)(COOH)$, $(CH_3)(CH_2)(CH_3CO)$	318	LLE	10	1.00	Arce et al. (1995)
propanoic acid, 2-pentanone	CH_n, COOH, CH_nCO	$(CH_3)(CH_2)(COOH)$, $(CH_3)(CH_2)_2(CH_3CO)$	298	LLE	12	0.00	Arce et al. (1995)
propanoic acid, 2-pentanone	CH_n, COOH, CH_nCO	$(CH_3)(CH_2)(COOH)$, $(CH_3)(CH_2)_2(CH_3CO)$	308	LLE	12	1.00	Arce et al. (1995)
propanoic acid, 2-pentanone	CH_n, COOH, CH_nCO	$(CH_3)(CH_2)(COOH)$, $(CH_3)(CH_2)_2(CH_3CO)$	318	LLE	12	1.00	Arce et al. (1995)
propanoic acid, 2-pentanone	CH_n, COOH, CH_nCO	$(CH_3)(CH_2)(COOH)$, $(CH_3)(CH_2)_2(CH_3CO)$	328	LLE	16	1.00	Arce et al. (1995)
– **water + acid + ether systems** –							
acetic acid, 2-methoxy-2-methylpropane	CH_n, COOH, CH_nO	$(CH_3)(COOH)$, $(CH_3)_3(C)(CH_3O)$	293	LLE	18	0.00	Miao et al. (2007)
acetic acid, 2-methoxy-2-methylpropane	CH_n, COOH, CH_nO	$(CH_3)(COOH)$, $(CH_3)_3(C)(CH_3O)$	298	LLE	18	0.00	Miao et al. (2007)
acetic acid, 2-methoxy-2-methylpropane	CH_n, COOH, CH_nO	$(CH_3)(COOH)$, $(CH_3)_3(C)(CH_3O)$	303	LLE	18	0.00	Miao et al. (2007)
acetic acid, 2-methoxy-2-methylpropane	CH_n, COOH, CH_nO	$(CH_3)(COOH)$, $(CH_3)_3(C)(CH_3O)$	308	LLE	18	0.10	Miao et al. (2007)
– **water + acid + ester systems** –							
acetic acid, ethyl acetate	CH_n, COOH, CCOO	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3COO)$	283	LLE	12	1.00	Colombo et al. (1999)
acetic acid, ethyl acetate	CH_n, COOH, CCOO	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3COO)$	298	LLE	12	0.00	Colombo et al. (1999)
acetic acid, ethyl acetate	CH_n, COOH, CCOO	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3COO)$	313	LLE	12	1.00	Colombo et al. (1999)
acetic acid, 1-butyl acetate	CH_n, COOH, CCOO	$(CH_3)(COOH)$, $(CH_3)(CH_2)_3(CH_3COO)$	304	LLE	18	0.00	Wang et al. (2007)
acetic acid, 1-butyl acetate	CH_n, COOH, CCOO	$(CH_3)(COOH)$, $(CH_3)(CH_2)_3(CH_3COO)$	332	LLE	16	1.00	Wang et al. (2007)
acetic acid, 1-butyl acetate	CH_n, COOH, CCOO	$(CH_3)(COOH)$, $(CH_3)(CH_2)_3(CH_3COO)$	366	LLE	16	1.00	Wang et al. (2007)
acetic acid, isobutyl acetate	CH_n, COOH, CCOO	$(CH_3)(COOH)$, $(CH_3)_2(CH_2)(CH)(CH_3COO)$	304	LLE	16	0.00	Wang et al. (2007)
acetic acid, isobutyl acetate	CH_n, COOH, CCOO	$(CH_3)(COOH)$, $(CH_3)_2(CH_2)(CH)(CH_3COO)$	332	LLE	16	1.00	Wang et al. (2007)
acetic acid, isobutyl acetate	CH_n, COOH, CCOO	$(CH_3)(COOH)$, $(CH_3)_2(CH_2)(CH)(CH_3COO)$	366	LLE	14	1.00	Wang et al. (2007)
– **water + acid + aromatic systems** –							
acetic acid, benzene	CH_n, COOH, ACH_n	$(CH_3)(COOH)$, $(ACH)_6$	298	LLE	10	0.00	Backes et al. (1990)
– **water + ketone + ether systems** –							
2-butanone, 2-butoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH, CH_nCO	$(CH_3)(CH_2)(CH_3CO)$, $(CH_3)(CH_2)_3(CH_2^{[OH]})(CH_2O)(OH)$	298	LLE	10	0.00	Newman et al. (1949)
– **water + ketone + ester systems** –							
acetone, ethyl acetate	CH_n, CH_nCO, CCOO	$(CH_3)(CH_3CO)$, $(CH_3)(CH_2)(CH_3COO)$	283	LLE	10	1.00	Choi et al. (1986)
– **water + ketone + aromatic systems** –							
acetone, phenol	CH_n, CH_nCO, ACH_n, ACOH	$(CH_3)(CH_3CO)$, $(ACH)_5(ACOH)$	323	LLE	24	1.00	Mafra and Krähenbühl (2006)
acetone, phenol	CH_n, CH_nCO, ACH_n, ACOH	$(CH_3)(CH_3CO)$, $(ACH)_5(ACOH)$	333	LLE	22	1.00	Mafra and Krähenbühl (2006)
– **water + ether + aromatic systems** –							
2-methoxy-2-methylpropane, benzene	CH_n, CH_nO, ACH_n	$(CH_3)_3(C)(CH_3O)$, $(ACH)_6$	298	LLE	30	0.00	Stephenson (1992)
– **water + ether + aldehyde systems** –							
diethyl ether, acetaldehyde	CH_n, CH_nO, CHO	$(CH_3)_2(CH_2)CH_2O$, $(CH_3)(CHO)$	288	LLE	10	0.20	Suska (1979)
– **water + ester + aromatic systems** –							
ethyl acetate, phenol	CH_n, CCOO, ACH_n, ACOH	$(CH_3)(CH_2)(CH_3COO)$, $(ACH)_5(ACOH)$	298	LLE	18	0.00	Alvarez Gonzalez et al. (1986)
1-butyl acetate, phenol	CH_n, CCOO, ACH_n, ACOH	$(CH_3)(CH_2)_3(CH_3COO)$, $(ACH)_5(ACOH)$	298	LLE	32	0.00	Takahashi et al. (1988)
1-butyl acetate, phenol	CH_n, CCOO, ACH_n, ACOH	$(CH_3)(CH_2)_3(CH_3COO)$, $(ACH)_5(ACOH)$	313	LLE	32	0.50	Takahashi et al. (1988)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
– **water-free systems** –							
ethanol, acetic acid	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(COOH)$	244–284	SLE(org)[d]	13	0.20	Carta and Dernini (1983)
ethanol, acetic acid	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(COOH)$	241–289	SLE(org)[d]	22	0.20	Pickering (1893)
ethanol, acetic acid	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(COOH)$	354–389	VLE	12	0.10	Reichl et al. (1998)
ethanol, acetic acid	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(COOH)$	351–386	VLE	16	0.10	Hirata et al. (1975)
ethanol, acetic acid	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(COOH)$	323	VLE	16	0.10	Miyamoto et al. (2001)
1-propanol, acetic acid	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})$ $(CH_2^{[OH]})(OH)$, $(CH_3)(COOH)$	254–287	SLE(org)[d]	13	0.20	Pickering (1893)
1-propanol, acetic acid	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})$ $(CH_2^{[OH]})(OH)$, $(CH_3)(COOH)$	370–387	VLE	14	1.00	Rius et al. (1959)
cyclohexanol, adipic acid	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_2^{[alc-tail]})_5(CH^{[OH]})(OH)$, $(CH_2)_4(COOH)_2$	299–352	SLE(org)[d]	12	0.10	Lihua et al. (2007)
ethanol, acetone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_3CO)$	154–173	SLE	6	0.20	Sapgir (1929)
ethanol, acetone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_3CO)$	344	VLE	9	1.00	Lee and Hu (1995)
ethanol, acetone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_3CO)$	353	VLE	9	1.00	Lee and Hu (1995)
ethanol, acetone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_3CO)$	363	VLE	9	1.00	Lee and Hu (1995)
ethanol, acetone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_3CO)$	373	VLE	9	1.00	Campbell et al. (1987)
ethanol, acetone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_3CO)$	398	VLE	11	1.00	Campbell et al. (1987)
ethanol, acetone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_3CO)$	423	VLE	10	1.00	Campbell et al. (1987)
ethanol, acetone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_3CO)$	330–350	VLE	9	1.00	Amer et al. (1956)
ethanol, 2-butanone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)(CH_3CO)$	298	VLE	12	0.00	Ohta et al. (1981)
ethanol, 2-butanone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)(CH_3CO)$	308–314	VLE	19	1.00	Martínez et al. (2008)
ethanol, 2-butanone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)(CH_3CO)$	348–351	VLE	19	1.00	Martínez et al. (2008)
ethanol, 2-butanone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)(CH_3CO)$	347–352	VLE	19	1.00	Wen and Tu (2007)
ethanol, 2-heptanone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)_4(CH_3CO)$	208–238	SLE(org)[d]	20	0.20	Fiege et al. (1996)
ethanol, 3-heptanone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_2(CH_2)_3(CH_2CO)$	204–236	SLE(org)[d]	20	0.20	Fiege et al. (1996)
ethanol, 4-heptanone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_2(CH_2)_3(CH_3CO)$	205–240	SLE(org)[d]	20	0.20	Fiege et al. (1996)
1-hexanol, 2-octanone	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_4 (CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)_5(CH_3CO)$	227–253	SLE(org)[d]	20	0.20	Abbas and Gmehling (2008)
ethanol, diethyl ether	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_2(CH_2)CH_2O$	151–157	SLE(org)[d]	4	0.20	Sapgir (1929)
ethanol, diethyl ether	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_2(CH_2)CH_2O$	149–157	SLE(org)[d]	13	0.20	Lalande (1934)
ethanol, diethyl ether	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_2(CH_2)CH_2O$	154–159	SLE(org)[d]	2	0.20	Sapgir (1929)
ethanol, diethyl ether	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_2(CH_2)CH_2O$	148–159	SLE(org)[d]	9	0.20	Lalande (1934)
ethanol, diethyl ether	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_2(CH_2)CH_2O$	342–378	VLE	10	0.20	Moeller et al. (1951)
ethanol, diethyl ether	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_2(CH_2)CH_2O$	363–382	VLE	10	0.20	Moeller et al. (1951)
ethanol, diethyl ether	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_2(CH_2)CH_2O$	378–400	VLE	10	0.20	Moeller et al. (1951)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
ethanol, 2-methoxy-2-methylpropane	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_3(C)(CH_3O)$	324–347	VLE	22	1.00	Al-Rub et al. (2002)
ethanol, 2-methoxy-2-methylpropane	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_3(C)(CH_3O)$	326–349	VLE	30	1.00	Al-Rub et al. (2002)
ethanol, 2-methoxy-2-methylpropane	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_3(C)(CH_3O)$	328–351	VLE	30	1.00	Park et al. (2002)
ethanol, 2-ethoxy-2-methylpropane	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_4(C)(CH_2O)$	298	VLE	56	0.00	Rarey et al. (1999)
ethanol, 2-ethoxy-2-methylpropane	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_4(C)(CH_2O)$	323	VLE	56	1.00	Rarey et al. (1999)
ethanol, 2-ethoxy-2-methylpropane	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_4(C)(CH_2O)$	333	VLE	21	1.00	Oh and Park (1998)
ethanol, 2-ethoxy-2-methylpropane	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_4(C)(CH_2O)$	338	VLE	56	1.00	Rarey et al. (1999)
ethanol, 2-ethoxy-2-methylpropane	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CH_nO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)_4(C)(CH_2O)$	363	VLE	52	1.00	Rarey et al. (1999)
ethanol, ethyl acetate	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CCOO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)(CH_3COO)$	158–190	SLE(org)[d]	7	0.20	Sapgir (1929)
ethanol, ethyl acetate	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CCOO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)(CH_3COO)$	313	VLE	14	1.00	Mertl (1972)
ethanol, ethyl acetate	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CCOO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)(CH_3COO)$	328	VLE	14	1.00	Mertl (1972)
ethanol, ethyl acetate	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CCOO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)(CH_3COO)$	343	VLE	15	1.00	Mertl (1972)
ethanol, ethyl acetate	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CCOO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)(CH_3COO)$	345–351	VLE	24	1.00	Calvar et al. (2005)
2-propanol, 1-butyl acetate	CH_n, $CH_n^{[alc]}$, $CH_n^{[OH]}$, OH, CCOO	$(CH_3^{[alc]})_2(CH^{[OH]})(OH)$, $(CH_3)(CH_2)_3(CH_3COO)$	355–399	VLE	27	0.20	Gonzalez (1996)
tert-Butanol, tert-butyl acetate	CH_n, $CH_n^{[alc]}$, OH, CCOO	$(CH_3^{[alc]})_3(C^{[OH]})(OH)$, $(CH_3)_3(C)(CH_3COO)$	356–369	VLE	21	1.00	Montón et al. (2005)
tert-Butanol, tert-butyl acetate	CH_n, $CH_n^{[alc]}$, OH, CCOO	$(CH_3^{[alc]})_3(C^{[OH]})(OH)$, $(CH_3)_3(C)(CH_3COO)$	319–324	VLE	20	1.00	Montón et al. (2005)
ethanol, benzene	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, ACH_n	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(ACH)_6$	160–279	SLE(org)[d]	22	0.20	Viala (1914)
ethanol, benzene	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, ACH_n	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(ACH)_6$	207–279	SLE(org)[d]	10	0.20	Tarasenkov (1930)
ethanol, benzene	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, ACH_n	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(ACH)_6$	202–277	SLE(org)[d]	44	0.20	Pickering (1893)
ethanol, benzene	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, ACH_n	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(ACH)_6$	328	VLE	17	1.00	Fu et al. (1995)
ethanol, benzene	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, ACH_n	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(ACH)_6$	333	VLE	17	1.00	Fu et al. (1995)
ethanol, benzene	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, ACH_n	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(ACH)_6$	341–350	VLE	17	1.00	Cabezas et al. (1985)
2-propanol, benzene	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH, ACH_n	$(CH_3^{[alc]})_2(CH^{[OH]})(OH)$, $(ACH)_6$	185–279	SLE(org)[d]	23	0.20	Perrakis (1925)
1-butanol, benzene	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, ACH_n	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2$ $(CH_2^{[OH]})(OH)$, $(ACH)_6$	192–279	SLE(org)[d]	19	0.20	Perrakis (1925)
cyclohexanol, benzene	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, ACH_n	$(CH_2^{[alc-tail]})_5(CH^{[OH]})(OH)$, $(ACH)_6$	241–265	SLE(org)[d]	11	0.20	Lohmann et al. (1997)
cyclohexanol, benzene	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, ACH_n	$(CH_2^{[alc-tail]})_5(CH^{[OH]})(OH)$, $(ACH)_6$	243–279	SLE(org)[d]	17	0.20	Lohmann et al. (1997)
cyclohexanol, benzene	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, ACH_n	$(CH_2^{[alc-tail]})_5(CH^{[OH]})(OH)$, $(ACH)_6$	245–289	SLE(org)[d]	9	0.20	Lohmann et al. (1997)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
ethanol, 2-hydroxybenzoic acid	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, ACH_n, ACOH, COOH	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(ACH)_4(AC)(ACOH)(COOH)$	298–348	SLE(org)^d	11	0.10	Shalmashi and Eliassi (2008)
ethanol, phenol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, ACH_n, ACOH	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(ACH)_5(ACOH)$	243–313	SLE(org)^d	9	0.20	Perrakis (1925)
ethanol, acetaldehyde	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CHO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CHO)$	146–158	SLE(org)^d	3	0.20	de Leeuw (1911)
ethanol, acetaldehyde	$CH_n CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CHO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CHO)$	283	VLE	5	0.01	d'Avila and Silva (1970)
ethanol, acetaldehyde	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CHO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CHO)$	288	VLE	5	0.01	d'Avila and Silva (1970)
ethanol, acetaldehyde	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CHO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CHO)$	293	VLE	5	0.00	d'Avila and Silva (1970)
ethanol, acetaldehyde	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CHO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CHO)$	303	VLE	5	0.01	d'Avila and Silva (1970)
ethanol, acetaldehyde	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CHO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CHO)$	302–350	VLE	5	0.01	Suska (1979)
ethanol, butyraldehyde	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CHO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)_2(CHO)$	323	VLE	9	1.0	Gmehling et al. (1988)
ethanol, butyraldehyde	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CHO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)_2(CHO)$	333	VLE	9	1.0	Gmehling et al. (1988)
ethanol, butyraldehyde	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CHO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)_2(CHO)$	343	VLE	9	1.0	Gmehling et al. (1988)
ethanol, butyraldehyde	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CHO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)_2(CHO)$	353	VLE	9	1.0	Gmehling et al. (1988)
ethanol, butyraldehyde	CH_n, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, CHO	$(CH_3^{[alc-tail]})(CH_2^{[OH]})(OH)$, $(CH_3)(CH_2)_2(CHO)$	346–350	VLE	15	1.0	Gmehling et al. (1988)
acetic acid, acetone	CH_n, COOH, $CH_n CO$	$(CH_3)(COOH)$, $(CH_3)(CH_3 CO)$	173	SLE(org)^d	1	0.20	Chesnokov (1969)
acetic acid, acetone	CH_n, COOH, $CH_n CO$	$(CH_3)(COOH)$, $(CH_3)(CH_3 CO)$	244–284	SLE(org)^d	8	0.20	Carta and Dernini (1983)
acetic acid, acetone	CH_n, COOH, $CH_n CO$	$(CH_3)(COOH)$, $(CH_3)(CH_3 CO)$	245–283	SLE(org)^d	5	0.20	Carta and Dernini (1983)
acetic acid, acetone	CH_n, COOH, $CH_n CO$	$(CH_3)(COOH)$, $(CH_3)(CH_3 CO)$	332–383	VLE	10	1.00	Othmer (1943)
acetic acid, acetone	CH_n, COOH, $CH_n CO$	$(CH_3)(COOH)$, $(CH_3)(CH_3 CO)$	308	VLE	12	0.10	Waradzin and Surovy (1975)
acetic acid, acetone	CH_n, COOH, $CH_n CO$	$(CH_3)(COOH)$, $(CH_3)(CH_3 CO)$	318	VLE	11	0.10	Waradzin and Surovy (1975)
acetic acid, acetone	CH_n, COOH, $CH_n CO$	$(CH_3)(COOH)$, $(CH_3)(CH_3 CO)$	328	VLE	11	0.10	Waradzin and Surovy (1975)
acetic acid, 2-butanone	CH_n, COOH, $CH_n CO$	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3 CO)$	242–290	SLE(org)^d	12	0.20	Dallos et al. (1986)
acetic acid, 2-butanone	CH_n, COOH, $CH_n CO$	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3 CO)$	353–391	VLE	40	1.00	Fu et al. (1986)
acetic acid, 2-butanone	CH_n, COOH, $CH_n CO$	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3 CO)$	353–388	VLE	22	0.00	Xie et al. (2009)
acetic acid, 2-butanone	CH_n, COOH, $CH_n CO$	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3 CO)$	303	VLE	12	0.00	Dallos et al. (1986)
acetic acid, 2-butanone	CH_n, COOH, $CH_n CO$	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3 CO)$	323	VLE	14	1.00	Dallos et al. (1986)
acetic acid, 2-butanone	CH_n, COOH, $CH_n CO$	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3 CO)$	351	VLE	9	1.00	Dallos et al. (1986)
butanoic acid, acetone	CH_n, COOH, $CH_n CO$	$(CH_3)(CH_2)_2(COOH)$, $(CH_3)(CH_3 CO)$	240–268	SLE(org)^d	12	0.20	Proust and Fernandez (1986)
butanoic acid, 2-butanone	CH_n, COOH, $CH_n CO$	$(CH_3)(CH_2)_2(COOH)$, $(CH_3)(CH_2)(CH_3 CO)$	240–268	SLE(org)^d	12	0.20	Proust and Fernandez (1986)
butanoic acid, 2-butanone	CH_n, COOH, $CH_n CO$	$(CH_3)(CH_2)_2(COOH)$, $(CH_3)(CH_2)(CH_3 CO)$	343	VLE	9	1.00	Rasmussen and Fredenslund (1977)
butanoic acid, 2-butanone	CH_n, COOH, $CH_n CO$	$(CH_3)(CH_2)_2(COOH)$, $(CH_3)(CH_2)(CH_3 CO)$	353	VLE	10	1.00	Rasmussen and Fredenslund (1977)
acetic acid, diethyl ether	CH_n, COOH, $CH_n O$	$(CH_3)(COOH)$, $(CH_3)_2(CH_2)CH_2 O$	207–289	SLE(org)^d	40	0.20	Pickering (1893)
acetic acid, diethyl ether	CH_n, COOH, $CH_n O$	$(CH_3)(COOH)$, $(CH_3)_2(CH_2)CH_2 O$	293–343	VLE	7	1.00	Meehan and Murphy (1965)
acetic acid, diethyl ether	CH_n, COOH, $CH_n O$	$(CH_3)(COOH)$, $(CH_3)_2(CH_2)CH_2 O$	299–351	VLE	7	1.00	Meehan and Murphy (1965)
acetic acid, diethyl ether	CH_n, COOH, $CH_n O$	$(CH_3)(COOH)$, $(CH_3)_2(CH_2)CH_2 O$	304–360	VLE	7	1.00	Meehan and Murphy (1965)
acetic acid, ethyl acetate	CH_n, COOH, CCOO	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3 COO)$	323	VLE	9	1.00	Miyamoto et al. (2001)
hexadecanoic acid (palmitic acid), ethyl acetate	CH_n, COOH, CCOO	$(CH_3)(CH_2)_{14}(COOH)$, $(CH_3)(CH_2)(CH_3 COO)$	243–273	SLE(org)^d	4	0.20	Kolb (1959)
octadecanoic acid (stearic acid), ethyl acetate	CH_n, COOH, CCOO	$(CH_3)(CH_2)_{16}(COOH)$, $(CH_3)(CH_2)(CH_3 COO)$	253–283	SLE(org)^d	4	0.20	Kolb (1959)

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Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
acetic acid, benzene	CH_n, COOH, ACH_n	$(CH_3)(COOH)$, $(ACH)_6$	264–289	SLE(org)[d]	20	0.20	Roloff (1895)
acetic acid, benzene	CH_n, COOH, ACH_n	$(CH_3)(COOH)$, $(ACH)_6$	274–289	SLE(org)[d]	8	0.20	Roloff (1895)
acetic acid, benzene	CH_n, COOH, ACH_n	$(CH_3)(COOH)$, $(ACH)_6$	313	VLE	9	0.20	Miyamoto et al. (2000)
acetic acid, benzene	CH_n, COOH, ACH_n	$(CH_3)(COOH)$, $(ACH)_6$	353–387	VLE	15	1.00	Haughton (1967)
acetic acid, benzene	CH_n, COOH, ACH_n	$(CH_3)(COOH)$, $(ACH)_6$	296–322	VLE	12	1.00	Carta et al. (1979)
acetic acid, acetaldehyde	CH_n, COOH, CHO	$(CH_3)(COOH)$, $(CH_3)(CHO)$	295–386	VLE	33	1.00	Shanghai-Inst. and Zhejiang (1978)
acetic acid, butyraldehyde	CH_n, COOH, CHO	$(CH_3)(COOH)$, $(CH_3)(CH_2)_2(CHO)$	323	VLE	9	1.00	Miyamoto et al. (2001)
propanoic acid, butyraldehyde	CH_n, COOH, CHO	$(CH_3)(CH_2)(COOH)$, $(CH_3)(CH_2)_2(CHO)$	323	VLE	9	1.00	Miyamoto et al. (2001)
acetone, 2-methoxy-2-methylpropane	CH_n, CH_nCO, CH_nO	$(CH_3)(CH_3CO)$, $(CH_3)_3(C)(CH_3O)$	322–326	VLE	19	1.00	Mejía et al. (2008)
2-butanone, 2-ethoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nCO, CH_nO, OH	$(CH_3)(CH_2)(CH_3CO)$, $(CH_3)(CH_2)(CH_2^{[OH]})(CH_2O)(OH)$	330	VLE	9	1.00	Naumann and Wagner (1986)
acetone, ethyl acetate	CH_n, CH_nCO, CCOO	$(CH_3)(CH_3CO)$, $(CH_3)(CH_2)(CH_3COO)$	330–348	VLE	16	1.00	Subrahmanyam and Murty (1964)
acetone, ethyl acetate	CH_n, CH_nCO, CCOO	$(CH_3)(CH_3CO)$, $(CH_3)(CH_2)(CH_3COO)$	328–348	VLE	16	1.00	Gilburd et al. (1979)
acetone, ethyl acetate	CH_n, CH_nCO, CCOO	$(CH_3)(CH_3CO)$, $(CH_3)(CH_2)(CH_3COO)$	313–330	VLE	12	1.00	Gilburd et al. (1981)
acetone, octadecanoic acid methyl ester (methyl stearate)	CH_n, CH_nCO, CCOO	$(CH_3)(CH_3CO)$, $(CH_3)(CH_2)_{16}(CH_3COO)$	265–311	SLE(org)[d]	6	0.10	Bailey et al. (1970)
acetone, octadecanoic acid ethyl ester (ethyl stearate)	CH_n, CH_nCO, CCOO	$(CH_3)(CH_3CO)$, $(CH_3)_2(CH_2)_{16}(CH_3COO)$	263–303	SLE(org)[d]	5	0.20	Bailey et al. (1970)
acetone, benzene	CH_n, CH_nCO, ACH_n	$(CH_3)(CH_3CO)$, $(ACH)_6$	318	VLE	11	1.00	Brown and Smith (1957)
acetone, benzene	CH_n, CH_nCO, ACH_n	$(CH_3)(CH_3CO)$, $(ACH)_6$	330–348	VLE	21	1.00	Kurihara et al. (1998)
2-heptanone, benzene	CH_n, CH_nCO, ACH_n	$(CH_3)(CH_2)_4(CH_3CO)$, $(ACH)_6$	228–279	SLE(org)[d]	13	0.20	Fiege et al. (1996)
2-heptanone, benzene	CH_n, CH_nCO, ACH_n	$(CH_3)(CH_2)_4(CH_3CO)$, $(ACH)_6$	228–238	SLE(org)[d]	8	0.20	Fiege et al. (1996)
3-heptanone, benzene	CH_n, CH_nCO, ACH_n	$(CH_3)_2(CH_2)_3(CH_2CO)$, $(ACH)_6$	228–279	SLE(org)[d]	13	0.20	Fiege et al. (1996)
3-heptanone, benzene	CH_n, CH_nCO, ACH_n	$(CH_3)_2(CH_2)_3(CH_2CO)$, $(ACH)_6$	225–236	SLE(org)[d]	8	0.20	Fiege et al. (1996)
4-heptanone, benzene	CH_n, CH_nCO, ACH_n	$(CH_3)_2(CH_2)_3(CH_2CO)$, $(ACH)_6$	227–241	SLE(org)[d]	9	0.20	Fiege et al. (1996)
4-heptanone, benzene	CH_n, CH_nCO, ACH_n	$(CH_3)_2(CH_2)_3(CH_2CO)$, $(ACH)_6$	238–279	SLE(org)[d]	11	0.20	Fiege et al. (1996)
acetone, acetaldehyde	CH_n, CH_nCO, CHO	$(CH_3)(CH_3CO)$, $(CH_3)(CHO)$	296–326	VLE	8	0.20	Tikhonova et al. (1970)
acetone, propionaldehyde	CH_n, CH_nCO, CHO	$(CH_3)(CH_3CO)$, $(CH_3)(CH_2)(CHO)$	322–329	VLE	13	1.00	Danciu (1970)
2-methoxyethanol, methyl acetate	CH_n, $CH_n^{[OH]}$, OH, CH_nO, CCOO	$(CH_2)(CH_2^{[OH]})(CH_3O)(OH)$, $(CH_3)(CH_3COO)$	298	VLE	9	0.00	Martin et al. (1994)
2-methoxyethanol, ethyl acetate	CH_n, $CH_n^{[OH]}$, OH, CH_nO, CCOO	$(CH_2)(CH_2^{[OH]})(CH_3O)(OH)$, $(CH_3)(CH_2)(CH_3COO)$	343	VLE	13	0.20	Chandak et al. (1977)
2-methoxyethanol, ethyl acetate	CH_n, $CH_n^{[OH]}$, OH, CH_nO, CCOO	$(CH_2)(CH_2^{[OH]})(CH_3O)(OH)$, $(CH_3)(CH_2)(CH_3COO)$	353	VLE	12	0.20	Chandak et al. (1977)
2-methoxyethanol, ethyl acetate	CH_n, $CH_n^{[OH]}$, OH, CH_nO, CCOO	$(CH_2)(CH_2^{[OH]})(CH_3O)(OH)$, $(CH_3)(CH_2)(CH_3COO)$	351–395	VLE	14	0.20	Chandak et al. (1977)
2-ethoxyethanol, methyl acetate	CH_n, $CH_n^{[OH]}$, OH, CH_nO, CCOO	$(CH_3)(CH_2)(CH_2^{[OH]})(CH_2O)(OH)$, $(CH_3)(CH_3COO)$	298	VLE	9	0.00	Martin et al. (1994)
2-ethoxyethanol, ethyl acetate	CH_n, $CH_n^{[OH]}$, OH, CH_nO, CCOO	$(CH_3)(CH_2)(CH_2^{[OH]})(CH_2O)(OH)$, $(CH_3)(CH_2)(CH_3COO)$	351–402	VLE	17	0.20	Thorat and Nageshwar (1988)
diethyl ether, benzene	CH_n, CH_nO, ACH_n	$(CH_3)_2(CH_2)_2CH_2O$, $(ACH)_6$	197–278	SLE(org)[d]	37	0.20	Pickering (1893)
2-butoxyethanol, benzene	CH_n, CH_nO, $CH_n^{[OH]}$, OH, ACH_n	$(CH_3)(CH_2)_3(CH_2^{[OH]})(CH_2O)(OH)$, $(ACH)_6$	217–279	SLE(org)[d]	18	0.20	Negadi et al. (2006)
1-methoxy-2-propanol, benzene	CH_n, $CH_n^{[OH]}$, OH, CH_nO, ACH_n	$(CH_3)_2(CH^{[OH]})(CH_3O)(OH)$, $(ACH)_6$	220–279	SLE(org)[d]	18	0.20	Negadi et al. (2006)
2-ethoxyethanol, phenol	CH_n, $CH_n^{[OH]}$, OH, CH_nO, ACH_n, ACOH	$(CH_3)(CH_2)(CH_2^{[OH]})(CH_2O)(OH)$, $(ACH)_5(ACOH)$	363	VLE	17	0.10	Chylinski et al. (2001)
2-ethoxyethanol, phenol	CH_n, $CH_n^{[OH]}$, OH, CH_nO, ACH_n, ACOH	$(CH_3)(CH_2)(CH_2^{[OH]})(CH_2O)(OH)$, $(ACH)_5(ACOH)$	373	VLE	17	0.10	Chylinski et al. (2001)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
2-ethoxyethanol, phenol	CH_n, $CH_n^{[OH]}$, OH, CH_nO, ACH_n, ACOH	$(CH_3)(CH_2)(CH_2^{[OH]})(CH_2O)$ (OH), $(ACH)_5(ACOH)$	383	VLE	17	0.10	Chylinski et al. (2001)
diethyl ether, acetaldehyde	CH_n, CH_nO, ACH_n, CHO	$(CH_3)_2(CH_2)(CH_2O)$, $(CH_3)(CHO)$	293–304	VLE	10	1.00	Suska (1979)
ethyl acetate, benzene	CH_n, CCOO, ACH_n	$(CH_3)(CH_2)(CH_3COO)$, $(ACH)_6$	350–353	VLE	19	1.00	Carr and Kropholler (1962)
ethyl acetate, 2-hydroxybenzoic acid	CH_n, CCOO, ACH_n, ACOH, COOH	$(CH_3)(CH_2)(CH_3COO)$, $(ACH)_4(AC)(ACOH)(COOH)$	298–348	SLE	11	1.00	Shalmashi and Eliassi (2008)
methyl acetate, butyraldehyde	CH_n, CCOO, CHO	$(CH_3)(CH_3COO)$, $(CH_3)(CH_2)_2(CHO)$	313	VLE	15	1.00	Radnai et al. (1987)
methyl acetate, butyraldehyde	CH_n, CCOO, CHO	$(CH_3)(CH_3COO)$, $(CH_3)(CH_2)_2(CHO)$	323	VLE	15	1.00	Radnai et al. (1987)
benzene, butyraldehyde	CH_n, ACH_n, CHO	$(ACH)_6$, $(CH_3)(CH_2)_2(CHO)$	353	VLE	5	1.00	Leu et al. (1989)
benzene, butyraldehyde	CH_n, ACH_n, CHO	$(ACH)_6$, $(CH_3)(CH_2)_2(CHO)$	393	VLE	6	1.00	Leu et al. (1989)

[a] Derived water activity data from differential scanning calorimetry (DSC) measurements at homogeneous freezing temperatures.

[b] M5 is a mixture of dicarboxylic acids consisting of: malic acid (2) + malonic acid (3) + maleic acid (4) + glutaric acid (5) + methylsuccinic acid (6).

[c] The chemical subgroup formulas of the M5 components are given in the table for the individual components, except for maleic acid, for which the subgroup formula is: $(CH=CH)(COOH)_2$.

[d] SLE data where the equilibrium is with respect to an organic compound in a solid (crystalline) state.

[e] Derived water activity data from total pressure measurements, for more information we refer to Ganbavale et al. (2014).

[f] Derived water activity data from Electrodynamic balance (EDB) measurements, for more information we refer to Ganbavale et al. (2014).

Table 2. Matrix of AIOMFAC short-range group interaction parameters. Parameter values for $a(i,j)$ (units of K) are from the literature [a], $b(i,j)$ (units of K), and $c(i,j)$ (dimensionless) are determined in this study.

group no. $j \rightarrow$ $i \downarrow$	main groups		1 CH_n	2 C=C	3 ACH_n	7 H_2O	8 ACOH	9 CH_nCO	10 CHO[aldehyde]	11 CCOO
1	CH_n	$a(i,j)$:	0.0	8.6020×10^1	6.1130×10^1	1.3180×10^3	1.3330×10^3	4.7640×10^2	6.7700×10^2	2.3210×10^2
		$b(i,j)$:	0.0	0.0	2.0000×10^2	8.7765×10^2	1.3330×10^3	-4.7640×10^2	2.0000×10^2	2.3210×10^2
		$c(i,j)$:	0.0	0.0 [b]	4.0000×10^{-1}	2.6360×10^0	2.6660×10^0	9.5280×10^{-1}	4.0000×10^{-1}	4.6420×10^{-1}
2	C=C	$a(i,j)$:	-3.5360×10^1	0.0	3.8810×10^1	2.7060×10^2	5.2610×10^2	1.8260×10^2	4.4880×10^2	3.7850×10^1
		$b(i,j)$:	0.0 [b]	0.0	0.0 [b]	0.0 [b]	0.0 [b]	0.0 [b]	0.0 [b]	0.0 [b]
		$c(i,j)$:	0.0 [b]	0.0	0.0 [b]	0.0 [b]	0.0 [b]	0.0 [b]	0.0 [b]	0.0 [b]
3	ACH_n	$a(i,j)$:	-1.1120×10^1	3.4460×10^0	0.0	9.0380×10^2	1.3290×10^3	2.5770×10^1	3.4730×10^2	5.9940×10^0
		$b(i,j)$:	5.3819×10^1	0.0 [b]	0.0	9.0380×10^2	-1.3290×10^3	-4.7477×10^1	-3.4730×10^2	0.0 [b]
		$c(i,j)$:	4.0000×10^{-1}	0.0 [b]	0.0	1.8076×10^0	-2.4726×10^0	0.0 [b]	0.0 [b]	0.0 [b]
7	H_2O	$a(i,j)$:	3.0000×10^2	4.9610×10^2	3.6230×10^2	0.0	3.2450×10^2	-1.9540×10^2	-1.1600×10^2	7.2870×10^1
		$b(i,j)$:	1.2542×10^1	0.0 [b]	-3.6230×10^2	0.0	5.4808×10^1	8.2298×10^1	-5.9018×10^1	4.4441×10^0
		$c(i,j)$:	-6.0000×10^{-1}	0.0 [b]	7.2460×10^{-1}	0.0	6.0210×10^{-1}	-4.0000×10^{-1}	0.0 [b]	-4.0000×10^{-1}
8	ACOH	$a(i,j)$:	2.7580×10^2	2.1750×10^2	2.5340×10^1	-6.0180×10^2	0.0	-3.5610×10^2	-2.7110×10^2	-4.4940×10^2
		$b(i,j)$:	2.7580×10^2	0.0 [b]	1.6367×10^1	6.1488×10^1	0.0	3.5610×10^2	0.0 [b]	3.9985×10^2
		$c(i,j)$:	3.2281×10^{-1}	0.0 [b]	-4.0000×10^{-1}	1.2036×10^0	0.0	0.0 [b]	0.0 [b]	0.0 [b]
9	CH_nCO	$a(i,j)$:	2.6760×10^1	4.2920×10^1	1.4010×10^2	4.7250×10^2	-1.3310×10^2	0.0	-3.7360×10^1	-2.1370×10^2
		$b(i,j)$:	4.5409×10^1	0.0 [b]	-1.8682×10^2	1.0675×10^2	2.0000×10^2	0.0	0.0 [b]	2.1370×10^2
		$c(i,j)$:	-4.0000×10^{-1}	0.0 [b]	0.0 [b]	-9.4500×10^{-1}	0.0 [b]	0.0	0.0 [b]	0.0 [b]
10	CHO[aldehyde]	$a(i,j)$:	5.0570×10^2	5.6300×10^1	2.3390×10^1	4.8080×10^2	-1.5560×10^2	1.2800×10^2	0.0	-1.1030×10^2
		$b(i,j)$:	5.0570×10^2	0.0 [b]	-2.0000×10^2	4.8080×10^2	0.0 [b]	0.0 [b]	0.0	0.0 [b]
		$c(i,j)$:	1.0114×10^0	0.0 [b]	0.0 [b]	0.0 [b]	0.0 [b]	0.0 [b]	0.0	0.0 [b]
11	CCOO	$a(i,j)$:	1.1480×10^2	1.3210×10^2	8.5840×10^1	2.0080×10^2	-3.6720×10^1	3.7220×10^2	1.8510×10^2	0.0
		$b(i,j)$:	2.0000×10^2	0.0 [b]	0.0 [b]	1.3043×10^2	5.5875×10^1	-2.2930×10^1	0.0 [b]	0.0
		$c(i,j)$:	4.0000×10^{-1}	0.0 [b]	0.0 [b]	-4.0160×10^{-1}	0.0 [b]	0.0 [b]	0.0 [b]	0.0
13	CH_nO[ether]	$a(i,j)$:	8.3360×10^1	2.6510×10^1	5.2130×10^1	-3.1470×10^2	-1.7850×10^2	1.9110×10^2	-7.8380×10^0	4.6130×10^2
		$b(i,j)$:	2.0000×10^2	0.0 [b]	-2.0000×10^2	-3.1470×10^2	0.0 [b]	0.0 [b]	0.0 [b]	-4.6130×10^2
		$c(i,j)$:	-1.0905×10^{-1}	0.0 [b]	-6.1186×10^{-2}	-6.2940×10^{-1}	0.0 [b]	0.0 [b]	0.0 [b]	-1.5826×10^{-1}
65	COOH	$a(i,j)$:	3.1530×10^2	1.2640×10^3	6.2320×10^1	-1.4588×10^2	-1.1000×10^1	-2.9780×10^2	-1.6550×10^2	-2.5630×10^2
		$b(i,j)$:	3.1530×10^2	0.0 [b]	-1.9014×10^1	3.8158×10^1	2.0000×10^2	-1.1715×10^2	-2.0000×10^2	2.5630×10^2
		$c(i,j)$:	6.3060×10^{-1}	0.0 [b]	3.5606×10^{-1}	-4.0000×10^{-1}	-3.3849×10^{-2}	-5.9560×10^{-1}	4.0000×10^{-1}	0.0 [b]
66	$CH_n^{[alc]}$	$a(i,j)$:	0.0 [b]	8.6020×10^1	6.1130×10^1	1.8900×10^3	1.3330×10^3	4.7640×10^2	6.7700×10^2	2.3210×10^2
		$b(i,j)$:	0.0 [b]	0.0 [b]	2.0000×10^2	1.8282×10^3	1.3330×10^3	-4.7640×10^2	2.0000×10^2	2.3210×10^2
		$c(i,j)$:	0.0 [b]	0.0 [b]	4.0000×10^{-1}	3.7800×10^0	2.6660×10^0	9.5280×10^{-1}	4.0000×10^{-1}	4.6420×10^{-1}
67	$CH_n^{[alc-tail]}$	$a(i,j)$:	0.0 [b]	8.6020×10^1	6.1130×10^1	1.3250×10^3	1.3330×10^3	4.7640×10^2	6.7700×10^2	2.3210×10^2
		$b(i,j)$:	0.0 [b]	0.0 [b]	2.0000×10^2	6.7344×10^2	1.3330×10^3	-4.7640×10^2	2.0000×10^2	2.3210×10^2
		$c(i,j)$:	0.0 [b]	0.0 [b]	4.0000×10^{-1}	-2.6500×10^0	2.6660×10^0	9.5280×10^{-1}	4.0000×10^{-1}	4.6420×10^{-1}
68	$CH_n^{[OH]}$	$a(i,j)$:	0.0 [b]	8.6020×10^1	6.1130×10^1	2.3140×10^3	1.3330×10^3	4.7640×10^2	6.7700×10^2	2.3210×10^2
		$b(i,j)$:	0.0 [b]	0.0 [b]	2.0000×10^2	-8.0335×10^1	1.3330×10^3	-4.7640×10^2	2.0000×10^2	2.3210×10^2
		$c(i,j)$:	0.0 [b]	0.0 [b]	4.0000×10^{-1}	-8.3200×10^{-1}	2.6660×10^0	9.5280×10^{-1}	4.0000×10^{-1}	4.6420×10^{-1}
69	OH	$a(i,j)$:	1.5640×10^2	4.5700×10^2	8.9600×10^1	2.7640×10^2	-2.5970×10^2	8.4000×10^1	-2.0360×10^2	1.0110×10^2
		$b(i,j)$:	2.0000×10^2	0.0 [b]	9.7617×10^1	2.7640×10^2	2.5970×10^2	2.0000×10^2	-2.0360×10^2	-6.4775×10^1
		$c(i,j)$:	-4.0000×10^{-1}	0.0 [b]	4.0000×10^{-1}	-5.5280×10^{-1}	2.7684×10^{-1}	4.0000×10^{-1}	-4.0720×10^{-1}	4.0000×10^{-1}

[a] The values of $a_{i,j}$ for OH, $CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$ interactions with H_2O are taken from Marcolli and Peter (2005). The $a_{i,j}$ values for COOH ↔ H_2O group interactions are taken from Peng et al. (2001), respectively. For all other functional groups the $a_{i,j}$ values from the revised parameter set of Hansen et al. (1991) are used.
[b] Main group interactions $b_{i,j}$ and $c_{i,j}$ are set to zero since appropriate data to determine these interactions are missing.

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Extended parameterization of the AIOMFAC model

G. Ganbavale et al.

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Table 2. Continued.

group no. $j \rightarrow$			13	65	66	67	68	69
$i \downarrow$	main groups		CH_nO[ether]	COOH	$CH_n^{[alc]}$	$CH_n^{[alc-tail]}$	$CH_n^{[OH]}$	OH
1	CH_n	$a(i,j)$:	2.5150×10^2	6.6350×10^2	0.0 [b]	0.0 [b]	0.0 [b]	9.8650×10^2
		$b(i,j)$:	1.5817×10^2	6.6350×10^2	0.0 [b]	0.0 [b]	0.0 [b]	9.8650×10^2
		$c(i,j)$:	1.8636×10^{-1}	1.3270×10^0	0.0 [b]	0.0 [b]	0.0 [b]	1.9730×10^0
2	C=C	$a(i,j)$:	2.1450×10^2	3.1890×10^2	-3.5360×10^1	-3.5360×10^1	-3.5360×10^1	5.2410×10^2
		$b(i,j)$:	0.0 [b]	0.0 [b]	0.0 [b]	0.0 [b]	0.0 [b]	0.0 [b]
		$c(i,j)$:	0.0 [b]	0.0 [b]	0.0 [b]	0.0 [b]	0.0 [b]	0.0 [b]
3	ACH_n	$a(i,j)$:	3.2140×10^1	5.3740×10^2	-1.1120×10^1	-1.1120×10^1	-1.1120×10^1	6.3610×10^2
		$b(i,j)$:	-4.3180×10^0	-5.3740×10^2	5.3819×10^1	5.3819×10^1	5.3819×10^1	-6.3610×10^2
		$c(i,j)$:	4.0000×10^{-1}	-1.3577×10^{-1}	4.0000×10^{-1}	4.0000×10^{-1}	4.0000×10^{-1}	1.2722×10^0
7	H_2O	$a(i,j)$:	5.4050×10^2	-6.9290×10^1	1.6230×10^2	3.6210×10^2	-8.9710×10^1	-1.5300×10^2
		$b(i,j)$:	1.7880×10^2	-8.6552×10^1	-2.0000×10^1	-2.3073×10^2	-2.0000×10^2	1.6393×10^2
		$c(i,j)$:	5.5486×10^{-1}	-4.0000×10^{-1}	3.6193×10^{-1}	-7.2420×10^{-1}	-4.0000×10^{-1}	-4.0000×10^{-1}
8	ACOH	$a(i,j)$:	-1.6290×10^2	4.0890×10^2	2.7580×10^2	2.7580×10^2	2.7580×10^2	-4.5160×10^2
		$b(i,j)$:	0.0 [b]	4.0890×10^2	2.7580×10^2	2.7580×10^2	2.7580×10^2	4.5160×10^2
		$c(i,j)$:	0.0 [b]	8.8840×10^{-2}	3.2281×10^{-1}	3.2281×10^{-1}	3.2281×10^{-1}	9.0320×10^{-1}
9	CH_nCO	$a(i,j)$:	-1.0360×10^2	6.6940×10^2	2.6760×10^2	2.6760×10^2	2.6760×10^2	1.6450×10^2
		$b(i,j)$:	0.0 [b]	-5.7894×10^2	4.5409×10^1	4.5409×10^1	4.5409×10^1	2.0000×10^2
		$c(i,j)$:	0.0 [b]	1.9383×10^{-1}	-4.0000×10^{-1}	-4.0000×10^{-1}	-4.0000×10^{-1}	4.0000×10^{-1}
10	CHO[aldehyde]	$a(i,j)$:	3.0410×10^2	4.9750×10^2	5.0570×10^2	5.0570×10^2	5.0570×10^2	5.2900×10^2
		$b(i,j)$:	0.0 [b]	4.9750×10^2	5.0570×10^2	5.0570×10^2	5.0570×10^2	-5.2900×10^2
		$c(i,j)$:	0.0 [b]	9.9500×10^{-1}	1.0114×10^0	1.0114×10^0	1.0114×10^0	-1.0580×10^0
11	CCOO	$a(i,j)$:	-2.3570×10^2	6.6020×10^2	1.1480×10^2	1.1480×10^2	1.1480×10^2	2.4540×10^2
		$b(i,j)$:	2.2988×10^0	-3.5339×10^1	2.0000×10^2	2.0000×10^2	2.0000×10^2	2.4540×10^2
		$c(i,j)$:	5.9724×10^{-2}	0.0 [b]	4.0000×10^{-1}	4.0000×10^{-1}	4.0000×10^{-1}	4.9080×10^{-1}
13	CH_nO[ether]	$a(i,j)$:	0.0	6.6460×10^2	8.3360×10^1	8.3360×10^1	8.3360×10^1	2.3770×10^2
		$b(i,j)$:	0.0	-6.6460×10^2	2.0000×10^2	2.0000×10^2	2.0000×10^2	2.3770×10^2
		$c(i,j)$:	0.0	7.3512×10^{-1}	-1.0905×10^{-1}	-1.0905×10^{-1}	-1.0905×10^{-1}	4.7540×10^{-1}
65	COOH	$a(i,j)$:	-3.3850×10^2	0.0	3.1530×10^2	3.1530×10^2	3.1530×10^2	-1.0303×10^2
		$b(i,j)$:	1.1390×10^1	0.0	3.1530×10^2	3.1530×10^2	3.1530×10^2	2.0000×10^2
		$c(i,j)$:	6.7700×10^{-1}	0.0	6.3060×10^{-1}	6.3060×10^{-1}	6.3060×10^{-1}	4.0000×10^{-1}
66	$CH_n^{[alc]}$	$a(i,j)$:	2.5150×10^2	6.6350×10^2	0.0	0.0 [b]	0.0 [b]	9.8650×10^2
		$b(i,j)$:	1.5817×10^2	6.6350×10^2	0.0	0.0 [b]	0.0 [b]	9.8650×10^2
		$c(i,j)$:	1.8636×10^{-1}	1.3270×10^0	0.0	0.0 [b]	0.0 [b]	1.9730×10^0
67	$CH_n^{[alc-tail]}$	$a(i,j)$:	2.5150×10^2	6.6350×10^2	0.0 [b]	0.0	0.0 [b]	9.8650×10^2
		$b(i,j)$:	1.5817×10^2	6.6350×10^2	0.0 [b]	0.0	0.0 [b]	9.8650×10^2
		$c(i,j)$:	1.8636×10^{-1}	1.3270×10^0	0.0 [b]	0.0	0.0 [b]	1.9730×10^0
68	$CH_n^{[OH]}$	$a(i,j)$:	2.5150×10^2	6.6350×10^2	0.0 [b]	0.0 [b]	0.0	9.8650×10^2
		$b(i,j)$:	1.5817×10^2	6.6350×10^2	0.0 [b]	0.0 [b]	0.0	9.8650×10^2
		$c(i,j)$:	1.8636×10^{-1}	1.3270×10^0	0.0 [b]	0.0 [b]	0.0	1.9730×10^0
69	OH	$a(i,j)$:	2.8060×10^2	2.2439×10^2	1.5640×10^2	1.5640×10^2	1.5640×10^2	0.0
		$b(i,j)$:	-2.6146×10^1	2.2439×10^2	2.0000×10^2	2.0000×10^2	2.0000×10^2	0.0
		$c(i,j)$:	-3.1087×10^{-1}	4.4878×10^{-1}	-4.0000×10^{-1}	-4.0000×10^{-1}	-4.0000×10^{-1}	0.0

[a] The values of $a_{i,j}$ for OH, $CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$ interactions with H_2O are taken from Marcolli and Peter (2005). The $a_{i,j}$ values for COOH ↔ H_2O group interactions are taken from Peng et al. (2001), respectively. For all other functional groups the $a_{i,j}$ values from the revised parameter set of Hansen et al. (1991) are used.
[b] Main group interactions $b_{i,j}$ and $c_{i,j}$ are set to zero since appropriate data to determine these interactions are missing.

Table A1. Bulk water activity (a_w) measurements[a] of water (1) + glycerol (2) solutions at three different temperatures. Solution compositions are given in mole fraction of the organic component (2), x_2.

x_2	a_w ($T = 289.15\,\text{K}$)	a_w ($T = 298.15\,\text{K}$)	a_w ($T = 313.15\,\text{K}$)
0.01769	0.976	0.980	0.980
0.03477	0.964	0.964	0.970
0.05128	0.956	0.953	0.955
0.06721	0.937	0.935	0.940
0.08263	0.916	0.920	0.920
0.09754	0.896	0.895	0.910
0.11199	0.872	0.875	0.883
0.12595	0.854	0.862	0.864
0.13950	0.838	0.841	0.856
0.15263	0.823	0.826	0.833
0.16960	0.802	0.802	0.815
0.22685	0.728	0.732	0.739
0.31338	0.622	0.628	0.628
0.43896	0.492	0.491	0.497
0.63774	0.297	0.298	0.299

[a] The accuracy of the water activity measurements is specified as ±0.015 in a_w.

Table A2. Bulk water activity (a_w) measurements[a] of water (1) + 2,5-hexanediol (2) solutions at three different temperatures. Solution compositions are given in mole fraction of the organic component (2), x_2.

x_2	a_w ($T = 289.15\,K$)	a_w ($T = 298.15\,K$)	a_w ($T = 313.15\,K$)
0.0167	0.971	0.978	0.975
0.0365	0.974	0.978	0.973
0.0616	0.943	0.955	0.972
0.0934	0.917	0.937	0.953
0.1325	0.897	0.912	0.933
0.1790	0.882	0.894	0.912
0.2734	0.825	0.849	0.860
0.3607	0.781	0.790	0.804
0.5630	0.605	0.620	0.618

[a] The accuracy of the water activity measurements is specified as ±0.015 in a_w.

Table A3. Bulk water activity (a_w) measurements[a] of water (1) + 1,2,6-hexanetriol (2) solutions at three different temperatures. Solution compositions are given in mole fraction of the organic component (2), x_2.

x_2	a_w ($T = 289.15\,\text{K}$)	a_w ($T = 298.15\,\text{K}$)	a_w ($T = 313.15\,\text{K}$)
0.014	0.975	0.988	0.985
0.032	0.957	0.974	0.973
0.055	0.944	0.962	0.966
0.080	0.919	0.934	0.943
0.114	0.890	0.895	0.909
0.171	0.834	0.847	0.853
0.216	0.784	0.802	0.802
0.340	0.664	0.673	0.681
0.539	0.456	0.458	0.465

[a] The accuracy of the water activity measurements is specified as ±0.015 in a_w.

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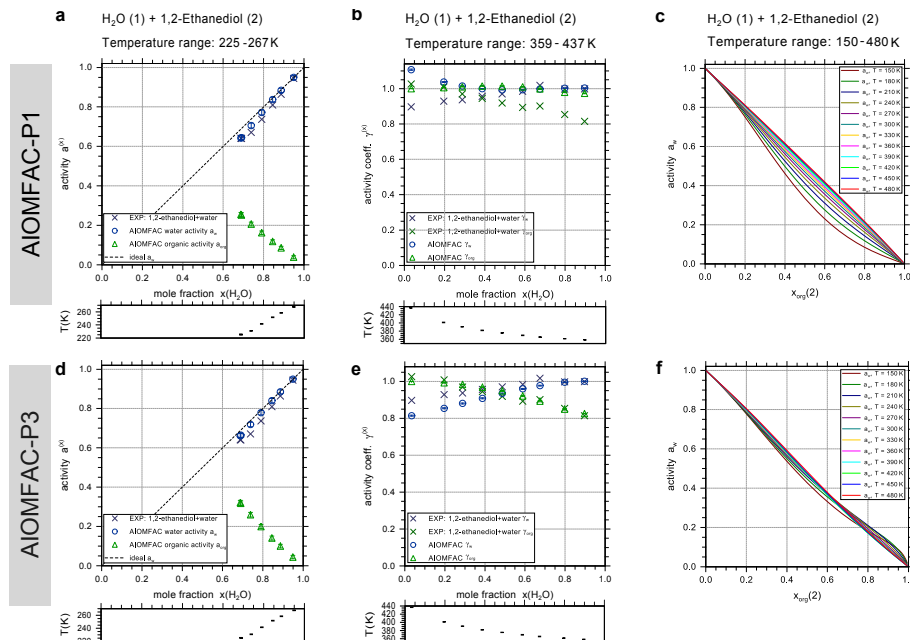Full Screen / Esc

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Table A4. Bulk water activity (a_{w}) measurements[a] of water (1) + 1,2,7,8-octantetrol (2) solutions at three different temperatures. Solution compositions are given in mole fraction of the organic component (2), x_2.

x_2	a_{w} ($T = 289.15\,\text{K}$)	a_{w} ($T = 298.15\,\text{K}$)	a_{w} ($T = 313.15\,\text{K}$)
0.0109	0.987	0.988	0.993
0.0245	0.976	0.977	0.981
0.0407	0.963	0.965	0.969
0.0650	0.944	0.946	0.953
0.0878	0.927	0.924	0.933
0.1329	0.877	0.887	0.901
0.1890	0.803	0.817	0.837
0.2911	0.605	0.643	0.667

[a] The accuracy of the water activity measurements is specified as ± 0.015 in a_{w}.

Table A5. Bulk water activity (a_w) measurements[a] of water (1) + 2,2,6,6-Tetrakis(hydroxymethyl)cyclohexanol (2) solutions at three different temperatures. Solution compositions are given in mole fraction of the organic component (2), x_2.

x_2	a_w ($T = 289.15$ K)	a_w ($T = 298.15$ K)	a_w ($T = 313.15$ K)
0.0999	0.990	0.992	0.993
0.1943	0.987	0.982	0.990
0.3029	0.973	0.974	0.979
0.3963	0.961	0.964	0.968
0.5010	0.929	0.938	0.942
0.6000	0.900	0.909	0.916
0.6519	0.881	0.887	0.895
0.7065	0.821	0.828	0.840

[a] The accuracy of the water activity measurements is specified as ±0.015 in a_w.

Table A6. Bulk water activity (a_w) measurements[a] of water (1) + vanillylmandelic acid (2) solutions at three different temperatures. Solution compositions are given in mole fraction of the organic component (2), x_2.

x_2	a_w ($T = 289.15$ K)	a_w ($T = 298.15$ K)	a_w ($T = 313.15$ K)
0.0102	0.997	0.999	0.996
0.0354	0.981	0.987	0.985
0.0844	0.963	0.965	0.965
0.1201	0.940	0.945	0.949
0.1712	0.891	0.898	0.906
0.2107	0.851	0.857	0.860

[a] The accuracy of the water activity measurements is specified as ±0.015 in a_w.

Table A7. Bulk water activity (a_w) measurements[a] of water (1) + raffinose (2) solutions at three different temperatures. Solution compositions are given in mole fraction of the organic component (2), x_2.

x_2	a_w ($T = 289.15\,\mathrm{K}$)	a_w ($T = 298.15\,\mathrm{K}$)	a_w ($T = 313.15\,\mathrm{K}$)
0.0089	0.993	0.993	0.992
0.0232	0.967	0.969	0.973
0.0364	0.938	0.944	0.948
0.0507	0.910	0.913	0.917
0.0781		0.835	

[a] The accuracy of the water activity measurements is specified as ±0.003 in a_w.

Table A8. Bulk water activity (a_w) measurements[a] of water (1) + sucrose (2) solutions at three different temperatures. Solution compositions are given in mole fraction of the organic component (2), x_2.

x_2	a_w ($T = 289.15$ K)	a_w ($T = 298.15$ K)	a_w ($T = 313.15$ K)
0.0104	0.992	0.992	0.998
0.0162	0.981	0.988	0.992
0.0230	0.977	0.977	0.985
0.0306	0.965	0.971	0.977
0.0394	0.952	0.955	0.963
0.0487	0.938	0.939	0.946
0.0606	0.906	0.914	0.922
0.0732	0.883	0.888	0.893

[a] The accuracy of the water activity measurements is specified as ±0.003 in a_w.

Figure 1. Database distribution for the water ↔ organic and organic ↔ organic interaction parameters. The table lists the total number of datasets (set count) available for each main group interaction at temperatures substantially different from the chosen reference temperature ($T_\ominus$ = 298.15 K). The total number of datasets available for each main group interaction pair are visualized by the green coloured bars. The percentile-wise colouring is used to visualize the lowest temperature (T_{low}, blue colour) and the highest temperature (T_{high}, red colour) (units of K) of the data points available for each main group interaction pair.
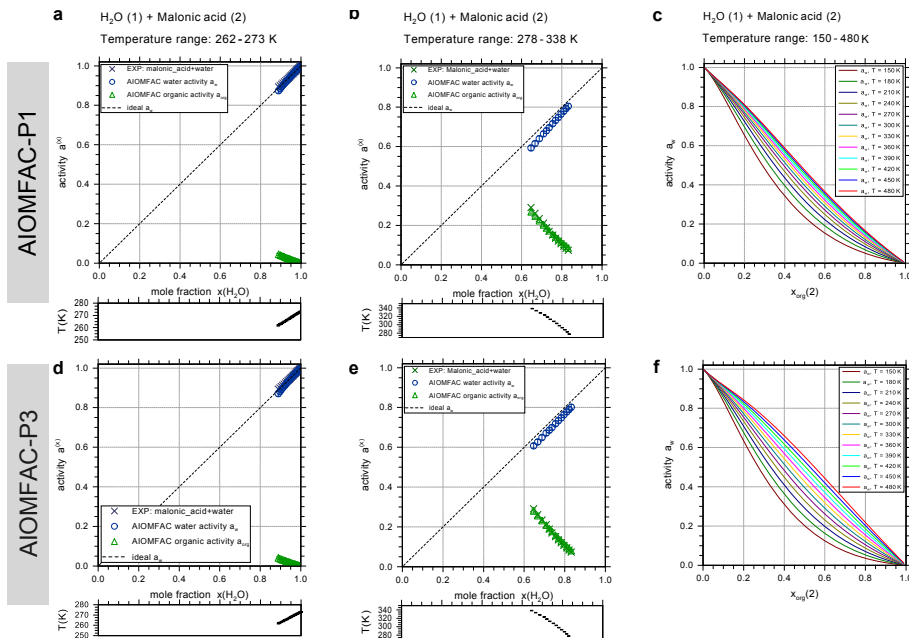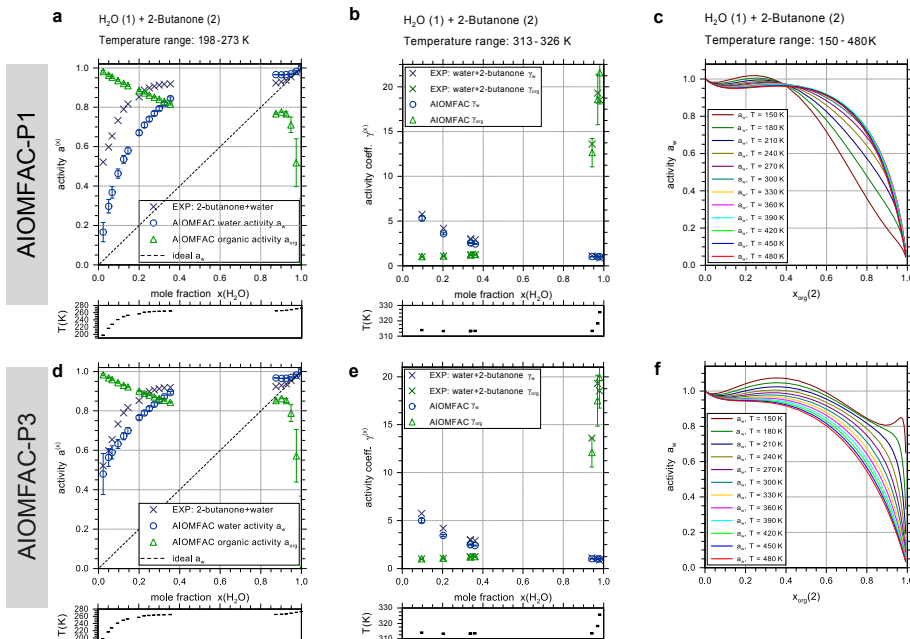
Figure 2. Measurements for water (1) + 1,2-ethanediol (2) solutions, corresponding calculations of AIOMFAC-P1 in **(a–c)** and AIOMFAC-P3 **(d–f)**. The coloured curves in **(c, f)** represents the temperature dependence of water activities predicted for the range from 150–480 K. **(a, d)** Low temperature experimental SLE data (crosses) are compared with the predictions for water activity at the same compositions and temperatures (blue circles). Predictions of the corresponding organic activities are shown as well (green triangles). The dashed line represents the hypothetical water activity of an ideal mixture. The error bars represent the model sensitivity to a composition variation by $x^{tol} = 0.01$. **(b, e)** show the model predictions of the activity coefficients compared to VLE data covering temperatures significantly higher than room temperature. The temperature of the individual data points are given in the boxes below the main panels. Experimental data: Ott et al. (1972) and Gmehling and Onken (2003a).

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Figure 3. Measurements for water (1) + acetic acid (2) solutions, corresponding calculations of AIOMFAC-P1 in and AIOMFAC-P3. The coloured curves in **(c, f)** represents the temperature dependence of water activities predicted for the range from 150–480 K. **(a, d)** Low temperature experimental SLE data (crosses) are compared with the predictions for water activity at the same compositions and temperatures (blue circles). Predictions of the corresponding organic activities are shown as well (green triangles). The dashed line represents the hypothetical water activity of an ideal mixture. The error bars represent the model sensitivity to a composition variation by $x^{tol} = 0.01$. **(b, e)** show the model predictions of the activity coefficients compared to VLE data covering temperatures significantly higher than room temperature. The temperature of the individual data points are given in the boxes below the main panels. Experimental data: Faucon (1910) and Narayana et al. (1985).
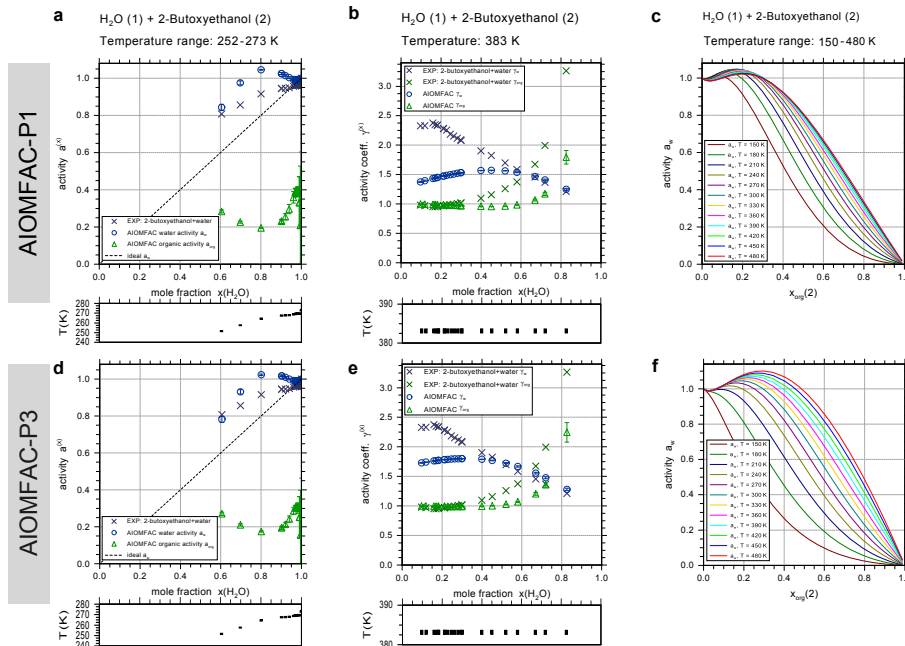
Figure 4. Measurements for water (1) + malonic acid (2) solutions, corresponding calculations of AIOMFAC-P1 in **(a–c)** and AIOMFAC-P3 in **(d–f)**. **(c, f)** show the temperature dependence of water activities predicted for the range from 150–480 K. **(a, d)** Low temperature experimental SLE data (crosses) are compared with the predictions for water activity at the same compositions and temperatures (blue circles). Predictions of the corresponding organic activities are shown as well (green triangles) while **(b, e)** show analogous data for the malonic acid melting curve. The error bars represent the model sensitivity to a composition variation by $x^{tol} = 0.01$. The dashed line represents the hypothetical water activity of an ideal mixture. The temperature of the individual data points are given in the boxes below the main panels. Experimental data: Braban et al. (2003) and Apelblat and Manzurola (1987).

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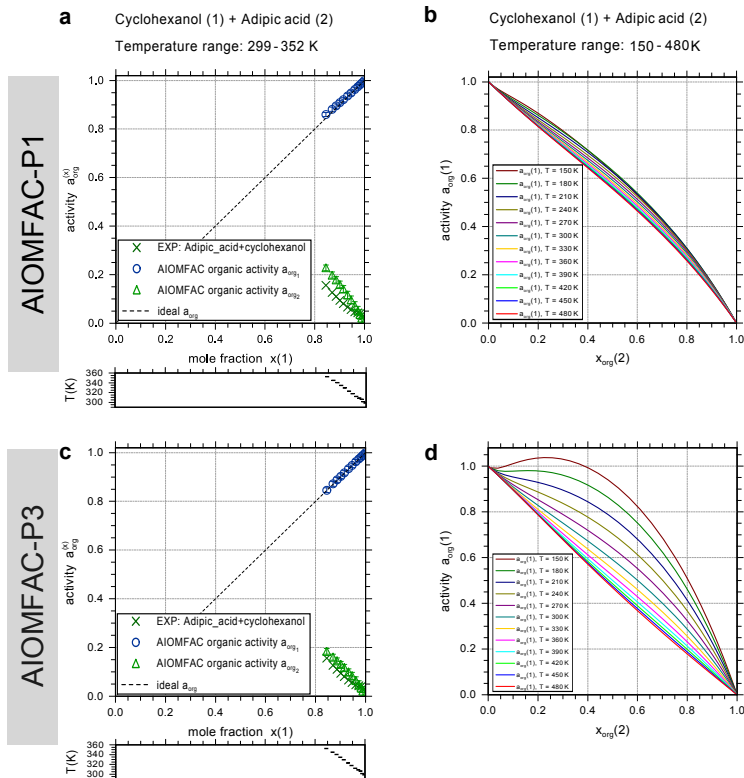Full Screen / Esc

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Figure 5. Measurements for water (1) + 2-butanone (2) solutions, corresponding calculations of AIOMFAC-P1 in **(a–c)** and AIOMFAC-P3 **(d–f)**. **(c, f)** show the temperature dependence of water activities predicted for the range from 150–480 K. **(a, d)** Low temperature experimental SLE data (crosses) are compared with the predictions for water activity at the same compositions and temperatures (blue circles). Predictions of the corresponding organic activities are shown as well (green triangles). The error bars represent the model sensitivity to a composition variation by $x^{tol} = 0.01$. The dashed line represents the hypothetical water activity of an ideal mixture. **(b, e)** show the model predictions of the activity coefficients compared to VLE data covering temperatures significantly higher than room temperature. The temperature of the individual data points are given in the boxes below the main panels. Experimental data: Lohmann et al. (1997) and Gmehling et al. (1981).

Figure 6. Measurements for 2-butoxyethanol + water solutions, corresponding calculations of AIOMFAC-P1 in **(a–c)** and AIOMFAC-P3 **(d–f)**. **(c, f)** show the temperature dependence of water activities predicted for the range from 150–480 K. **(a, d)** Low temperature experimental SLE data (crosses) are compared with the predictions for water activity at the same compositions and temperatures (blue circles). Predictions of the corresponding organic activities are shown as well (green triangles). The error bars represent the model sensitivity to a composition variation by $x^{tol} = 0.01$. The dashed line represents the hypothetical water activity of an ideal mixture. **(b, e)** show the model predictions of the activity coefficients compared to VLE data covering temperatures significantly higher than room temperature. The temperature of the individual data points are given in the boxes below the main panels. Experimental data: Koga et al. (1994) and Schneider and Wilhelm (1959).
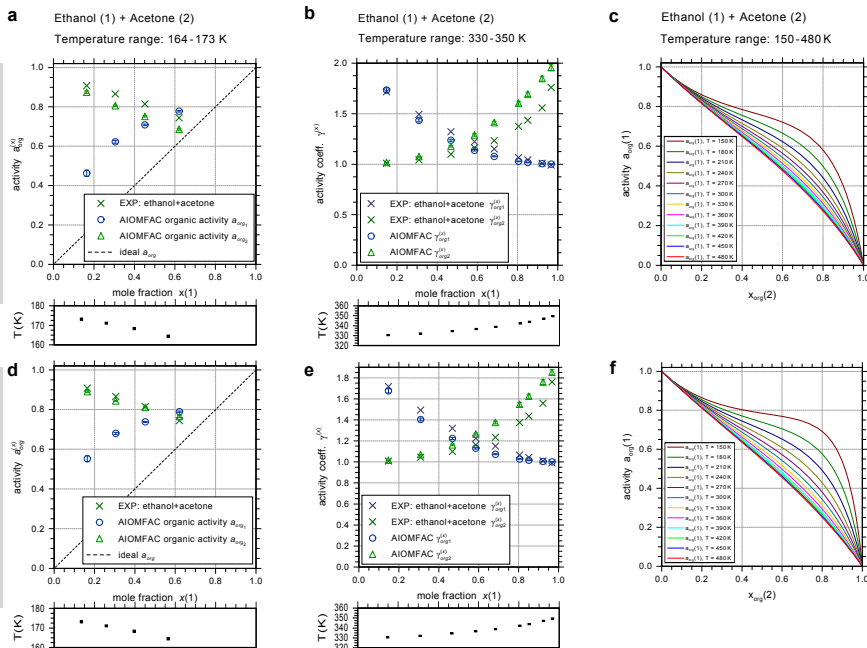
Figure 7. Measurements for cyclohexanol (1) + adipic acid (2) solutions, corresponding calculations of AIOMFAC-P1 in **(a, b)** and AIOMFAC-P3 **(c, d)**. **(b, d)** represent the temperature dependence predictions from AIOMFAC-P1 and AIOMFAC-P3 for temperature range of 150–480 K. **(a, c)** SLE of adipic acid shown vs. mole fraction of cyclohexanol (component 1). The error bars represent the model sensitivity to a composition variation by x^{tol} = 0.01. The dashed line is the ideal solution curve for component 1. The temperature of the individual data points are given in the boxes below the main panels. Experimental data: Lihua et al. (2007).

Figure 8. Measurements for ethanol (1) + acetone (2) solutions, corresponding calculations of AIOMFAC-P1 in **(a–c)** and AIOMFAC-P3 **(d, e)**. **(c, f)** show the temperature dependence as predicted by AIOMFAC-P1 and AIOMFAC-P3 for the temperature range of 150–480 K. **(a, d)** Low temperature experimental SLE data (crosses), shown as mole fraction of ethanol, $x(1)$, vs. activity ($a_{\text{org2}}^{(x)}$) of acetone. The error bars represent the model sensitivity to a composition variation by $x^{\text{tol}} = 0.01$. The dashed line is the ideal solution curve for component 1. **(b, e)** show the model predictions of the activity coefficients compared to VLE data covering temperatures significantly higher than room temperature. The temperature of the individual data points are given in the boxes below the main panels. Experimental data: Sapgir (1929) and Amer et al. (1956).
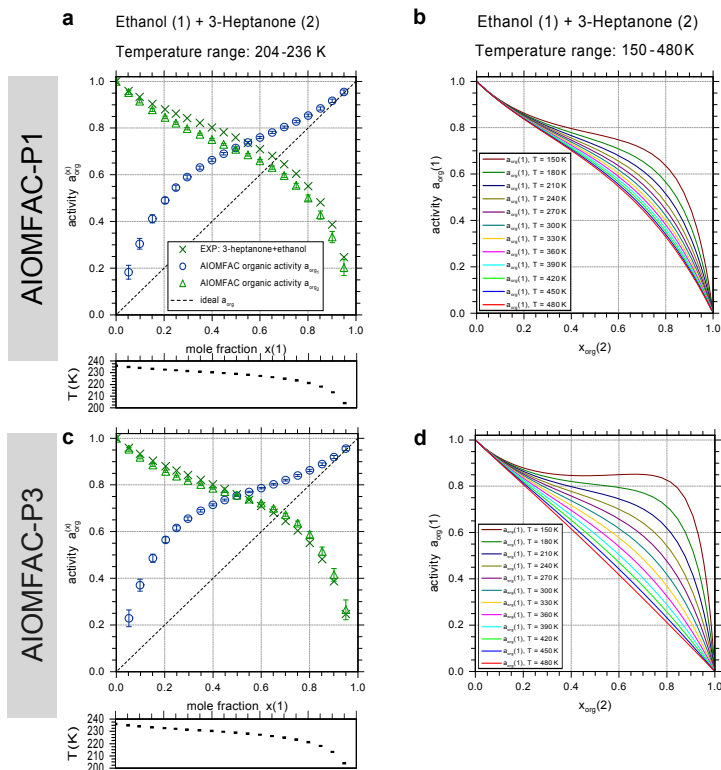
Figure 9. Measurements for ethanol (1) + 3-heptanone (2) solutions, corresponding calculations of AIOMFAC-P1 in **(a, b)** and AIOMFAC-P3 **(c, d)**. **(b, d)** shows the temperature dependence predictions from AIOMFAC-P1 and AIOMFAC-P3 for temperature range of 150–480 K. The SLE data in **(a, c)** show the composition (mole fraction of ethanol) against activity of 3-heptanone. The error bars represent the model sensitivity to a composition variation by $x^{tol} = 0.01$. The dashed line is the ideal solution curve for component 1. Experimental data: Fiege et al. (1996).
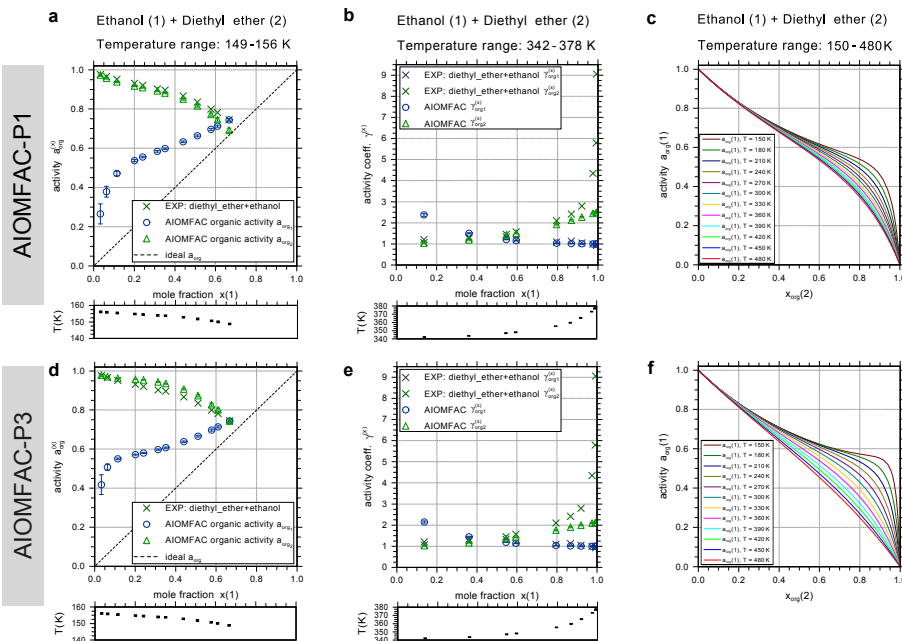
Figure 10. Measurements for ethanol (1) + diethyl ether (2) solutions, corresponding calculations of AIOMFAC-P1 and AIOMFAC-P3. **(c, f)** show the temperature dependence of the ethanol activity, as predicted by AIOMFAC-P1 and AIOMFAC-P3 for the temperature range 150–480 K. **(a, d)** Experimental SLE data (crosses) compared with model predictions (triangles) for the activity of diethyl ether in the very low temperature range 149 to 156 K. The dashed line is the ideal solution curve for component 1. **(b, e)** show the model predictions of the activity coefficients compared to VLE data covering temperatures significantly higher than room temperature. The temperature of the individual data points are given in the boxes below the main panels. The error bars represent the model sensitivity to a composition variation by $x^{tol} = 0.01$. Experimental data: Lalande (1934) and Moeller et al. (1951).

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