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

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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. To this end we introduce a new parameterisation for the temperature dependence. The improved temperature dependence parameterisation is derived from classical thermodynamic theory by describing effects from changes in molar enthalpy and heat capacity of a multi-component 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 28 % in comparison to the previous model version, when both versions are compared to our database of experimentally determined activity coefficients and related thermodynamic data. When comparing the previous and new AIOMFAC model parameterisations to the subsets of experimental data with all temperatures below 274 K or all temperatures above 322 K (i.e. outside a 25 K margin of the reference temperature of 298 K), applying the new parameterisation leads to 37 % improvement in each of the two temperature ranges considered. The new parameterisation of AIOMFAC agrees well with a large number of experimental data sets. Larger model–measurement discrepancies were found particularly for some of the systems containing multi-functional organic compounds. The affected systems were typically also poorly represented at room temperature and further improvements will be necessary to achieve better performance of AIOMFAC in these cases (assuming the experimental data are reliable). The performance of the AIOMFAC parameterisation is typically better for systems containing relatively small organic compounds and larger deviations may occur in mixtures where molecules of high structural complexity such as highly oxygenated compounds or molecules of high molecular mass (e.g. oligomers) prevail. Nevertheless, the new parameterisation enables the calculation of activity coefficients for 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 lifetime (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 (here liquid also refers to a homogeneous, yet potentially highly viscous amorphous phase), a crystalline solid, or a mixture of solid and liquid phases (when assumption of equilibrium is appropriate) 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). Furthermore, if the formation of crystalline phases is ignored intentionally in such calculations, metastable equilibria between the gas phase and supersaturated liquid solutions can be predicted. Phase equilibria calculations 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 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 multi-functional 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) re-parameterised 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 (absolute uncertainties in a_w) in case of most of the data at higher temperature and ±0.05 in a_w for all data collected 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. In addition, the new AIOMFAC parameterisation introduced in this work leads also to substantial improvements in activity coefficient calculations at temperatures significantly higher than room temperature, which is of interest for applications in other fields of science and engineering, such as distillation.

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 multi-component 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 multi-component organic + water systems. We will refer to the new AIOMFAC version, with an im-

proved temperature dependence parameterisation with two additional main group interaction terms, as AIOMFAC-P3, indicating a three-term parameterisation in the short-range (modified 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. Given the focus on organic + water systems, this work does not address the temperature dependence of interaction terms related to inorganic electrolyte/ionic components included in AIOMFAC. A few organic functional groups that have been considered explicitly in the AIOMFAC model development in the past are not included in this work. The excluded organic functionalities are the following: hydroperoxide, peroxy acid peroxide, peroxyacyl nitrate, and organonitrate, all introduced in the AIOMFAC model by Zuend and Seinfeld (2012) based on work by Compernolle et al. (2009). Note that these functional groups are available in AIOMFAC, but on the basis of the AIOMFAC-P1 model parameterisation only.

The thermodynamic group-contribution model AIOMFAC allows thermodynamically consistent calculations of activity coefficients at temperatures close to 298 K and covers multi-component 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. An estimate for the appropriate temperature range of AIOMFAC, when in addition to organic compounds and water also dissolved inorganic ions are included, is 298 ± 10 K. However, due to a rather weak temperature dependence of activity coefficients in aqueous electrolyte solutions, for many mixtures, the AIOMFAC model may also be applicable in a wider temperature range to good approximation (also relative to other uncertainties associated with a group-contribution model prediction). 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 characterised 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):

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

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 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, based on the approach and UNIFAC parameters determined by Compernolle et al. (2009), Zuend and Seinfeld (2012) introduced in AIOMFAC the functional groups hydroperoxide, peroxy acid, 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).

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

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

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

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

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

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

In these equations, x_j is the mole fraction of component j, and $\nu_t^{(j)}$ 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 the following:

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

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. $\nu_t^{(j)}$ is the number of subgroups of type t in molecule j. The residual activity coefficient of subgroup t is as follows:

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

where

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

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).

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

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) data sets. 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):

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

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 equilibria 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 Δg°, change in molar enthalpy Δh° and change in molar heat capacity Δc_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):

$$R \ln K_p = -\frac{\Delta g_{T_\ominus}^\circ}{T_\ominus} + \Delta h_{T_\ominus}^\circ \left[\frac{1}{T_\ominus} - \frac{1}{T}\right] + \Delta c_{p,T_\ominus}^\circ \left[\frac{T_\ominus}{T} - 1 + \ln\frac{T}{T_\ominus}\right], \tag{15}$$

where $T_\ominus$ is a reference temperature at which the changes in Δg°, Δh° and Δc_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 $T_\ominus = 298.15\,\text{K}$. 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 $\Delta g_{T_\ominus}^\circ$ as well as a part of the changes related to $\Delta h_{T_\ominus}^\circ$ (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 simultaneously the AIOMFAC

group interaction parameters $b_{n,m}$ and $c_{n,m}$ for pertaining organic functional 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 the goal to describe a wide variety of organic compounds at relevant atmospheric temperatures, we focus on the aqueous systems of oxidised 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$_n$CO), aldehyde (CHO), ether (CH$_n$O), ester (CCOO), alkenyl (C=C), aromatic carbon (ACH$_n$), aromatic carbon-alcohol (ACOH) (a phenol group), and water (H$_2$O). 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 neighbouring 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 multi-functional 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$_2$O 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., http://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 data sets at temperatures substantially different from 298 K available for each main group pair interaction. The green bars indicate the maximum number of overall data sets including all data types 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 data points are available, is indicated. In addition, listed are the median and arithmetic mean values of the assigned initial data set weighting values (w_d^{init}) pertaining to each main group interaction pair. The combination of these values serves as an approximate measure of the data quality. A higher median value (median(w_d^{init}) $\geq\sim$ 1), paired with a large number of data sets and a wide temperature range covered, indicates the availability of reliable thermodynamic equilibrium data for the model parameterisation. For certain group interactions, the data coverage and reliability is clearly lacking, which was considered in the model parameterisation.

The database overall consists of 677 data sets covering different data types, for monofunctional and multi-functional organic molecules in aqueous and water-free mixtures of binary and ternary systems. Table 1 lists the data sets 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

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" data sets used (where $w_d^{init} > 0$) for the short-range parameterisation of organic main group $\leftrightarrow$ water and organic $\leftrightarrow$ 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	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})(CH_2^{[OH]})(OH)$	263–270	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	$(CH_3^{[alc]})(CH_2^{[alc-tail]})(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$	215–259	SLE	10	5.00	Lohmann et al. (1997)
2-butanol	$CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_2^{[alc-tail]})(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$	240–273	SLE	2	5.00	Lohmann et al. (1997)
2-butanol	$CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})(CH_2^{[alc-tail]})(CH_2^{[alc-tail]})(CH^{[OH]})(OH)$	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)
tert-butanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, OH	$(CH_3^{[alc]})_3(C^{[OH]})(OH)$	331–339	VLE	15	1.00	Gmehling and Onken (1977)
tert-butanol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, 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)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
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)
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-ethanediol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, 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)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
1,5-pentanediol	$CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH	$(CH_2^{[alc-tail]})_3(CH_2^{[OH]})_2$ $(OH)_2$	298	a_w (bulk)	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
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-octanetetrol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, 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-octanetetrol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, 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-octanetetrol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, 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-octanetetrol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, 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-octanetetrol	$CH_n^{[alc]}$, $CH_n^{[OH]}$, 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)
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)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
oxalic acid	COOH	$(\text{COOH})_2$	272–273	SLE	4	5.00	Braban et al. (2003)
oxalic acid	COOH	$(\text{COOH})_2$	277–308	SLE(org)[d]	11	0.00	Braban et al. (2003)
oxalic acid	COOH	$(\text{COOH})_2$	278–338	SLE(org)[d]	13	0.00	Apelblat and Manzurola (1987)
oxalic acid	COOH	$(\text{COOH})_2$	298	a_w	14	0.00	Peng et al. (2001)
oxalic acid	COOH	$(\text{COOH})_2$	284–352	SLE(org)[d]	8	0.00	Omar and Ulrich (2006)
malic acid	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH	$(\text{CH}_2)(\text{CH}^{[\text{OH}]})(\text{COOH})_2\,(\text{OH})$	278–338	SLE(org)[d]	13	0.2	Apelblat and Manzurola (1987)
malic acid	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH	$(\text{CH}_2)(\text{CH}^{[\text{OH}]})(\text{COOH})_2\,(\text{OH})$	262–273	SLE	16	2.00	Beyer et al. (2008)
malic acid	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH	$(\text{CH}_2)(\text{CH}^{[\text{OH}]})(\text{COOH})_2\,(\text{OH})$	298	a_w	6	0.00	Maffia and Meirelles (2001)
malonic acid	CH$_n$, COOH	$(\text{CH}_2)(\text{COOH})_2$	262–273	SLE	22	5.00	Braban et al. (2003)
malonic acid	CH$_n$, COOH	$(\text{CH}_2)(\text{COOH})_2$	278–338	SLE(org)[d]	13	0.2	Apelblat and Manzurola (1987)
malonic acid	CH$_n$, COOH	$(\text{CH}_2)(\text{COOH})_2$	298	a_w	6	0.00	Peng et al. (2001)
malonic acid	CH$_n$, COOH	$(\text{CH}_2)(\text{COOH})_2$	298	a_w	6	0.00	Maffia and Meirelles (2001)
malonic acid	CH$_n$, COOH	$(\text{CH}_2)(\text{COOH})_2$	298	a_w	7	0.00	Peng et al. (2001)
succinic acid	CH$_n$, COOH	$(\text{CH}_2)_2(\text{COOH})_2$	273	SLE	9	5.00	Beyer et al. (2008)
succinic acid	CH$_n$, COOH	$(\text{CH}_2)_2(\text{COOH})_2$	296–447	SLE(org)[d]	10	0.20	Lin et al. (2007)
succinic acid	CH$_n$, COOH	$(\text{CH}_2)_2(\text{COOH})_2$	278–338	SLE(org)[d]	13	0.20	Apelblat and Manzurola (1987)
succinic acid	CH$_n$, COOH	$(\text{CH}_2)_2(\text{COOH})_2$	298	a_w	5	0.00	Maffia and Meirelles (2001)
succinic acid	CH$_n$, COOH	$(\text{CH}_2)_2(\text{COOH})_2$	298	a_w	9	0.00	Peng et al. (2001)
glutaric acid	CH$_n$, COOH	$(\text{CH}_2)_3(\text{COOH})_2$	271–273	SLE	5	5.00	Beyer et al. (2008)
glutaric acid	CH$_n$, COOH	$(\text{CH}_2)_3(\text{COOH})_2$	279–336	SLE(org)[d]	24	0.10	Apelblat and Manzurola (1989)
glutaric acid	CH$_n$, COOH	$(\text{CH}_2)_3(\text{COOH})_2$	277–298	SLE(org)[d]	23	0.10	Beyer et al. (2008)
glutaric acid	CH$_n$, COOH	$(\text{CH}_2)_3(\text{COOH})_2$	298	a_w	34	0.00	Peng et al. (2001)
glutaric acid	CH$_n$, COOH	$(\text{CH}_2)_3(\text{COOH})_2$	291	a_w	57	0.00	Zardini et al. (2008)
citric acid	CH$_n$, C$^{[\text{OH}]}$, COOH, OH	$(\text{CH}_2)_2(\text{C}^{[\text{OH}]})(\text{COOH})_3\,(\text{OH})$	278–338	SLE(org)[d]	13	0.0	Apelblat and Manzurola (1987)
citric acid	CH$_n$, C$^{[\text{OH}]}$, COOH, OH	$(\text{CH}_2)_2(\text{C}^{[\text{OH}]})(\text{COOH})_3\,(\text{OH})$	291	a_w	90	0.00	Zardini et al. (2008)
citric acid	CH$_n$, C$^{[\text{OH}]}$, COOH, OH	$(\text{CH}_2)_2(\text{C}^{[\text{OH}]})(\text{COOH})_3(\text{OH})$	298	a_w	25	0.00	Peng et al. (2001)
adipic acid	CH$_n$, COOH	$(\text{CH}_2)_4(\text{COOH})_2$	278–338	SLE(org)[d]	13	0.20	Apelblat and Manzurola (1987)
pimelic acid	CH$_n$, COOH	$(\text{CH}_2)_5(\text{COOH})_2$	279–342	SLE(org)[d]	21	0.20	Apelblat and Manzurola (1989)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	191–230	$a_\text{w}(T_\text{hom})$[a]	6	1.00	Zobrist et al. (2008)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	255–271	SLE	6	5.00	Zobrist et al. (2008)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	233	$a_\text{w}(\text{EDB})$[f]	3	0.20	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	236	$a_\text{w}(\text{EDB})$[f]	2	0.20	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	244	$a_\text{w}(\text{EDB})$[f]	6	0.50	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	253	$a_\text{w}(\text{EDB})$[f]	3	0.50	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	253	$a_\text{w}(p^\text{tot})$	5	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	255	$a_\text{w}(p^\text{tot})$	3	0.50	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	258	$a_\text{w}(p^\text{tot})$	3	0.50	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	260	$a_\text{w}(p^\text{tot})$	4	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	263	$a_\text{w}(\text{EDB})$[f]	2	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	263	$a_\text{w}(\text{EDB})$[f]	5	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	265	$a_\text{w}(p^\text{tot})$	3	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	268	$a_\text{w}(p^\text{tot})$	3	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	268	$a_\text{w}(\text{EDB})$[f]	8	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	270	$a_\text{w}(p^\text{tot})$	3	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	273	$a_\text{w}(p^\text{tot})$	3	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	273	$a_\text{w}(\text{EDB})$[f]	10	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	275	$a_\text{w}(p^\text{tot})$	3	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	278	$a_\text{w}(p^\text{tot})$	5	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	279	a_w (bulk)	9	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	280	$a_\text{w}(p^\text{tot})$	5	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	283	$a_\text{w}(p^\text{tot})$	5	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	285	$a_\text{w}(p^\text{tot})$	5	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	288	$a_\text{w}(p^\text{tot})$	5	1.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	289	$a_\text{w}(\text{EDB})$[f]	10	0.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	289	a_w (bulk)	10	0.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	290	$a_\text{w}(p^\text{tot})$	5	0.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	298	a_w (bulk)	10	0.00	Ganbavale et al. (2014)
M5[b]	CH$_n$, CH$_n^{[\text{OH}]}$, COOH, OH, C=C	c	313	a_w (bulk)	10	0.00	Ganbavale et al. (2014)

– water + ketone systems –

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
acetone	CH$_n$, CH$_n$CO	$(\text{CH}_3)(\text{CH}_3\text{CO})$	221–273	SLE	17	5.00	Jakob (1994)
acetone	CH$_n$, CH$_n$CO	$(\text{CH}_3)(\text{CH}_3\text{CO})$	298	VLE	13	0.00	Gmehling et al. (1988)
acetone	CH$_n$, CH$_n$CO	$(\text{CH}_3)(\text{CH}_3\text{CO})$	308	VLE	13	1.00	Gmehling et al. (1988)
acetone	CH$_n$, CH$_n$CO	$(\text{CH}_3)(\text{CH}_3\text{CO})$	318	VLE	13	1.00	Gmehling et al. (1988)
acetone	CH$_n$, CH$_n$CO	$(\text{CH}_3)(\text{CH}_3\text{CO})$	323	VLE	13	1.00	Gmehling et al. (1988)
acetone	CH$_n$, CH$_n$CO	$(\text{CH}_3)(\text{CH}_3\text{CO})$	328	VLE	13	1.00	Gmehling et al. (1988)
acetone	CH$_n$, CH$_n$CO	$(\text{CH}_3)(\text{CH}_3\text{CO})$	373	VLE	20	1.00	Griswold and Wong (1952)
acetone	CH$_n$, CH$_n$CO	$(\text{CH}_3)(\text{CH}_3\text{CO})$	295–321	VLE	10	1.00	Othmer and Benenati (1945)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
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	0.00	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	$(CH_3)(CH_2)(CH_n^{[OH]})(CH_2O)(OH)$	343	VLE	20	0.50	Chiavone-Filho et al. (1993)
2-ethoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)(CH_n^{[OH]})(CH_2O)(OH)$	363	VLE	18	0.50	Chiavone-Filho et al. (1993)
2-ethoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)(CH_n^{[OH]})(CH_2O)(OH)$	373–407	VLE	34	0.50	Hirata and Hoshino (1982)
2-ethoxyethanol	CH_n, $CH_n^{[OH]}$, CH_nO, OH	$(CH_3)(CH_2)(CH_n^{[OH]})(CH_2O)(OH)$	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)
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)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
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)
tert-butyl acetate	CH_n, CCOO	$(CH_3)_3 (C) (CH_3COO)$	273–354	solubil.	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	0.00	this work
raffinose	CH_n, $CH_n^{[OH]}$, OH, CHO[ether]	$(C)(CH)(CH_2^{[OH]})_3(CH^{[OH]})_8$ $(CH_2O)(CHO[ether])_4(OH)_{11}$	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)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
levoglucosan	CH_n, $CH_n^{[OH]}$, OH, CHO[ether]	$(CH)(CH^{[OH]})_3(CH_2O)$ (CHO[ether]) $(OH)_3$	187–230	$a_w(T_{\text{hom}})^a$	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	$CH_2^{[OH]}$, OH, COOH	$(CH_2^{[OH]})(OH)(COOH)$	206–230	$a_w(T_{\text{hom}})^a$	4	1.00	Ganbavale et al. (2014)
glycolic acid	$CH_2^{[OH]}$, OH, COOH	$(CH_2^{[OH]})(OH)(COOH)$	259–271	SLE	4	5.00	Ganbavale et al. (2014)
glycolic acid	$CH_2^{[OH]}$, 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	$a_w(T_{\text{hom}})^a$	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)
2-methoxyacetic acid	CH_n, COOH, CH_nO	$(CH_2)(CH_3O)(COOH)$	194–232	$a_w(T_{\text{hom}})^a$	5	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH_n, COOH, CH_nO	$(CH_2)(CH_3O)(COOH)$	251–271	SLE	3	2.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH_n, COOH, CH_nO	$(CH_2)(CH_3O)(COOH)$	268	$a_w(p^{\text{tot}})$	4	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH_n, COOH, CH_nO	$(CH_2)(CH_3O)(COOH)$	270	$a_w(p^{\text{tot}})$	4	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH_n, COOH, CH_nO	$(CH_2)(CH_3O)(COOH)$	273	$a_w(p^{\text{tot}})$	4	0.50	Ganbavale et al. (2014)
2-methoxyacetic acid	CH_n, COOH, CH_nO	$(CH_2)(CH_3O)(COOH)$	275	$a_w(p^{\text{tot}})$	5	0.50	Ganbavale et al. (2014)
2-methoxyacetic acid	CH_n, COOH, CH_nO	$(CH_2)(CH_3O)(COOH)$	278	$a_w(p^{\text{tot}})$	10	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH_n, COOH, CH_nO	$(CH_2)(CH_3O)(COOH)$	279	a_w (bulk)	10	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH_n, COOH, CH_nO	$(CH_2)(CH_3O)(COOH)$	280	$a_w(p^{\text{tot}})$	10	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH_n, COOH, CH_nO	$(CH_2)(CH_3O)(COOH)$	283	$a_w(p^{\text{tot}})$	10	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH_n, COOH, CH_nO	$(CH_2)(CH_3O)(COOH)$	285	$a_w(p^{\text{tot}})$	10	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH_n, COOH, CH_nO	$(CH_2)(CH_3O)(COOH)$	288	$a_w(p^{\text{tot}})$	10	1.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH_n, COOH, CH_nO	$(CH_2)(CH_3O)(COOH)$	289	a_w (bulk)	10	0.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH_n, COOH, CH_nO	$(CH_2)(CH_3O)(COOH)$	290	a_w (bulk)	10	0.00	Ganbavale et al. (2014)
2-methoxyacetic acid	CH_n, COOH, CH_nO	$(CH_2)(CH_3O)(COOH)$	298	a_w (bulk)	9	0.00	Ganbavale et al. (2014)
2-ethoxyethyl acetate	CH_n, CH_nO, CCOO	$(CH_3)(CH_2)(CH_2O)_2$ (CH_3COO)	208–233	$a_w(T_{\text{hom}})^a$	3	1.00	Ganbavale et al. (2014)
2-ethoxyethyl acetate	CH_n, CH_nO, CCOO	$(CH_3)(CH_2)(CH_2O)_2$ (CH_3COO)	271–272	SLE	3	2.00	Ganbavale et al. (2014)
2-ethoxyethyl acetate	CH_n, CH_nO, CCOO	$(CH_3)(CH_2)(CH_2O)_2$ (CH_3COO)	276–368	solubli.	12	1.00	Carvoli and Delogu (1986)
resorcinol	ACH_n, ACOH	$(ACH)_4$ $(ACOH)_2$	223–232	$a_w(T_{\text{hom}})^a$	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_nO, OH	$(CH_3)(CH_2)_2(CH_2O)_2$ (OH)	211–233	$a_w(T_{\text{hom}})^a$	3	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH_n, CH_nO, OH	$(CH_3)(CH_2)_2(CH_2O)_2$ (OH)	260–272	SLE	4	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH_n, CH_nO, OH	$(CH_3)(CH_2)_2(CH_2O)_2$ (OH)	265	$a_w(p^{\text{tot}})$	5	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH_n, CH_nO, OH	$(CH_3)(CH_2)_2(CH_2O)_2$ (OH)	268	$a_w(p^{\text{tot}})$	5	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH_n, CH_nO, OH	$(CH_3)(CH_2)_2(CH_2O)_2$ (OH)	270	$a_w(p^{\text{tot}})$	5	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH_n, CH_nO, OH	$(CH_3)(CH_2)_2(CH_2O)_2$ (OH)	273	$a_w(p^{\text{tot}})$	5	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH_n, CH_nO, OH	$(CH_3)(CH_2)_2(CH_2O)_2$ (OH)	275	$a_w(p^{\text{tot}})$	6	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH_n, CH_nO, OH	$(CH_3)(CH_2)_2(CH_2O)_2$ (OH)	278	$a_w(p^{\text{tot}})$	9	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH_n, CH_nO, OH	$(CH_3)(CH_2)_2(CH_2O)_2$ (OH)	279	a_w (bulk)	12	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH_n, CH_nO, OH	$(CH_3)(CH_2)_2(CH_2O)_2$ (OH)	280	$a_w(p^{\text{tot}})$	9	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH_n, CH_nO, OH	$(CH_3)(CH_2)_2(CH_2O)_2$ (OH)	283	$a_w(p^{\text{tot}})$	9	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH_n, CH_nO, OH	$(CH_3)(CH_2)_2(CH_2O)_2$ (OH)	285	$a_w(p^{\text{tot}})$	9	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH_n, CH_nO, OH	$(CH_3)(CH_2)_2(CH_2O)_2$ (OH)	288	$a_w(p^{\text{tot}})$	9	0.10	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH_n, CH_nO, OH	$(CH_3)(CH_2)_2(CH_2O)_2$ (OH)	289	a_w (bulk)	12	0.00	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH_n, CH_nO, OH	$(CH_3)(CH_2)_2(CH_2O)_2$ (OH)	290	a_w (bulk)	9	0.00	Ganbavale et al. (2014)
2-(2-ethoxyethoxy)ethanol	CH_n, CH_nO, OH	$(CH_3)(CH_2)_2(CH_2O)_2$ (OH)	298	a_w (bulk)	12	0.00	Ganbavale et al. (2014)
vanillylmandelic acid	ACH_n, ACOH, $CH_n^{[OH]}$, COOH, CH_nO, OH	$(ACH)_3(AC)_2(ACOH)(CH_3O)$ $(CH^{[OH]})(OH)(COOH)$	214–232	$a_w(T_{\text{hom}})^a$	4	1.00	Zobrist et al. (2008)
vanillylmandelic acid	ACH_n, ACOH, $CH_n^{[OH]}$, COOH, CH_nO, OH	$(ACH)_3(AC)_2(ACOH)(CH_3O)$ $(CH^{[OH]})(OH)(COOH)$	267–272	SLE	4	5.00	Zobrist et al. (2008)
vanillylmandelic acid	ACH_n, ACOH, $CH_n^{[OH]}$, COOH, CH_nO, OH	$(ACH)_3(AC)_2(ACOH)(CH_3O)$ $(CH^{[OH]})(OH)(COOH)$	289	a_w (bulk)	6	0.00	this work
vanillylmandelic acid	ACH_n, ACOH, $CH_n^{[OH]}$, COOH, CH_nO, OH	$(ACH)_3(AC)_2(ACOH)(CH_3O)$ $(CH^{[OH]})(OH)(COOH)$	298	a_w (bulk)	6	0.00	this work
vanillylmandelic acid	ACH_n, ACOH, $CH_n^{[OH]}$, COOH, CH_nO, OH	$(ACH)_3(AC)_2(ACOH)(CH_3O)$ $(CH^{[OH]})(OH)(COOH)$	313	a_w (bulk)	6	1.00	this work

– water + alcohol + alcohol systems –

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	$(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})_2$ $(CH_2^{[OH]})(OH)$, $(CH_3^{[alc-tail]})(CH_2^{[alc-tail]})$ $(CH_2^{[OH]})(OH)$	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)
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)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
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	$(CH_3^{[alc]})(CH_3^{[alc-tail]})$ $(CH^{[alc-tail]})(CH^{[OH]})(OH)$, $(CH_3)(COOH)$	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	$(CH_3^{[alc]})(CH_3^{[alc-tail]})$ $(CH^{[alc-tail]})(CH^{[OH]})(OH)$, $(CH_3)(COOH)$	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, $CH_3^{[alc]}$, $CH_n^{[alc-tail]}$, $CH_n^{[OH]}$, OH, COOH	$(CH_3^{[alc]})(CH_3^{[alc-tail]})$ $(CH^{[alc-tail]})(CH^{[OH]})(OH)$, $(CH_2)_2(C^{[OH]})(COOH)_3(OH)$	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)
– water + alcohol + ketone systems –							
tert-butanol, 4-methyl-2-pentanone	CH_n, $CH_n^{[alc]}$, $CH_n^{[OH]}$, OH, CH_nCO	$(CH_3^{[alc]})_3(C^{[OH]})(OH)$, $(CH_3)_2(CH_2)(CH)(CH_3CO)$	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	$(CH_3^{[alc]})_3(C^{[OH]})(OH)$, $(CH_3)_2(CH_2)(CH)(CH_3CO)$	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	$(CH_3^{[alc]})_3(C^{[OH]})(OH)$, $(CH_3)_2(CH_2)(CH)(CH_3CO)$	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	$(CH_3^{[alc]})_3(C^{[OH]})(OH)$, $(CH_3)_2(CH_2)(CH)(CH_3CO)$	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)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
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)
– 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)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
– 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)
– 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)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
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)
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)
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	$CH_nCH_n^{[alc-tail]}$, $CH_n^{[OH]}$, 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)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)	T (K)	Data type	N_d	w_d^{init}	Reference
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_nCO	$(CH_3)(COOH)$, $(CH_3)(CH_3CO)$	173	SLE(org)[d]	1	0.20	Chesnokov (1969)
acetic acid, acetone	CH_n, COOH, CH_nCO	$(CH_3)(COOH)$, $(CH_3)(CH_3CO)$	244–284	SLE(org)[d]	8	0.20	Carta and Dernini (1983)
acetic acid, acetone	CH_n, COOH, CH_nCO	$(CH_3)(COOH)$, $(CH_3)(CH_3CO)$	245–283	SLE(org)[d]	5	0.20	Carta and Dernini (1983)
acetic acid, acetone	CH_n, COOH, CH_nCO	$(CH_3)(COOH)$, $(CH_3)(CH_3CO)$	332–383	VLE	10	1.00	Othmer (1943)
acetic acid, acetone	CH_n, COOH, CH_nCO	$(CH_3)(COOH)$, $(CH_3)(CH_3CO)$	308	VLE	12	0.10	Waradzin and Surovy (1975)
acetic acid, acetone	CH_n, COOH, CH_nCO	$(CH_3)(COOH)$, $(CH_3)(CH_3CO)$	318	VLE	11	0.10	Waradzin and Surovy (1975)
acetic acid, acetone	CH_n, COOH, CH_nCO	$(CH_3)(COOH)$, $(CH_3)(CH_3CO)$	328	VLE	11	0.10	Waradzin and Surovy (1975)
acetic acid, 2-butanone	CH_n, COOH, CH_nCO	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3CO)$	242–290	SLE(org)[d]	12	0.20	Dallos et al. (1986)
acetic acid, 2-butanone	CH_n, COOH, CH_nCO	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3CO)$	353–391	VLE	40	1.00	Fu et al. (1986)
acetic acid, 2-butanone	CH_n, COOH, CH_nCO	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3CO)$	353–388	VLE	22	0.00	Xie et al. (2009)
acetic acid, 2-butanone	CH_n, COOH, CH_nCO	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3CO)$	303	VLE	12	0.00	Dallos et al. (1986)
acetic acid, 2-butanone	CH_n, COOH, CH_nCO	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3CO)$	323	VLE	14	1.00	Dallos et al. (1986)
acetic acid, 2-butanone	CH_n, COOH, CH_nCO	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3CO)$	351	VLE	9	1.00	Dallos et al. (1986)
butanoic acid, acetone	CH_n, COOH, CH_nCO	$(CH_3)(CH_2)_2(COOH)$, $(CH_3)(CH_3CO)$	240–268	SLE(org)[d]	12	0.20	Proust and Fernandez (1986)
butanoic acid, 2-butanone	CH_n, COOH, CH_nCO	$(CH_3)(CH_2)_2(COOH)$, $(CH_3)(CH_2)(CH_3CO)$	240–268	SLE(org)[d]	12	0.20	Proust and Fernandez (1986)
butanoic acid, 2-butanone	CH_n, COOH, CH_nCO	$(CH_3)(CH_2)_2(COOH)$, $(CH_3)(CH_2)(CH_3CO)$	343	VLE	9	1.00	Rasmussen and Fredenslund (1977)
butanoic acid, 2-butanone	CH_n, COOH, CH_nCO	$(CH_3)(CH_2)_2(COOH)$, $(CH_3)(CH_2)(CH_3CO)$	353	VLE	10	1.00	Rasmussen and Fredenslund (1977)
acetic acid, diethyl ether	CH_n, COOH, CH_nO	$(CH_3)(COOH)$, $(CH_3)_2(CH_2)CH_2O$	207–289	SLE(org)[d]	40	0.20	Pickering (1893)
acetic acid, diethyl ether	CH_n, COOH, CH_nO	$(CH_3)(COOH)$, $(CH_3)_2(CH_2)CH_2O$	293–343	VLE	7	1.00	Meehan and Murphy (1965)
acetic acid, diethyl ether	CH_n, COOH, CH_nO	$(CH_3)(COOH)$, $(CH_3)_2(CH_2)CH_2O$	299–351	VLE	7	1.00	Meehan and Murphy (1965)
acetic acid, diethyl ether	CH_n, COOH, CH_nO	$(CH_3)(COOH)$, $(CH_3)_2(CH_2)CH_2O$	304–360	VLE	7	1.00	Meehan and Murphy (1965)
acetic acid, ethyl acetate	CH_n, COOH, CCOO	$(CH_3)(COOH)$, $(CH_3)(CH_2)(CH_3COO)$	323	VLE	9	1.00	Miyamoto et al. (2001)
hexadecanoic acid (palmitic acid), ethyl acetate	CH_n, COOH, CCOO	$(CH_3)(CH_2)_{14}(COOH)$, $(CH_3)(CH_2)(CH_3COO)$	243–273	SLE(org)[d]	4	0.20	Kolb (1959)
octadecanoic acid (stearic acid), ethyl acetate	CH_n, COOH, CCOO	$(CH_3)(CH_2)_{16}(COOH)$, $(CH_3)(CH_2)(CH_3COO)$	253–283	SLE(org)[d]	4	0.20	Kolb (1959)
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)

Table 1. Continued.

Organic compounds	Org. main groups	Chemical formula (subgroups)		T (K)	Data type	N_d	w_d^{init}	Reference
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	$(CH_3)_2(CH_2)CH_2O$, $(ACH)_6$		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	$(CH_3)(CH_2)(CH^{[OH]})(CH_3O)$ (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)
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 the following: 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 as follows: $(CH=CH)(COOH)_2$.
[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).

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 data sets 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, $a_w^{\mathrm{SLE}}(T, p)$, is given by (Koop et al., 2000):

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

where $\mu_w^{\mathrm{S}}(T)$ and $\mu_w^{\circ,\mathrm{L}}(T)$ 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.

$$\mu_w^{\mathrm{S}}(T) - \mu_w^{\circ,\mathrm{L}}(T) = 210\,368 + 131.438\,T \tag{18}$$
$$- 3.32\,373 \times 10^6\,T^{-1} - 41\,729.1\ln(T).$$

The parameterisation in Eq. (18) represents the thermodynamically consistent function for use with Eq. (17) valid at low (ambient) pressure in the temperature range $150 < T < 273$ 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; Dománska et al., 2009):

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

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

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. $i \downarrow$	$j \rightarrow$ 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^b	2.0000×10^2	1.2481×10^3	1.3330×10^3	-4.7640×10^2	2.0000×10^2	-2.0762×10^1
		$c(i,j)$:	0.0	0.0^b	3.0257×10^{-1}	5.2720×10^0	3.1475×10^0	1.9056×10^0	4.2165×10^{-1}	9.2840×10^{-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
		$b(i,j)$:	1.9504×10^1	0.0^b	0.0	9.0380×10^2	-1.3290×10^3	-1.8718×10^2	-3.4730×10^2	0.0^b
		$c(i,j)$:	8.0000×10^{-1}	0.0^b	0.0	2.3228×10^0	-5.3160×10^0	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
		$b(i,j)$:	2.07691×10^0	0.0^b	-3.6230×10^2	0.0	2.6456×10^2	4.5845×10^1	-2.9366×10^1	-1.3512×10^1
		$c(i,j)$:	-1.2000×10^0	0.0^b	1.2682×10^0	0.0	-1.2980×10^0	-8.0000×10^{-1}	0.0^b	-8.0000×10^{-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	2.0000×10^2	9.8265×10^1	0.0	3.5610×10^2	0.0^b	3.5689×10^2
		$c(i,j)$:	9.7679×10^{-1}	0.0^b	-4.9742×10^{-1}	-2.0012×10^{-1}	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
		$b(i,j)$:	-5.0597×10^1	0.0^b	-1.8962×10^1	1.1460×10^2	2.0000×10^2	0.0	0.0^b	2.1370×10^2
		$c(i,j)$:	-8.0000×10^{-1}	0.0^b	0.0^b	-1.8900×10^0	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
		$b(i,j)$:	5.0569×10^2	0.0^b	-2.0000×10^2	4.8080×10^2	0.0^b	0.0^b	0.0	0.0^b
		$c(i,j)$:	-2.0228×10^0	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	7.7173×10^1	1.9950×10^2	-1.1627×10^2	0.0^b	0.0
		$c(i,j)$:	8.0000×10^{-1}	0.0^b	0.0^b	-8.0320×10^{-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	-4.5906×10^2
		$c(i,j)$:	8.0000×10^{-1}	0.0^b	8.0000×10^{-1}	-1.2588×10^0	0.0^b	0.0^b	0.0^b	-9.6038×10^{-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	-4.4703×10^0	4.7584×10^1	-7.4212×10^2	2.0332×10^1	2.5630×10^2	0.0^b
		$c(i,j)$:	1.2612×10^0	0.0^b	8.0000×10^{-1}	-8.0000×10^{-1}	4.0284×10^{-2}	-1.1912×10^0	8.0000×10^{-1}	0.0^b
66	$CH_n^{[alc]}$	$a(i,j)$:	0.0^c	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^c	0.0^b	2.0000×10^2	1.8900×10^3	1.3330×10^3	-4.7640×10^2	2.0000×10^2	-2.0762×10^1
		$c(i,j)$:	0.0^c	0.0^b	3.0257×10^{-1}	7.5600×10^0	3.1475×10^0	1.9056×10^0	4.2165×10^{-1}	9.2840×10^{-1}
67	$CH_n^{[alc-tail]}$	$a(i,j)$:	0.0^c	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^c	0.0^b	2.0000×10^2	1.3250×10^3	1.3330×10^3	-4.7640×10^2	2.0000×10^2	-2.0762×10^1
		$c(i,j)$:	0.0^c	0.0^b	3.0257×10^{-1}	2.9603×10^0	3.1475×10^0	1.9056×10^0	4.2165×10^{-1}	9.2840×10^{-1}
68	$CH_n^{[OH]}$	$a(i,j)$:	0.0^c	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^c	0.0^b	2.0000×10^2	-2.1510×10^3	1.3330×10^3	-4.7640×10^2	2.0000×10^2	-2.0762×10^1
		$c(i,j)$:	0.0^c	0.0^b	3.0257×10^{-1}	-1.6464×10^0	3.1475×10^0	1.9056×10^0	4.2165×10^{-1}	9.2840×10^{-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	2.0000×10^2	2.7640×10^2	2.5970×10^2	1.9847×10^2	-2.0360×10^2	2.0000×10^2
		$c(i,j)$:	-8.0000×10^{-1}	0.0^b	8.0000×10^{-1}	-1.1056×10^0	9.7596×10^{-1}	8.0000×10^{-1}	-1.2530×10^{-1}	8.0000×10^{-1}

Table 2. Continued.

group no. $i \downarrow$	main groups		13 $CH_nO[ether]$	65 COOH	66 $CH_n^{[alc]}$	67 $CH_n^{[alc-tail]}$	68 $CH_n^{[OH]}$	69 OH
1	CH_n	$a(i,j)$:	2.5150×10^2	6.6350×10^2	0.0 [c]	0.0 [c]	0.0 [c]	9.8650×10^2
		$b(i,j)$:	-1.7943×10^2	6.6350×10^2	0.0 [c]	0.0 [c]	0.0 [c]	9.8650×10^2
		$c(i,j)$:	5.5434×10^{-1}	2.6540×10^0	0.0 [c]	0.0 [c]	0.0 [c]	2.1976×10^0
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
		$b(i,j)$:	-1.2963×10^1	-5.3740×10^2	1.9504×10^1	1.9504×10^1	1.9504×10^1	-6.3610×10^2
		$c(i,j)$:	8.0000×10^{-1}	-1.4576×10^{-1}	8.0000×10^{-1}	8.0000×10^{-1}	8.0000×10^{-1}	2.5444×10^0
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
		$b(i,j)$:	3.5503×10^2	-1.4082×10^2	-2.0000×10^2	-1.7373×10^2	-2.0000×10^2	1.0086×10^2
		$c(i,j)$:	-1.8480×10^0	-8.0000×10^{-1}	-7.9977×10^{-1}	-1.4484×10^0	-8.0000×10^{-1}	-8.0000×10^{-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]	1.7894×10^{-1}	9.7679×10^{-1}	9.7679×10^{-1}	9.7679×10^{-1}	1.8064×10^{-1}
9	CH_nCO	$a(i,j)$:	-1.0360×10^2	6.6940×10^2	2.6760×10^1	2.6760×10^1	2.6760×10^1	1.6450×10^2
		$b(i,j)$:	0.0 [b]	-6.6935×10^2	-50597×10^1	-5.0597×10^1	-50597×10^1	2.0000×10^2
		$c(i,j)$:	0.0 [b]	-2.6776×10^0	-8.0000×10^{-1}	-8.0000×10^{-1}	-8.0000×10^{-1}	8.0000×10^{-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	5.0569×10^2	5.0569×10^2	5.0569×10^2	-5.2900×10^2
		$c(i,j)$:	0.0 [b]	1.9900×10^0	-2.0228×10^0	-2.0228×10^0	-2.0228×10^0	-2.1160×10^0
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
		$b(i,j)$:	-2.1770×10^2	-4.2917×10^2	2.0000×10^2	2.0000×10^2	2.0000×10^2	2.4540×10^2
		$c(i,j)$:	-9.4280×10^{-1}	0.0 [b]	8.0000×10^{-1}	8.0000×10^{-1}	8.0000×10^{-1}	9.8160×10^{-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	2.6560×10^0	8.0000×10^{-1}	8.0000×10^{-1}	8.0000×10^{-1}	9.5080×10^{-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
		$b(i,j)$:	-1.4574×10^2	0.0	3.1530×10^2	3.1530×10^2	3.1530×10^2	2.0000×10^2
		$c(i,j)$:	3.1930×10^{-1}	0.0	1.2612×10^0	1.2612×10^0	1.2612×10^0	8.0000×10^{-1}
66	$CH_n^{[alc]}$	$a(i,j)$:	2.5150×10^2	6.6350×10^2	0.0	0.0 [c]	0.0 [c]	9.8650×10^2
		$b(i,j)$:	-1.7943×10^2	6.6350×10^2	0.0	0.0 [c]	0.0 [c]	9.8650×10^2
		$c(i,j)$:	5.5434×10^{-1}	2.6540×10^0	0.0	0.0 [c]	0.0 [c]	2.1976×10^0
67	$CH_n^{[alc-tail]}$	$a(i,j)$:	2.5150×10^2	6.6350×10^2	0.0 [c]	0.0	0.0 [c]	9.8650×10^2
		$b(i,j)$:	-1.7943×10^2	6.6350×10^2	0.0 [c]	0.0	0.0 [c]	9.8650×10^2
		$c(i,j)$:	5.5434×10^{-1}	2.6540×10^0	0.0 [c]	0.0	0.0 [c]	2.1976×10^0
68	$CH_n^{[OH]}$	$a(i,j)$:	2.5150×10^2	6.6350×10^2	0.0 [c]	0.0 [c]	0.0	9.8650×10^2
		$b(i,j)$:	-1.7943×10^2	6.6350×10^2	0.0 [c]	0.0 [c]	0.0	9.8650×10^2
		$c(i,j)$:	5.5434×10^{-1}	2.6540×10^0	0.0 [c]	0.0 [c]	0.0	2.1976×10^0
69	OH	$a(i,j)$:	2.8060×10^1	2.2439×10^2	1.5640×10^2	1.5640×10^2	1.5640×10^2	0.0
		$b(i,j)$:	-1.2899×10^2	2.2439×10^2	2.0000×10^2	2.0000×10^2	2.0000×10^2	0.0
		$c(i,j)$:	-8.0000×10^{-1}	8.9756×10^{-1}	-8.0000×10^{-1}	-8.0000×10^{-1}	-8.0000×10^{-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 $\leftrightarrow$ H_2O group interactions are taken from Peng et al. (2001). 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 interaction parameters $b_{i,j}$ and $c_{i,j}$ are set to zero since appropriate data to determine these interactions are missing.

[c] Interaction parameters between different types of alkyl main groups (CH_n, $CH_n^{[alc]}$, $CH_n^{[alc-tail]}$, and $CH_n^{[OH]}$) are set to zero.

when there is a solid–solid phase transition (change of polymorphic form) between T and $T_{m,i}$. Note that if more than one solid–solid phase transition is present in the temperature range of interest, additional terms (of the form of the second term) need to be added in Eq. (19) to account for each of these phase changes. 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 $\Delta h_{\text{m},i}$ and $\Delta c_{p,\text{m},i}$ are obtained from tabulated experimental data (Domalski and Hearing, 1996; Dean, 1999). We note that for certain organic compounds rather large uncertainties in the physicochemical property values used in Eq. (19) will translate into large uncertainties in the calculated SLE activity values, particularly when the target temperature is far from the melting point temperature at standard pressure. In this work, such uncertainties were assessed based on the comparison of derived activity values with activity values from other data types for the same system, and by means of preliminary model fits of AIOMFAC-P3. Affected data sets were either assigned a much lower weighting or zero weighting (removing the data set from the fit).

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 multi-functional organic solutions are provided in Ganbavale et al. (2014). Measured water activities were then used directly for the AIOMFAC-P3 parameter determination – with the exception of data within ± 10 K from 298 K.

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, multi-component 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 the composition of the two liquid phases in equilibrium at a certain temperature. A direct calculation and comparison of activities in coexisting phases is possible at experimental LLE compositions, i.e. measured mole fractions x_j^{α} and x_j^{β} of the two liquid phases α and β at equilibrium. According to the reference state definitions of AIOMFAC, different independent components j should have the same activities in coexisting phases, i.e. $a_j^{(x),\alpha} = a_j^{(x),\beta}$. This data type can therefore be implemented in the model fit by minimising 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.

Furthermore, we also performed AIOMFAC-based predictions of the phase compositions at LLE using the method of Zuend and Seinfeld (2013), particularly for the graphical comparison of measured and predicted tie-line LLE data. To perform such predictions, an initial composition point is required from which a liquid–liquid equilibrium calculation is performed in order to determine whether the initial mixture composition is stable as a single homogeneous phase or whether two coexisting liquid phases represent the stable equilibrium state (according to the model) and what the compositions of the two phases are in the LLE case. An initial mixture composition with mole fraction x_j^{init} of component j on a unstable / metastable point of an experimental tie-line can be generated by the following:

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

Such LLE predictions from an initial composition are computationally more expensive than the relative activity difference calculations used in the model fit, yet offer a different view on the performance of the model for applications of phase separation / phase composition computations. For more details about the LLE computations with AIOMFAC we 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 are usually obtained by performing measurements either at isobaric or isothermal conditions. VLE data considered in the model include binary water + organic systems and binary
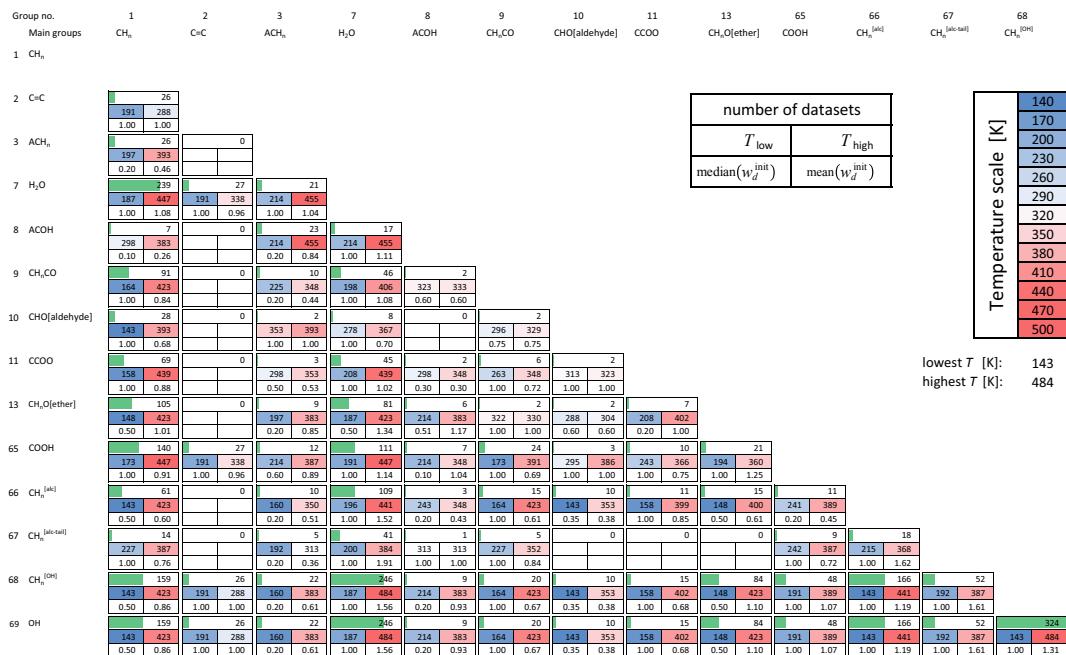
Figure 1. Database distribution for the water ↔ organic and organic ↔ organic interaction parameters. The table lists for each main group interaction pair at temperatures substantially different from the reference temperature, $T_{\ominus} = 298.15\,\mathrm{K}$, i.e. per data set d: $T_{d,\mathrm{low}} < 289\,\mathrm{K}$ or $T_{d,\mathrm{high}} > 307\,\mathrm{K}$, the following information. Top boxes: the total number of data sets available, visualised by the green bars. Middle boxes: the lowest temperature (T_{low}) and the highest temperature (T_{high}) (units of K) of the data points using a percentile-wise colour scale. Bottom boxes: the median and arithmetic mean of the assigned initial data set weighting values (w_d^{init}) of the data sets involved.

Legend — number of datasets; T_{low} | T_{high}; median(w_d^{init}) | mean(w_d^{init}).
Temperature scale [K]: 140, 170, 200, 230, 260, 290, 320, 350, 380, 410, 440, 470, 500.
lowest T [K]: 143; highest T [K]: 484.

Each cell lists three lines: top = number of data sets; middle = T_{low}, T_{high}; bottom = median, mean of w_d^{init}.

Row group	1 CHn	2 C=C	3 ACHn	7 H2O	8 ACOH	9 CHnCO	10 CHO	11 CCOO	13 CH2O[ether]	65 COOH	66 CHn[alc]	67 CHn[alc-tail]
2 C=C	26; 191,288; 1.00,1.00											
3 ACHn	26; 197,393; 0.20,0.46	0										
7 H2O	239; 187,447; 1.00,1.08	27; 191,338; 1.00,0.96	21; 214,455; 1.00,1.04									
8 ACOH	7; 298,383; 0.10,0.26		0; 214,455; 0.20,0.84	23; 214,455; 1.00,1.11								
9 CH3CO	91; 164,423; 1.00,0.84		0; 225,348; 0.20,0.44	10; 198,406; 1.00,1.08	46; 323,333; 0.60,0.60	2						
10 CHO[aldehyde]	28; 143,393; 1.00,0.68		0; 353,393; 1.00,1.00	2; 278,367; 1.00,0.70	8	0; 296,329; 0.75,0.75	2					
11 CCOO	69; 158,439; 1.00,0.88		0; 298,353; 0.50,0.53	3; 208,439; 1.00,1.02	45; 298,348; 0.30,0.30	2; 263,348; 1.00,0.72	6; 313,323; 1.00,1.00	2				
13 CH2O[ether]	105; 148,423; 0.50,1.01		0; 197,383; 0.20,0.85	9; 187,423; 0.50,1.34	81; 214,383; 0.51,1.17	6; 322,330; 1.00,1.00	2; 288,304; 0.60,0.60	2; 208,402; 0.20,1.00	7			
65 COOH	140; 173,447; 1.00,0.91	27; 191,338; 1.00,0.96	12; 214,387; 0.60,0.89	111; 191,447; 1.00,1.14	7; 214,348; 0.10,1.04	24; 173,391; 1.00,0.69	3; 295,386; 1.00,0.75	10; 243,366; 1.00,0.75	21; 194,360; 1.00,1.25			
66 CHn[alc]	61; 143,423; 0.50,0.60		0; 160,350; 0.20,0.51	10; 196,441; 1.00,1.52	109; 243,348; 0.20,0.43	3; 164,423; 1.00,0.61	15; 143,353; 0.35,0.38	11; 158,399; 1.00,0.85	15; 148,400; 0.50,0.61	11; 241,389; 0.20,0.45		
67 CHn[alc-tail]	14; 227,387; 1.00,0.76		0; 192,313; 0.20,0.36	5; 200,384; 1.00,1.91	41; 313,313; 1.00,1.00	1; 227,352; 1.00,0.84	5	0	0; 242,387; 1.00,0.72	9; 215,368; 1.00,1.62	18	
68 CHn[OH]	159; 143,423; 0.50,0.86	26; 191,288; 1.00,1.00	22; 160,383; 0.20,0.61	246; 187,484; 1.00,1.56	9; 214,383; 0.20,0.93	20; 164,423; 1.00,0.67	10; 143,353; 0.35,0.38	15; 158,402; 1.00,0.68	84; 148,423; 0.50,1.10	48; 191,389; 1.00,1.07	166; 143,441; 1.00,1.19	52; 192,387; 1.00,1.61
69 OH	159; 143,423; 0.50,0.86	26; 191,288; 1.00,1.00	22; 160,383; 0.20,0.61	246; 187,484; 1.00,1.56	9; 214,383; 0.20,0.93	20; 164,423; 1.00,0.67	10; 143,353; 0.35,0.38	15; 158,402; 1.00,0.68	84; 148,423; 0.50,1.10	48; 191,389; 1.00,1.07	166; 143,441; 1.00,1.19	52; 192,387; 1.00,1.61

(Row 69 OH additionally includes column 68 CHn[OH]: 324; 143,484; 1.00,1.31.)

data for water-free organic (1) + organic (2) systems. Since isobaric measurements are usually conducted at 1 atm ($= 101.325\,\mathrm{kPa}$) 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:

$$\gamma_j^{(x)} = \frac{p_j}{p_j^{\circ}(T)\,x_j}, \qquad p_j = y_j\,p. \qquad (21)$$

Here, p_j is the partial pressure of component j, and $p_j^{\circ}(T)$ 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 $p_j^{\circ}(T)$ 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 ex-

ceptions 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. For glycerol, fugacity corrections were not applied; instead, given the large amount of data sets covering functional groups of alcohols, the glycerol VLE data sets were assigned a very small weighting, essentially excluding their influence on the parameter fit. 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 minimisation (Zuend et al., 2011):

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

Here, $w_{d,u}$ is the weighting value of a data point and the sums cover all data points u in all data sets d considered. $Q_{d,u}^{\mathrm{ref}}$ is a reference quantity, directly determined from experiments (e.g. a 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. $Q_{d,u}^{\mathrm{calc}}$ represents the corresponding quantity calculated with the model at the given conditions. $Q_{d,u}^{\mathrm{tol}}$ is a tolerance quantity (> 0) which represents the measurement uncertainty or model sensitivity and has the same units as $Q_{d,u}^{\mathrm{ref}}$. 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 $x^{\mathrm{tol}} = 0.01$. 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 Data set 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 data sets 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 data sets with a large number of data points, as well as preventing an immoderate high weighting of data sets with a small number of data points, Zuend et al. (2011) propose a simplified procedure of assigning individual weighting to data sets on the basis of data type

and number of data points N_d in a data set:

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

where w_d^{init} is an initial weighting of data set 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 data set. The weighting of individual data points that are part of large data sets 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 data sets 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 $w_d^{\mathrm{init}} = 5.0$ while the SLE organic activity (SLE(org)) data sets (i.e. SLE data where an organic compound forms the solid in equilibrium with the liquid solution) are given an initial weighting of $w_d^{\mathrm{init}} = 0.2$ 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 differential scanning calorimetry (DSC) measurements at homogeneous freezing temperatures (T_{hom}) are assigned $w_d^{\mathrm{init}} = 1.0$ (considering some uncertainties associated with the T_{hom} determination from DSC measurements). The weighting of all types of data sets 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 data sets are assigned an initial weighting of $w_d^{\mathrm{init}} = 1.0$. However, data sets 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: $\Delta T_{\mathrm{low}} = |T_{\mathrm{low}} - T_{\ominus}|$ or $\Delta T_{\mathrm{high}} = \left| T_{\mathrm{high}} - T_{\ominus} \right| > 40\,\mathrm{K}$ and $\Delta T = \left| T_{\mathrm{low}} - T_{\mathrm{high}} \right| >$

40 K, where T_{low} and T_{high} are the lowest and highest temperatures covered by the data points involved (see Fig. 1) and $T_\ominus = 298.15$ K is the reference temperature. Similarly, the $c_{m,n}$ parameters for the main groups are determined only if $\Delta T_{low} > 80$ K or $\Delta T_{high} > 80$ K and if $\Delta T > 80$ 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. In the temperature range of interest here, molar heat capacity changes (units of $J\,mol^{-1}\,K^{-1}$) are roughly 2 to 3 orders of magnitude smaller in value than changes in molar enthalpy (units of $J\,mol^{-1}$). 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 minimisation problem is a challenging task for any global optimisation method. For the parameter optimisation, 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 data sets dominate the parameter optimisation due to potential numerical issues or other reasons, such as inconsistent data sets and outliers, a large number of trial parameter optimisation runs were carried out. To solve the parameter optimisation problem, we use the formulation introduced by Zuend et al. (2011) by using a combination of algorithms to solve the parameter optimisation 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 (Bound Optimization BY Quadratic Approximation) 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 data sets to the objective function value (Eq. 22) were used to identify potential inconsistencies among data sets, 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 AIOMFAC 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. As discussed in Sect. 4.1, the database and therefore the values of F_{obj} (Eq. 22) evaluated with both AIOMFAC-P3 and AIOMFAC-P1 for comparison, do not include data sets with data points exclusively near room temperature (298 ± 10 K). In this section, we compare the model performance of the new AIOMFAC-P3 version, with AIOMFAC-P1 (original AIOMFAC version) based on overall quantitative measures followed by a discussion of 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 28 % in terms of F_{obj} in comparison to AIOMFAC-P1 (542 data sets involved). As stated earlier, AIOMFAC-P1 uses the temperature-dependence expression of standard UNIFAC and represents the AIOMFAC performance using only $a_{m,n}$ interaction parameters. 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.

For the purpose of evaluating the improvement of the new parameterisation it is of interest to compare the performance of the two AIOMFAC model versions for different subsets of the database covering separately low and high temperature ranges and certain aspects of the complexity of molecular structures involved ("monofunctional" vs. "multi-functional" organic components). We define the value $F_{obj,\,low\text{-}T}$ calculated as the objective function value based on Eq. (22) when exclusively considering data sets with $T_{high} < 274$ K. That is, the subset of the database including only data sets containing data points with a maximum temperature below 274 K (at least 25 K below the reference temperature of 298 K). This serves to represent the low-temperature range in our comparison. Analogously, to represent the high-temperature range (at least 25 K above 298 K), we define $F_{obj,\,high\text{-}T}$ by exclusively considering the data sets with $T_{low} > 322$ K. The minimum distance of 25 K from the reference temperature was chosen such that there is (i) a clear difference between the low and high temperature ranges considered, yet that (ii) still
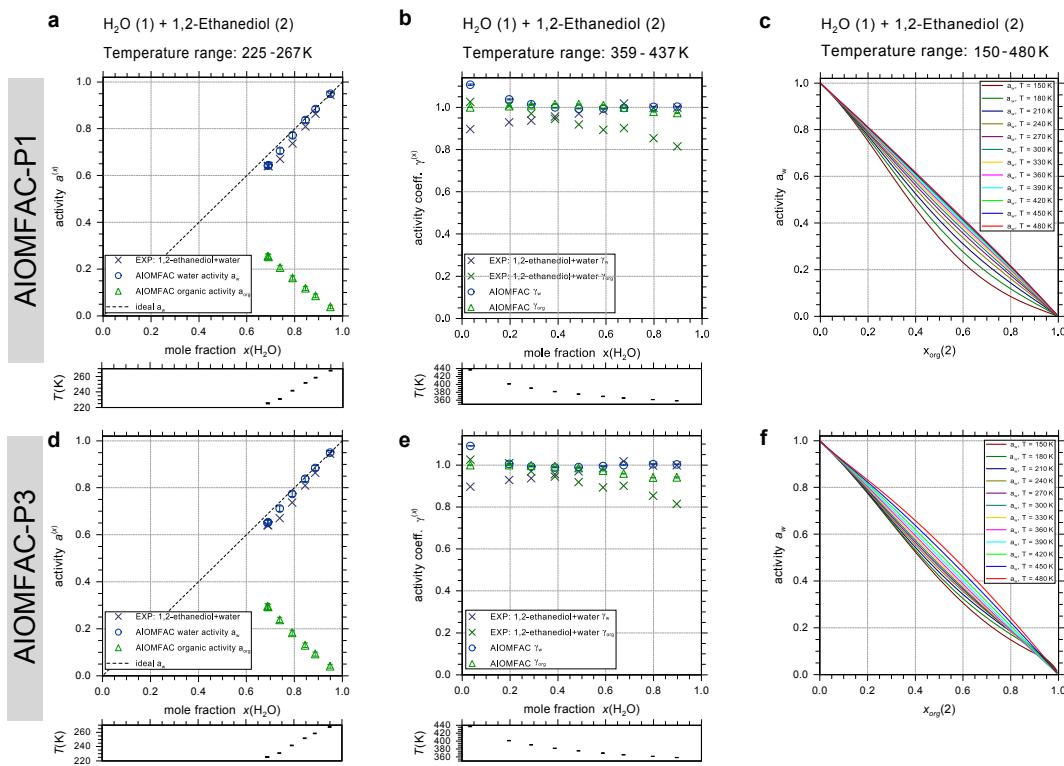
Figure 2. SLE and VLE measurements for water $(1) + 1,2$-ethanediol (2) solutions and corresponding calculations of AIOMFAC-P1 **(a–c)** or AIOMFAC-P3 **(d–f)**. The coloured curves in **(c, f)** represent the temperature dependence of water activities predicted for the range 150–480 K. **(a, d)** Low 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 $x^{tol} = 0.01$. Panels **(b, e)** show the model predictions of the activity coefficients compared to VLE data covering temperatures significantly higher than room temperature. The temperatures 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).

many data sets are included in the comparison (especially given that low-temperature SLE-derived water activity data usually starts at the melting point temperature of pure water-ice). Based on this distinction into low and high temperature ranges and from the evaluation of $F_{obj, \, low-T}$ and $F_{obj, \, high-T}$ with both AIOMFAC versions, it is found that AIOMFAC-P3 improves similarly in both temperature ranges relative to AIOMFAC-P1. For the low-temperature range the improvement of AIOMFAC-P3 is 37 % (152 data sets involved; $F_{obj, \, low-T}$ (AIOMFAC-P3) = 10.207), while for the high-temperature range the improvement is 37 % (223 data sets involved; $F_{obj, \, high-T}$ (AIOMFAC-P3) = 37.554). The better improvement in the lower and higher temperature ranges compared to the overall improvement (of 28 %) is not surprising. This is simply because the two additional fit parameters in AIOMFAC-P3 have a relatively small effect on the model performance in the ± 25 K range around the reference temperature. Therefore, the AIOMFAC-P3 improvement relative to AIOMFAC-P1 is better when the data sets covering the temperature range close to room temperature are excluded from the comparison (to clarify: these data are not excluded

from the AIOMFAC-P3 fit – except for data sets within the 10 K margin around 298 K, which are also not considered in the overall model performance comparison).

We further differentiate the low and high temperature subsets of the database each into two classes of (i) data sets containing monofunctional organic compounds only and (ii) data sets containing at least one multi-functional organic compound. The terminology applied here is to call an organic compound "monofunctional" when its molecular structure contains only one oxygen-bearing subgroup (e.g. phenol, 2-butanol, or palmitic acid), while glycerol, sucrose, 2-ethoxyethanol, glutaric acid, vanillylmandelic acid, and resorcinol are examples for multi-functional compounds included in our database (see Table 1). Despite this terminology, in AIOMFAC/UNIFAC the compounds termed monofunctional here are typically also composed of several types of subgroups (e.g. different CH_n and ACH_n groups in addition to an oxygen-bearing subgroup). Multi-functional oxygenated compounds are often found as major contributors to the total mass of the organic aerosol fraction (e.g. Hallquist et al., 2009). The results from
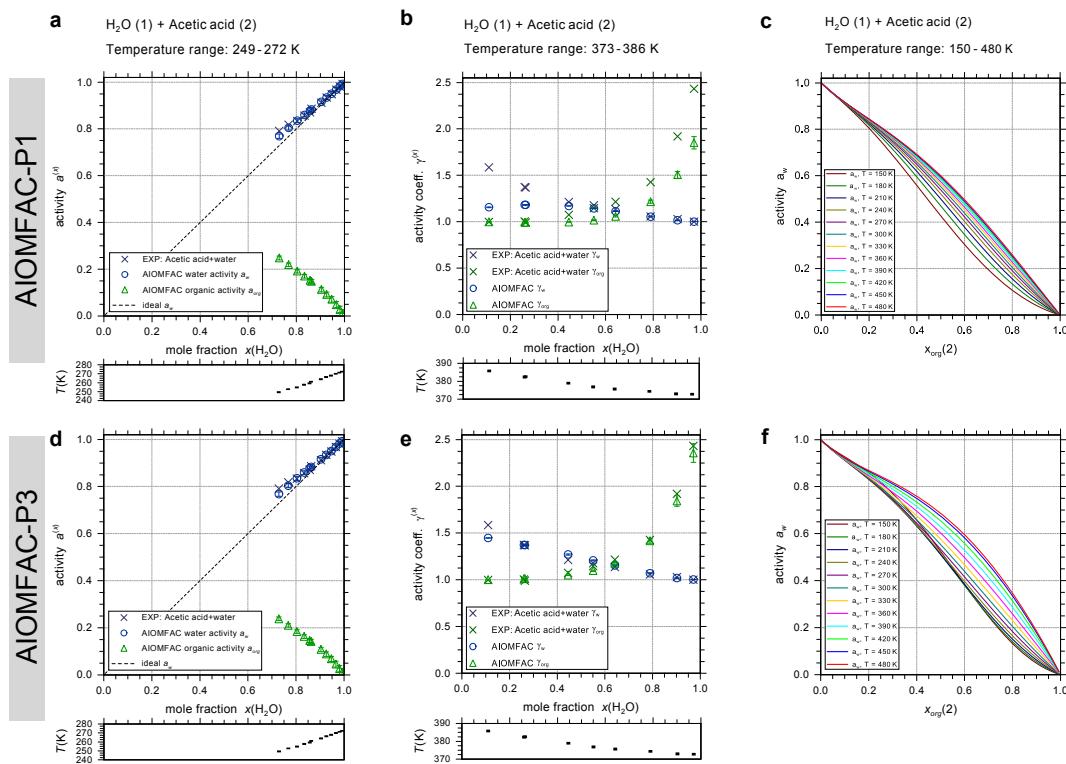
Figure 3. SLE and VLE measurements for water (1) + acetic acid (2) solutions and corresponding calculations of AIOMFAC-P1 **(a–c)** or AIOMFAC-P3 **(d–f)**. The coloured curves in **(c, f)** represent the temperature dependence of water activities predicted for the range 150–480 K. **(a, d)** Low temperature 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 $x^{tol} = 0.01$. Panels **(b, e)** show the model predictions of the activity coefficients compared to VLE data covering temperatures significantly higher than room temperature. The temperatures of the individual data points are given in the boxes below the main panels. Experimental data: Faucon (1910) and Narayana et al. (1985).

the evaluation with these subclasses in terms of average improvement of AIOMFAC-P3 compared to AIOMFAC-P1 for the low-temperature range are as follows: 55 % (46 data sets; $F_{obj,\,low\text{-}T,mono}(\text{AIOMFAC-P3}) = 5.197$) for the subset of data sets with monofunctional compounds and -7 % (106 data sets; $F_{obj,\,low\text{-}T,multi}(\text{AIOMFAC-P3}) = 5.010$), i.e. a decline in agreement, in the case of data sets with multi-functional compounds. For the high-temperature range the average improvement is as follows: 35 % (162 data sets; $F_{obj,\,high\text{-}T,mono}(\text{AIOMFAC-P3}) = 31.237$) for monofunctional and 43 % (61 data sets; $F_{obj,\,high\text{-}T,multi}(\text{AIOMFAC-P3}) = 6.317$) for the data sets involving multi-functional compounds. Note that these percentages reflect a weighted average improvement of AIOMFAC-P3 (weighting depends on the w_d^{init} values). There are some data sets for which the AIOMFAC-P3 parameterisation shows an improvement over AIOMFAC-P1 and in return there are some data sets for which the AIOMFAC-P1 parameterisation shows better agreement. In the case of the low-temperature range comparisons for the subset of data sets containing monofunctional compounds, AIOMFAC-P3

leads to improvement in the case of 34 data sets vs. a decline in the case of 12 data sets. For the low-temperature range subset of data sets containing multi-functional compounds, AIOMFAC-P3 leads to improvement in case of 50 data sets but to decline in case of 56 data sets.

Thus, while this evaluation shows that AIOMFAC-P3 leads to improvement with the experimental data considering the whole database, as well as for the subsets of low and high temperature ranges, the new parameterisation does also lead to a decline in agreement for a number of data sets with respect to the performance of the original AIOMFAC-P1 parameterisation. This is is partly due to the nature of applying a global parameter optimisation aiming at the simultaneous improvement of the weighted model–measurement deviations based on Eq. (22), which entails the possibility for reduced agreement for some systems as long as the overall model–measurement agreement increases. Moreover, the AIOMFAC-P1 parameterisation shows already good agreement with a part of the experimental data sets at low and high temperatures. For this fraction of data sets any changes in model prediction due to a new parameterisation may eas-
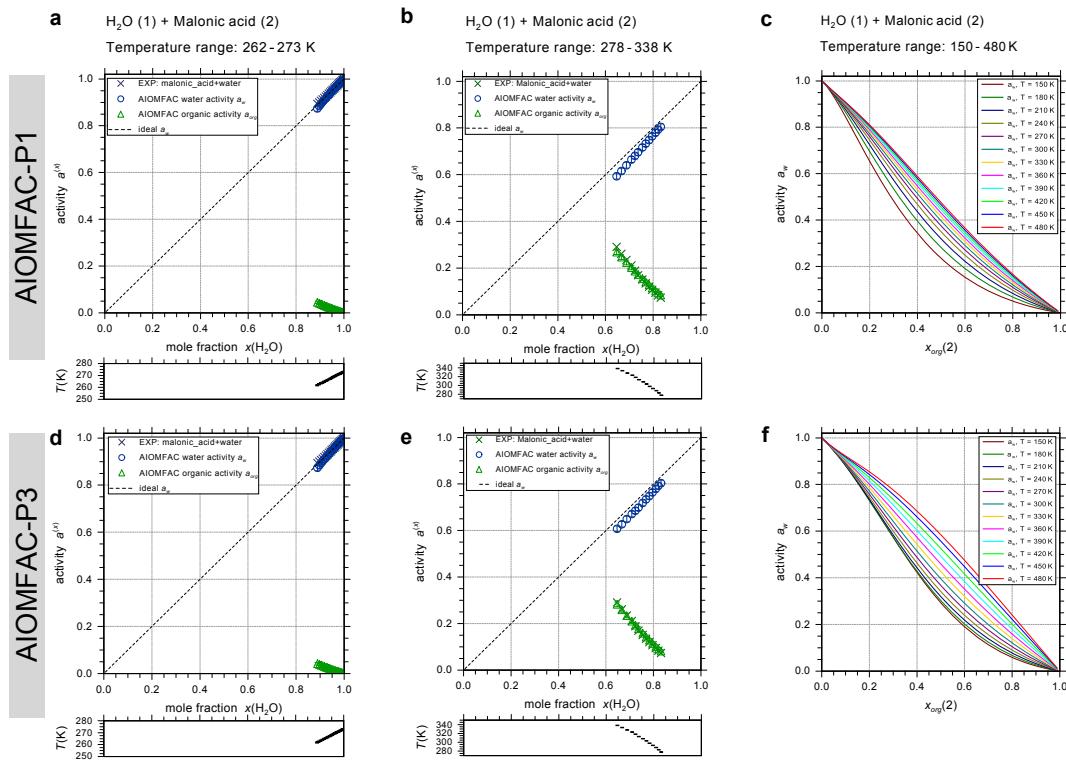
Figure 4. SLE measurements for water (1) + malonic acid (2) solutions and corresponding calculations of AIOMFAC-P1 **(a–c)** or AIOMFAC-P3 **(d–f)**. Panels **(c, f)** show the temperature dependence of water activities predicted for the range 150–480 K. **(a, d)** Low temperature experimental SLE data (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 SLE 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 temperatures 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).

ily lead to a decline rather than an improved agreement with experimental data. However, as long as the changes in the model predictions are small for these systems, a decline in agreement relative to AIOMFAC-P1 could still mean that AIOMFAC-P3 performs well. Nevertheless, there are also data sets for which both AIOMFAC parameterisations show relatively large discrepancies (e.g. the water + 2-butoxyethanol system further discussed below). For such systems, additional improvements of the AIOMFAC model are conceivable – either by a new fit of certain $a_{m,n}$ interaction parameters (kept untouched in this work) or by introduction of additional (special) subgroups that help to account for the effects of certain intra- and inter-molecular subgroup–subgroup interactions (e.g. intramolecular hydrogen-bonding among oxygenated functional groups in close proximity). A thorough evaluation of these options and improvement of AIOMFAC in this direction is the topic of future work.

In the following, the two AIOMFAC parameterisations are compared for a selection of aqueous organic mixtures and water-free organic mixtures. Again, it should be noted that the model was not just fitted to the selection of data sets 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 data set only) would represent those data better, but 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 better represented by AIOMFAC-P3 in comparison to AIOMFAC-P1 even though both models show deviations from the experimental VLE-derived activity coefficients at low and high mole fraction of water. 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. In
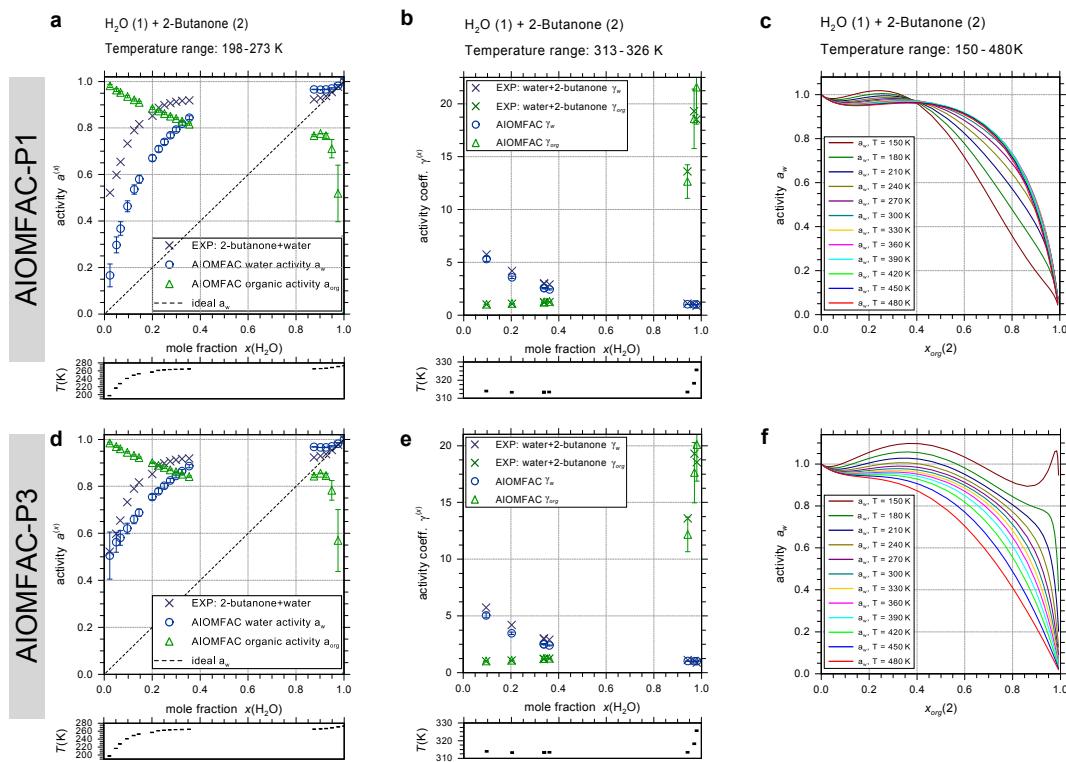
Figure 5. SLE and VLE measurements for water (1) + 2-butanone (2) solutions and corresponding calculations of AIOMFAC-P1 **(a–c)** or AIOMFAC-P3 **(d–f)**. Panels **(c, f)** show the temperature dependence of water activities predicted for the range 150–480 K. **(a, d)** Low temperature experimental 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. Panels **(b, e)** show the model predictions of the activity coefficients compared to VLE data covering temperatures significantly higher than room temperature. The temperatures 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).

comparison to AIOMFAC-P1, the resulting temperature dependence from low to high x_{org} is slightly smaller in the case of the AIOMFAC-P3 parameterisation (f).

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 are 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. The AIOMFAC-P1 parameterisation tends to underestimate the activity coefficients of water and acetic acid, particularly at high and low mole fractions of water. 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, 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 in the range 330–480 K.

This steeper slope of 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 functional groups in common with the acetic acid + water system.

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 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 temperatures of the pure component or the SLE at the highest concentration of the organic component, 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 close to and above room temperature) is well represented in both AIOMFAC-P1 and AIOMFAC-P3 (b, e). No VLE data are available for aqueous
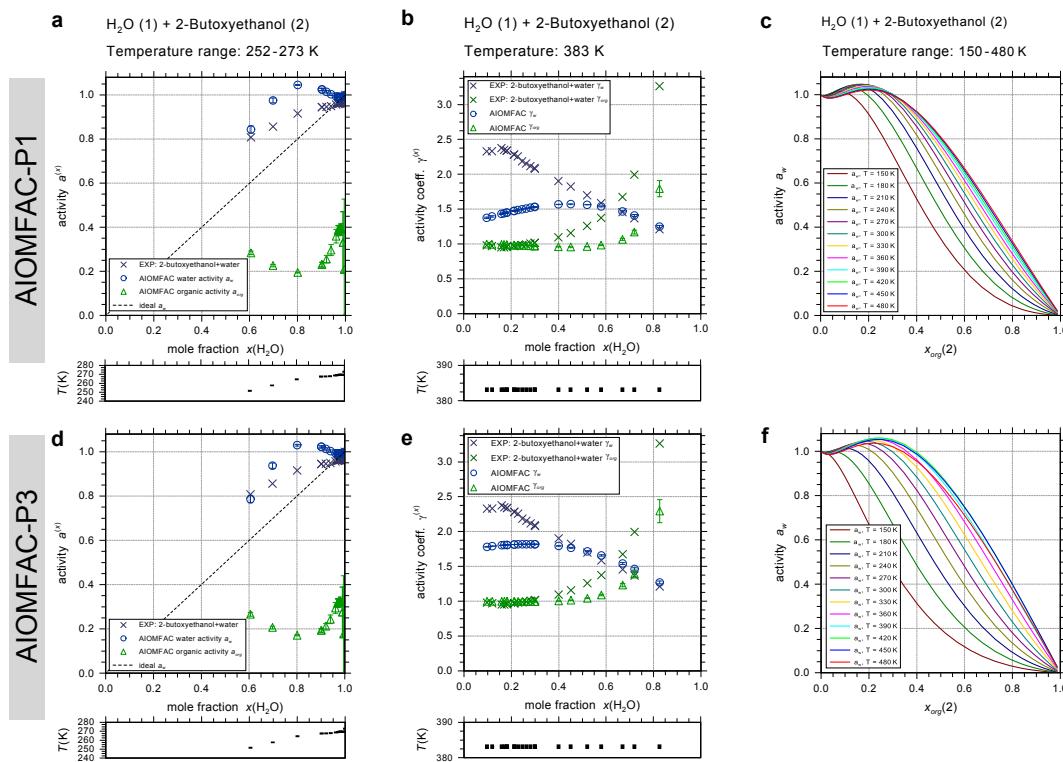
Figure 6. SLE and VLE measurements for 2-butoxyethanol + water solutions and corresponding calculations of AIOMFAC-P1 **(a–c)** or AIOMFAC-P3 **(d–f)**. Panels **(c, f)** show the temperature dependence of water activities predicted for the range 150–480 K. **(a, d)** Low temperature experimental SLE 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 $x^{\text{tol}} = 0.01$. The dashed line represents the hypothetical water activity of an ideal mixture. Panels **(b, e)** show the model predictions of the activity coefficients compared to VLE data covering temperatures significantly higher than room temperature. The temperatures 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).

malonic acid at higher temperatures and hence could not be compared. AIOMFAC-P3 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 (b) and AIOMFAC-P3 (e) 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 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 green a_{w} curve at $T = 180$ K, liquid–liquid phase separation is predicted at $a_{\text{w}} = 0.98$ in the composition range between $x_{\text{org}}(2\text{-butanone}) = 0.05$ and $x_{\text{org}}(2\text{-butanone}) = 0.61$. 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 $0.35 < x$ $(\text{H}_2\text{O}) < 0.85$.

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 $a_{\text{w}} > 1$ 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 (a) and (d) (see also local minima in a_{w} curves of panels c, f). Note that the model
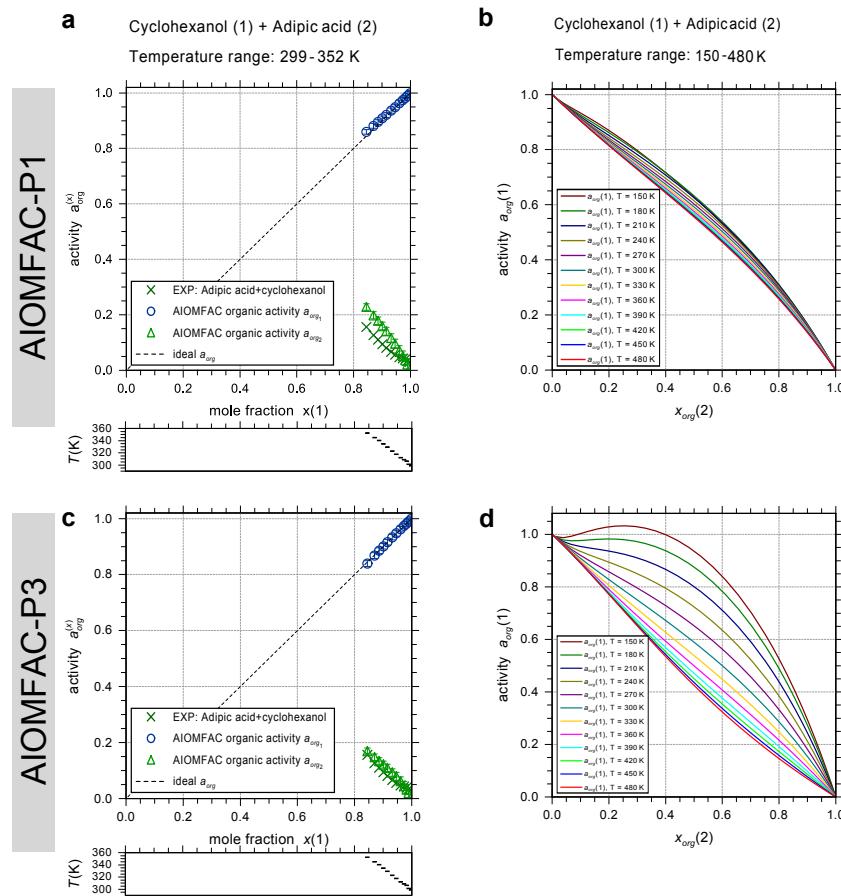
Figure 7. SLE measurements for cyclohexanol (1) + adipic acid (2) solutions and corresponding calculations of AIOMFAC-P1 **(a, b)** or AIOMFAC-P3 **(c, d)**. Panels **(b, d)** represent the temperature dependence predictions from AIOMFAC-P1 and AIOMFAC-P3 for the temperature range 150–480 K. **(a, c)** 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 temperatures of the individual data points are given in the boxes below the main panels. Experimental data: Lihua et al. (2007).

predictions in these figures do not include phase separation computations on purpose, since the experimental data are for a homogeneous 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). The observed disagreement between both models and the experimental data is mainly due to the fact that there is already a clear discrepancy between AIOMFAC (both versions) and the experimental data near room temperature. Since there is already disagreement at the reference temperature (298.15 K), the new model parameters for improved temperature dependence ($b_{m,n}$ and $c_{m,n}$) cannot (and should not) remove this model–measurement discrepancy. This system illustrates that a re-parameterisation of certain $a_{m,n}$ group interaction parameters may be necessary to improve AIOMFAC for this and similar systems.

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 ~ 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 (b) and does not predict a phase separation in the range shown.

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
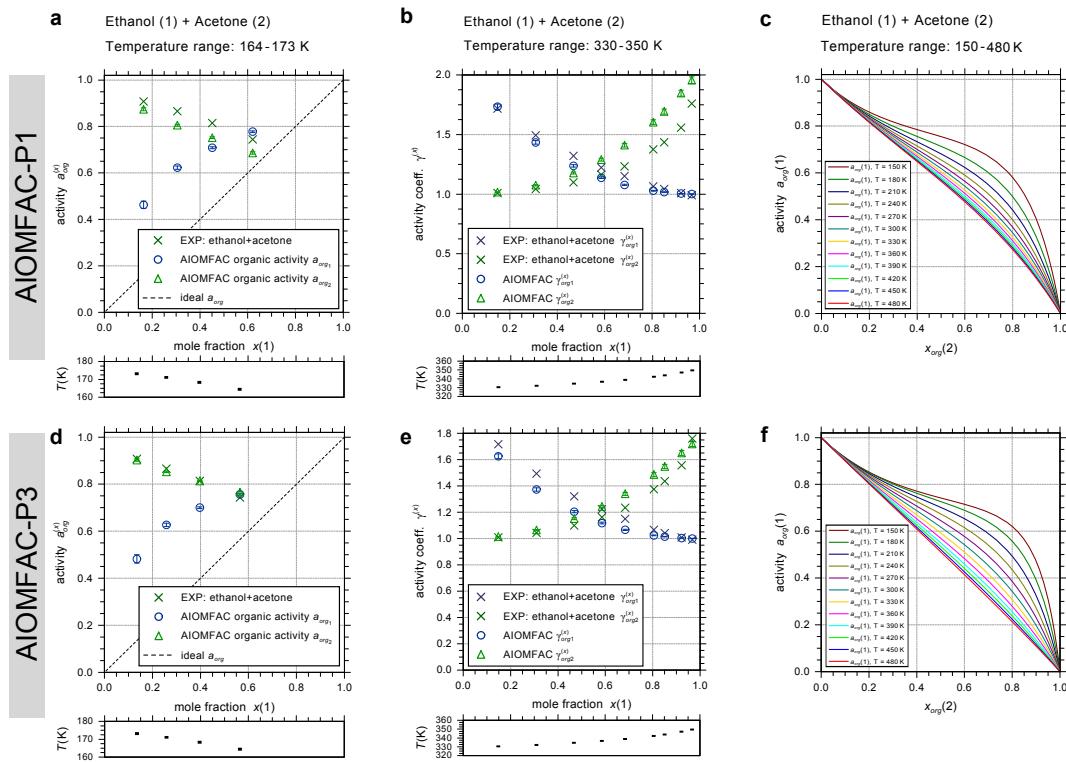
Figure 8. SLE and VLE measurements for ethanol (1) + acetone (2) solutions and corresponding calculations of AIOMFAC-P1 **(a–c)** or AIOMFAC-P3 **(d–f)**. Panels **(c, f)** show the temperature dependence as predicted by AIOMFAC-P1 and AIOMFAC-P3 for the temperature range 150–480 K. **(a, d)** Low temperature experimental SLE data (crosses), shown as mole fraction of ethanol, x(1), vs. activity ($a_{\mathrm{org2}}^{(x)}$) of acetone. The error bars represent the model sensitivity to a composition variation by $x^{\mathrm{tol}} = 0.01$. The dashed line is the ideal solution curve for component 1. Panels **(b, e)** show the model predictions of the activity coefficients compared to VLE data covering temperatures significantly higher than room temperature. The temperatures of the individual data points are given in the boxes below the main panels. Experimental data: Sapgir (1929) and Amer et al. (1956).

agreement with the experimental SLE-derived data (d), 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 $\gamma_{\mathrm{org2}}^{(x)}$ (activity coefficient of component 2, i.e. acetone) in the predictions of 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 (d).

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 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 in the range $0.15 < x(\text{ethanol}) < 0.6$, while AIOMFAC-P1 tends to underpredict the experimental data. In contrast, at higher temperatures (~ 350 to 380 K) covered by experimental VLE data (b and e), the predicted activity coefficients $\gamma_{\mathrm{org}}^{(x)}$ (diethyl ether) at high mole fractions of ethanol (component 1) 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
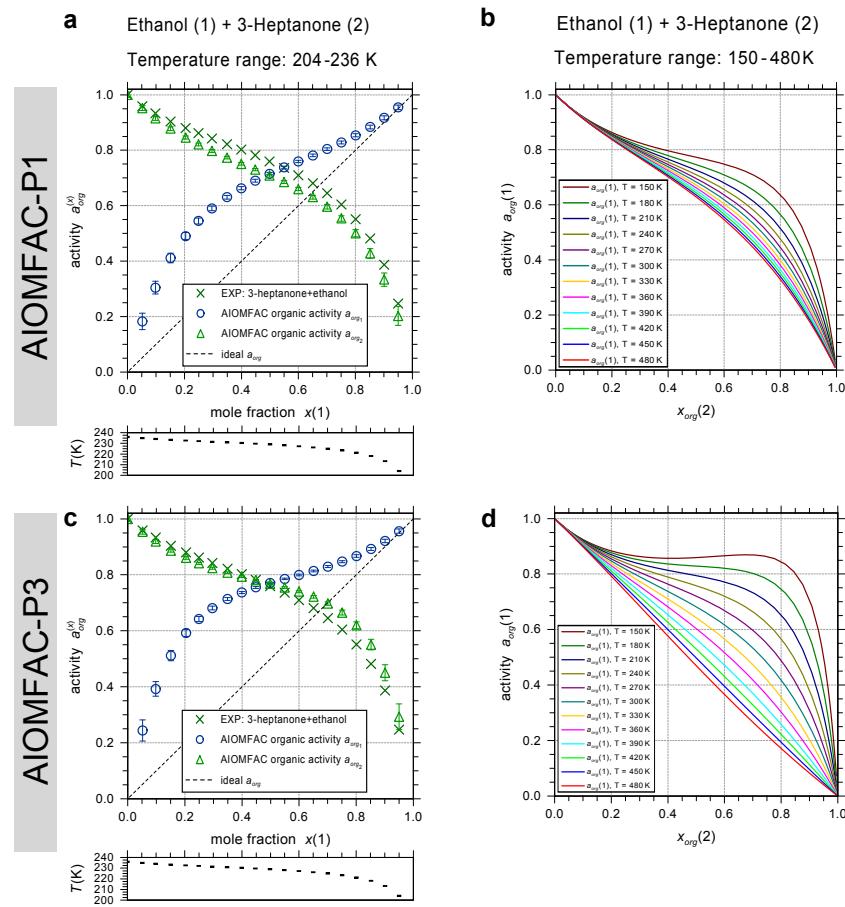
Figure 9. SLE measurements for ethanol $(1) + 3$-heptanone (2) solutions and corresponding calculations of AIOMFAC-P1 **(a, b)** or AIOMFAC-P3 **(c, d)**. Panels **(b, d)** show the temperature dependence predictions from AIOMFAC-P1 and AIOMFAC-P3 for the temperature range 150–480 K. The SLE data in **(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).

group interaction parameterisation of AIOMFAC-P3 in comparison to AIOMFAC-P1. As is visible from panels (c) 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.

While an extensive database was compiled to allow for an improvement of the AIOMFAC model with respect to its performance at temperatures substantially lower and higher than room temperature, there are still limitations present in the general coverage of the extended temperature range by experimental data. The complexity of organic molecules
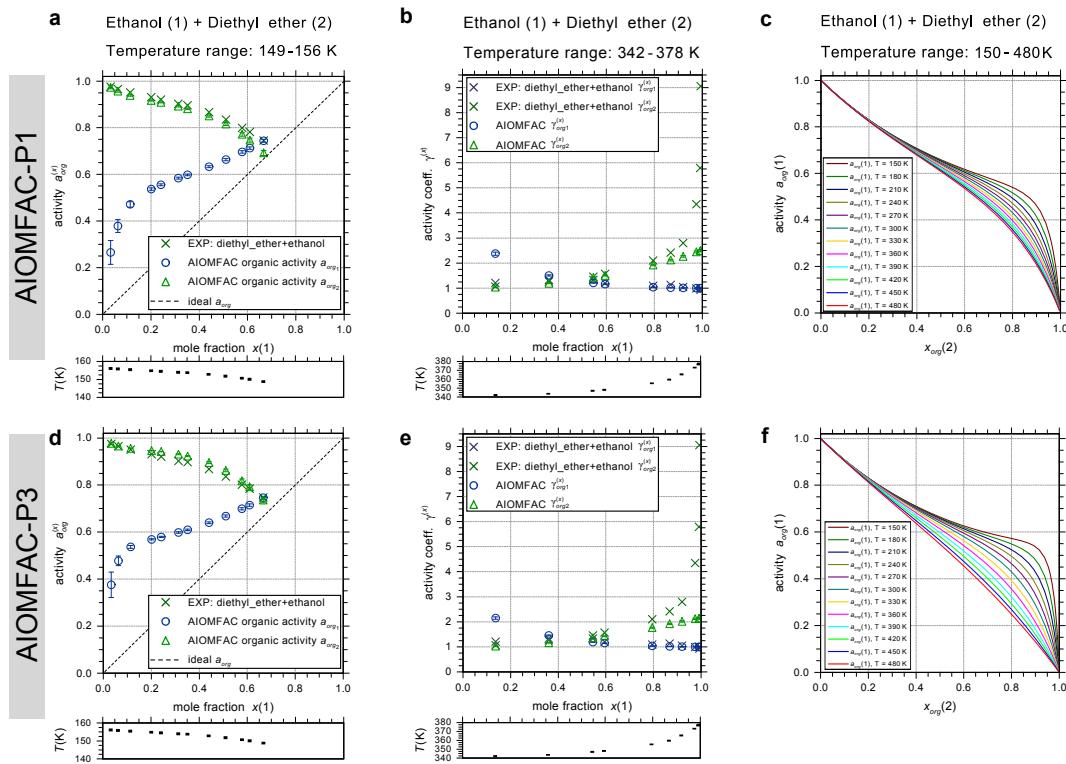
Figure 10. SLE and VLE measurements for ethanol (1) + diethyl ether (2) solutions and corresponding calculations of AIOMFAC-P1 **(a–c)** or AIOMFAC-P3 **(d–f)**. Panels **(c, f)** show the temperature dependence of the ethanol activity, as predicted by AIOMFAC-P1 and AIOMFAC-P3 for the temperature range 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. Panels **(b, e)** show the model predictions of the activity coefficients compared to VLE data covering temperatures significantly higher than room temperature. The temperatures 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 $x^{\text{tol}} = 0.01$. Experimental data: Lalande (1934) and Moeller et al. (1951).

in terms of their physical and chemical properties such as size, shape and combinations of functional groups, particularly the number and proximity of oxygen-bearing functionalities, are important factors that influence the quality of AIOMFAC predictions. Of interest for atmospheric aerosol systems are data sets containing multi-functional organic compounds, such as sugar-like compounds, di- and polycarboxylic acids, hydroxylated ketones and functionalized aromatic compounds. We have added many experimental thermodynamic equilibrium data sets that cover systems containing such compounds (e.g. sorbitol, 1,2,7,8-octanetetrol, sucrose, raffinose, citric acid, malonic acid, 2-isopropoxyethanol, vanillylmandelic acid, etc.; see Table 1 for a complete list), yet overall the database remains dominated by small, monofunctional organic compounds. This possibly limits the accuracy of AIOMFAC-P3 for predicting activity coefficients in multi-component systems containing multi-functional, high-molecular mass species. This is a disadvantage not just for AIOMFAC-P3 or this work, but generally rooted in the very limited amount of experimental data covering such systems (especially at temperatures much lower/higher than 298 K). Due to this, the accuracy of

AIOMFAC predictions is expected to decrease with increasing complexity of organic compounds.

As discussed in more detail at the beginning of Sect. 5, it is found that the new temperature dependence parameterisation shows particular improvement for the majority of systems containing monofunctional compounds both in the low and high temperature ranges (the temperature ranges at least 25 K above/below 298 K). In case of the mixtures containing multi-functional compounds present in our database, the improvement for the low-temperature range in comparison to AIOMFAC-P1 is more diverse: for about half of the data sets a small improvement is found while for the other half a reduced agreement is the result of the parameter optimisation. For some systems containing multi-functional compounds, the model–measurement agreement is not good with either AIOMFAC version (e.g. in case of the aqueous 2-butoxyethanol system shown in Fig. 6). For such systems and corresponding main group interactions, further improvement of AIOMFAC may only be achieved by a refitting of certain $a_{m,n}$ interaction parameters involved.

It is known that the standard UNIFAC parameterisation and model expressions need to be modified for aque-

ous oligomer/polymer solutions to achieve good model–measurement agreement (e.g. Ninni et al., 1999). This has been done in previous work targeting specific types of polymers, including the introduction of specific UNIFAC groups fitted to experimental data exclusively of such polymer systems (e.g. Ninni et al., 1999). The introduced AIOMFAC-P3 parameterisation has as purpose general applicability, as is the case for AIOMFAC-P1. Therefore, it is expected that the AIOMFAC model may perform rather poorly when used for predicting activity coefficients in oligomer/polymer solutions. For such systems, the application of specifically fitted models is recommended. 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 carbonalcohol, 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 data sets. 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. In addition, larger discrepancies in model–measurement agreement were found in particular for some of the systems containing multi-functional organic compounds. The affected systems were typically also poorly represented at room temperature. Further investigations will be needed to thoroughly address these issues and achieve better performance of AIOMFAC in such cases over the full temperature range of interest.

The performance of the AIOMFAC parameterisation is typically better for systems containing relatively small organic compounds and substantial deviations may occur in mixtures when molecules of high structural complexity such as highly oxygenated compounds or molecules of high molecular mass (e.g. oligomers and polymers) prevail. 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 multi-component 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, 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 (absolute range) 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 in a_w (absolute range). 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 ("vanillylmandelic 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 solutions are tabulated in Appendix Tables A1–A8.

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 ($T = 289.15$ K)	a_w ($T = 298.15$ K)	a_w ($T = 313.15$ 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 (absolute range) 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 (absolute range) 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 ($T = 289.15$ K)	a_w ($T = 298.15$ K)	a_w ($T = 313.15$ 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 (absolute range) in a_w.

Table A4. Bulk water activity (a_w) measurements[a] of water (1) + 1,2,7,8-octanetetrol (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 ($T = 313.15\,K$)
0.0109	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 (absolute range) 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 (absolute range) 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 (absolute range) 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 ($T = 289.15\,\text{K}$)	a_w ($T = 298.15\,\text{K}$)	a_w ($T = 313.15\,\text{K}$)
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 (absolute range) 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 ($T = 289.15\,\text{K}$)	a_w ($T = 298.15\,\text{K}$)	a_w ($T = 313.15\,\text{K}$)
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 (absolute range) in a_w.

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