Recommended Liquid–Liquid Equilibrium Data. Part 4. 1-Alkanol–Water Systems

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The recommended liquid–liquid equilibrium (LLE) data for 19 binary 1-alkanol–water systems have been obtained after critical evaluation of all data (527 data sets) reported in the open literature up to the end of 2004. An equation for prediction of the 1-alkanol solubility was developed. The predicted 1-alkanol solubility was used for calculation of water solubility in the second liquid phase. The LLE calculations were done with the equation of state appended with a chemical term proposed by Góral. The recommended data were presented in the form of individual pages containing tables and all the references. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2203354]

Key words: 1-alkanols; water; liquid–liquid equilibria; binary systems; recommended data; predicted data.

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1. Introduction

The objective of this article is to provide selected and critically evaluated liquid–liquid equilibrium (LLE) data for binary 1-alkanol–water systems, taken from the open litera-

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ture up to the end of 2004 and completed with predicted data. In this work we investigated 527 data sets obtained from 157 references.

Solubility data for alkanol–water systems were the object of IUPAC Commission on Solubility Data and presented as Volume 15 of the IUPAC Solubility Data Series edited by Barton.[165] This work takes into account new data published since that time as well as new methods of the data evaluation.

When each system is evaluated in isolation, the estimation of data quality can be difficult, especially in cases of scarce or disagreeing data. The solubility of higher alkanols in water are very low and consequently even small experimental errors may lead to substantial relative errors in the measured solubility, which in some cases reach 100% or more. To help clarify these uncertainties, this work continues the approach presented in the previous articles by Mączyński *et al.*[166] and Góral *et al.*[167,168] for hydrocarbon–water systems. This approach consists of the calculation of "reference data" using solubility information from all the investigated systems. The calculation of reference data consists of two steps:

(1) The solubility of 1-alkanols in water is approximated with a smoothing equation described in the next section. This equation depends not only on the number of carbon atoms of the alkanol but it also contains empirical constants, which are derived from simultaneous regression of the solubility data for all investigated alkanols.

(2) The solubility of water in 1-alkanols is calculated using LLE calculations. The input data for these calculations are the alkanol in water solubility predicted by the smoothing equation. The LLE calculations use a correlating method based on equation of state modified to account for the role of hydrogen bonding in solvion.[169]

In these two steps an extensive body of experimental data is described with a few adjustable parameters providing an additional framework for comparison of experimental data and help in the recognition of systematic error. The solubility calculated by these two steps is used as the reference values in evaluations.

2. Solubility of 1-Alkanol in Water

The solubility of 1-alkanols in water, expressed as mole fraction (x_1) along the three-phase equilibrium line, resembles the solubility of alkanes in water (except in the critical region). This is illustrated by Fig. 1, in which experimental points for 1-octanol in water are compared to solubility curve calculated for pentane.[166]

The solubility curve in both systems has a minimum. The solubility at the minimum ($x_{1,\min}$) decreases within each homologous series as shown in Fig. 2, where the minimum solubility in the series of normal 1-alkanols is compared with the minimum solubility calculated for the corresponding n-alkanes.[166]

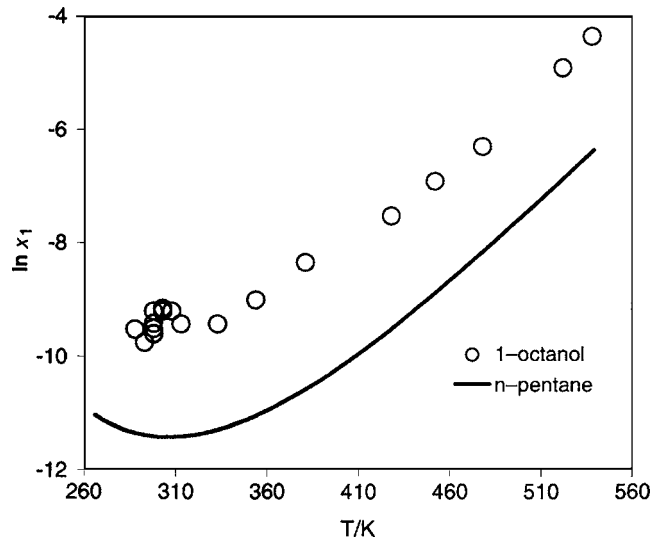

FIG. 1. Logarithm of mole fraction of solute in water ($\ln x_1$) vs temperature (T). Comparison between solubility of 1-octanol and n-pentane in water.

The temperature of the minimum ($T_{\min}$) is constant for a given class of hydrocarbon+water mixtures: e.g., $T_{\min}$ =306 K for alkanes, $T_{\min}$=298 K for cycloalkanes, and $T_{\min}$=280 K for alkylbenzenes.[166–168] One might expect that alkanols would be charcterized by an even lower value of $T_{\min}$ but this is not the case. In the series of the alkanols $T_{\min}$ decreases gradually with increasing length of the 1-alkanol molecule starting from $T_{\min}$=330 K for 1-pentanol.

The equation for the solubility of alkanols in water, derived in the following, takes into account that only a fraction of an alkanol dissolved in water exists in the form of free molecules not joined to others by hydrogen bonds. These free molecules are called monomers here in analogy to associations such as dimers, trimers, etc. It is assumed that solubility of the monomers in water along the three-phase equi-

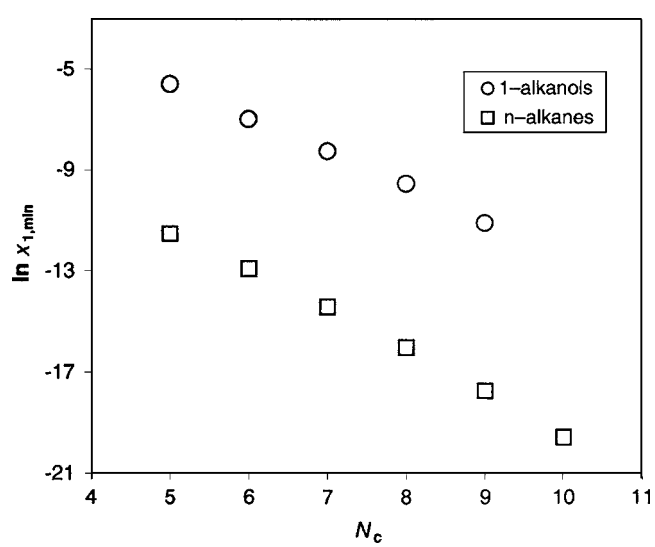

FIG. 2. Comparison of solubility in water for series of normal 1-alkanols and n-alkanes. Logarithm of mole fraction of the solute in water at minimum of the solubility ($\ln x_{1,\min}$) vs number of carbon atoms of the solute (N_c).

librium line can be described by the equation used previously for the solubility of hydrocarbons in water. This equation adopted for the monomers can be written as follows:

$$\partial \ln(N_1/n)/\partial(1/T) = -h_1/R, \tag{1}$$

where N_1 is number of moles of the monomer in solution consisting of n total number of moles and h_1 is heat of solution of the monomer. The monomers are in chemical equilibrium with various associations of the alkanol. Hence, the total amount of the alkanol dissolved in water is higher than N_1 and corresponds to the total moles of alkanol (n_1). Using the definition:

$$\beta = N_1/n_1. \tag{2}$$

One can rearrange Eq. (1) into the following form:

$$\partial \ln x_1/\partial(1/T) = -h_1/R - \partial \ln \beta/\partial(1/T), \tag{3}$$

where x_1 is the mole fraction of an alkanol in water along the three-phase equilibrium line. In analogy to the alkane + water systems, it is assumed that h_1 depends linearly on T going through zero at some temperature T^0. Thus h_1/R in Eq. (3) can be approximated with the following equation:

$$h_1/R = C_1(T - T^0), \tag{4}$$

where C_1 is an adjustable parameter depending on alkanol.

For the second term in Eq. (3), the following approximation is used:

$$\partial \ln \beta/\partial(1/T)\ (\mathrm{K}) = 2400. \tag{5}$$

The approximation of Eq. (5) is valid at sufficiently low temperatures, say below 370 K. This can be seen from an analysis of the association model used in this work for LLE calculations. Equations (4) and (5) introduced into Eq. (3) give, after rearrangement,

$$\partial \ln x_1/\partial(1/T) = -C_1(T - T_{1,\min}), \tag{6}$$

where $T_{1,\min}$ is defined by

$$T_{1,\min}\ (\mathrm{K}) = T^0\ (\mathrm{K}) + 2400/C_1, \tag{7}$$

where $T_{1,\min}$ is a temperature at which the differential in Eq. (6) is equal to zero. Thus $T_{1,\min}$ is a temperature corresponding to the minimum of the solubility of the 1-alkanol. Equation (6) has the same form as the equation used for solubility of alkanes,[166] but $T_{1,\min}$ is no longer constant as it depends on C_1, which in turn depends on the number of carbon atoms of the alkanol. This explains the change of $T_{1,\min}$ observed in alkanol + water systems.

Integration of Eq. (6) gives the following equation, which describes the solubility of alkanols in water as a function of temperature:

$$\ln x_1 = \ln x_{1,\min} + C_1 \mathrm{f}(T_{1,\min}/T), \tag{8a}$$

where

$$\mathrm{f}(T_{1,\min}/T) = T_{1,\min}/T - \ln(T_{1,\min}/T) - 1. \tag{8b}$$

The same type of equation was used previously[166] for alkane + water systems but contrary to the alkane systems Eq. (8a) when applied for alkanols is valid only at temperatures sufficiently distant from the critical temperature of solubility. It was found that all investigated 1-alkanol + water systems can be approximated simultaneously with Eq. (8a) provided that the adjustable parameters $\ln x_{1,\min}$ and C_1 are treated as linear functions of the number of carbon atoms, N_c

$$\ln x_{1,\min} = d_1 + d_2 N_c, \tag{9}$$

$$C_1 = d_3 + d_4 N_c. \tag{10}$$

Equations (9) and (10) allow rewriting Eq. (8) in the form:

$$\ln x_1 = (d_1 + d_2 N_c) + (d_3 + d_4 N_c)\mathrm{f}(T_{1,\min}/T). \tag{11}$$

The coefficients d_1, d_2, d_3, and d_4 in Eq. (11) as well as T^0 in definition (7) were determined by simultaneous regression of the experimental data for normal 1-alkanols from 1-pentanol to 1-hexadecanol at at temperatures from the freezing point of water to approximately 60 K below the critical temperature of solubility. Altogether 242 experimental points were used in the regression. After the regression the most outlying point was removed and the remaining points were regressed once more. This procedure was repeated until the deviation of the most outlying point in the remaining data set did not exceed three times the estimated standard deviation. This procedure removed 22 of 242 initial points. The following values of the parameters were obtained:

$$d_1 = 1.249, \quad d_2 = -1.365, \quad d_3 = 7.7, \quad d_4 = 4.2,$$

$$T^0/\mathrm{K} = 246.4. \tag{12}$$

Equation (11) works well up to 60 K below the critical temperature of solubility (T_{2c}) as is shown in Fig. 3 but the data above the boiling point of water were reported only by one source (with exception of pentanol). For the higher alkanols shown in Fig. 4, there are no measurements at high temperatures. Therefore it is concluded that reliability of Eq. (11) is not sufficiently tested at $T > 373$ K.

It was found that Eq. (11) [with parameters defined by Eq. (12)] can also be applied for branched 1-alkanols provided

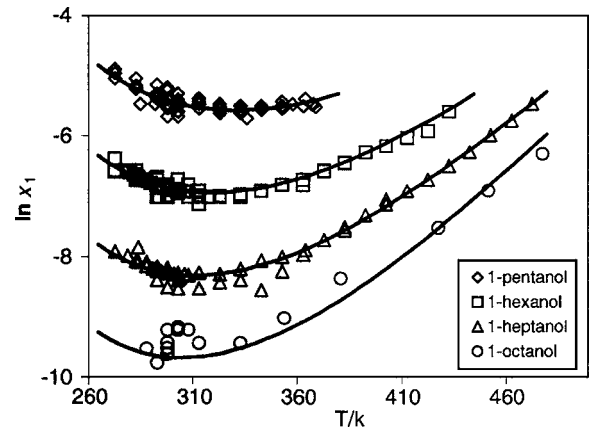

FIG. 3. Logarithm of mole fractions of alkanols in water ($\ln x_1$) vs temperature (T). Experimental points and approximating curves calculated with Eq. (11) with parameters defined by Eq. (12).

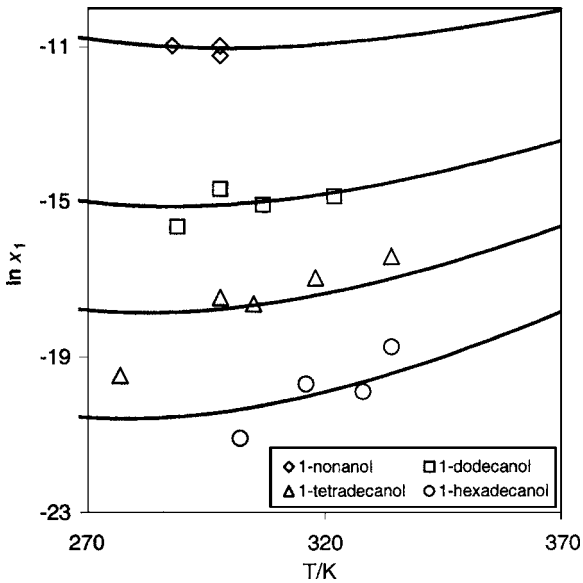

FIG. 4. Logarithm of mole fractions of alkanols in water ($\ln x_1$) vs temperature (T). Experimental points and approximating curves calculated with Eq. (11) with parameters defined by Eq. (12).

that instead of N_c "effective" values N_c^* are used. In a first step N_c^* for each branched 1-alkanol was adjusted, via Eqs. (11) and (12), to the experimental solubility points. It was found that the determined values of N_c^* as well as N_c for normal 1-alkanols are related in the same way to the excluded volumes of the alkanols. In this work, the excluded volume, as used in the Redlich-Kwong equation of state, is used. It is calculated from critical temperature (T_c) and critical pressure (P_c) with the equation:

$$b = 0.08664RT_c/P_c. \tag{13}$$

The parameter b was used instead of N_c in previous articles[166–168] devoted to hydrocarbon+water systems. Using b enables a description of n-alkanes, cycloalkanes, and branched alkanes with a set of two equations analogous to Eqs. (9) and (10). The situation in 1-alkanol+water systems is not exactly the same because $x_{1,\min}$ in the series of 1-alkanols does not correspond to the same temperature and parameter b as defined by Eq. (13) is influenced by autoassociation of the alkanols. These are probably the reasons that Eqs. (9) and (10) are simpler when related to N_c instead of b. As a consequence of this choice, it is necessary to use N_c^* for branched 1-alkanols.

It was found that N_c is linearly dependent on $\sqrt{b}$ for the investigated normal 1-alkanols:

$$N_c = c_1 + c_2\sqrt{b}, \tag{14}$$

where $c_1 = -7.98$ and c_2 $(\mathrm{mol/cm^3})^{0.5} = 1.242$. Values of N_c^* lie on a parallel, slightly shifted line:

$$N_c^* = (c_1 + c_2\sqrt{b}) - 0.07. \tag{15}$$

Table 1 gives values of N_c^* of the branched 1-alkanols investigated in this work calculated from Eq. (15). It is interesting that values of N_c^* calculated with Eq. (15) and used in Eq. (11) are able to predict minor differences in solubility of isomers. An example is shown in Fig. 5.

The standard deviation of the experimental points, $s(\ln x_{1,\mathrm{exp}})$, was estimated with the equation:

TABLE 1. Data for calculation of the 1-alkanol solubility by means of Eq. (8a) or (18) with parameters $T_{1,\min}$, $\ln x_{1,\min}$, and C_1 calculated from the predictive equations (7), (9), (10), (12), and (15)

Name	$T_{1,\min}$	$\ln x_{1,\min}$	C_1	D_1	α_1	T_{2c}	N_c^*
1-Butanol	330.0	−4.12	27.71	0.911	−30	398.0	
2-Methyl-1-propanol	330.0	−4.03	32.34	0.858	−30	406.3	
2,2-Dimethyl-1-propanol	333.8	−5.17	27.4				4.70
2-Methyl-1-butanol	332.3	−5.33	27.9				4.82
3-Methyl-1-butanol	331.7	−5.38	28.1				4.86
1-Pentanol	330.0	−5.58	29.7	1.299	−20	459.8	5
2-Ethyl-1-butanol	322.0	−6.56	31.7				5.72
1-Hexanol	319.3	−6.94	32.9	0.713	−20	490.5	6
2-Methyl-1-pentanol	321.0	−6.70	32.1				5.82
2,2-Dimethyl-1-butanol	321.2	−6.67	32.1				5.69
1-Heptanol	311.1	−8.31	37.1	0.440	−40	517.7	7
2-Ethyl-1-hexanol	306.4	−9.25	40.0				7.69
1-Octanol	304.5	−9.67	41.30	1.239	−50	545.0	8
1-Nonanol	299.1	−11.04	45.5				9
1-Decanol	294.7	−12.40	49.7				10
1-Undecanol	290.9	−13.77	53.9				11
1-Dodecanol	287.7	−15.13	58.1				12
1-Tetradecanol	282.5	−17.86	66.50				14
1-Hexadecanol	278.4	−20.59	74.90				16

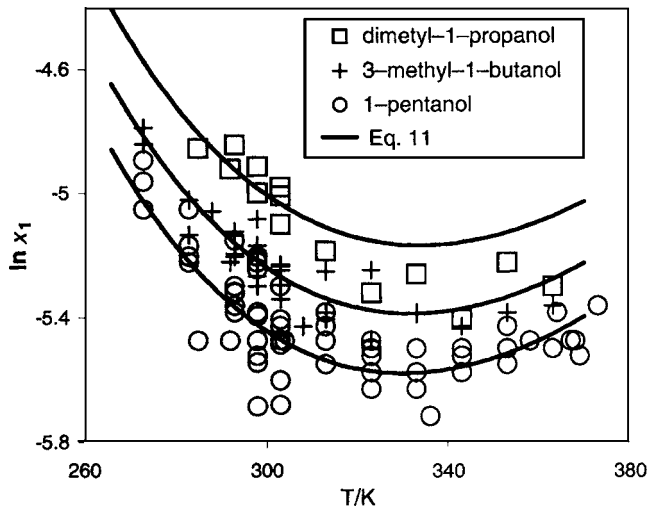

FIG. 5. Comparison between experimental solubility of three isomeric pentanols in water and approximating curves calculated with Eq. (11).

$$s(\ln x_{1,\mathrm{exp}}) = \left[\sum_{k=1}^{m} (\ln x_{1,\mathrm{exp}} - \ln x_{1,\mathrm{calc}})_k^2/(m-n) \right]^{0.5}, \quad (16)$$

where $\ln x_{1,\mathrm{exp}}$ are experimental values, $\ln x_{1,\mathrm{calc}}$ are calculated from Eq. (11), m is the number of experimental points, and n is the number of adjustable parameters. After removing outlying points, by the procedure described earlier, the average standard deviation of the experimental points for alkanols C_5–C_8 was as follows:

$$s(\ln x_{1,\mathrm{exp}}) = 0.10, \quad (17)$$

which corresponds to relative standard deviation of $x_{1,\mathrm{exp}}$ of approximately 10%.

The alkanol solubility calculated from Eq. (11) is called here "reference values." For evaluations presented here it is assumed that data are in good agreement with the reference value when the difference between the experimental mole fraction and the reference value does not exceed one standard deviation, e.g., 10% for C_5–C_8 alkanols. The solubility of higher alkanols are lower and more difficult to measure as is shown by the scatter of points in Fig. 4. The corresponding standard deviation for these points is 20%, therefore, for the C_9–C_{12} alkanols limit of 20% is assumed. This limit is further increased up to 35% for 1-tetradecanol and 1-hexadecanol.

Equation (11) is not applicable for a solubility of 1-butanol and 2-methyl-1-propanol. Fortunately these systems were investigated by many laboratories. For the solubility of 1-butanol over 200 and for the solubility of 2-methyl-1-propanol over 100 points are reported. This allows selecting the recommended data using a smoothing equation as the reference. The experimental points for these systems were smoothed by Eq. (8) with an additional empirical term, which has a negligible value at low and medium temperatures but is growing rapidly when the temperature approaches the critical temperature of solubility (T_{2c}). This additional term extends applicability of the smoothing equation up to approximately 5 K below T_{2c}:

$$\ln x_1 = \ln x_{1,\mathrm{min}} + C_1 f(T_{1,\mathrm{min}}/T) + D_1 \exp[\alpha_1(1 - T/T_{2c})]. \quad (18)$$

Equation (18) was used also for other 1-alkanols, which where measured up to the critical point but in this case only D_1 and α_1 were adjusted to the points of the given system whereas $\ln x_{1,\mathrm{min}}$, C_1, and $T_{1,\mathrm{min}}$ were determined with the general equations (7), (9), (10), and (12) used in Eq. (11).

3. Solubility of Water in 1-Alkanol

Reference values for the solubility of water in an alkanol were calculated using LLE between the two coexisting liquid phases. The calculations were done by a method developed by Góral.[169] This method yields equations for chemical potentials of the components derived from equation of state with an added chemical term (EOSC), which accounts for hydrogen bonding. Application of the EoSC for water systems is described in Refs. 166–168. The input information for the LLE correlation is the solubility of 1-alkanol in water (x_1), calculated with Eq. (11) or (18). The output is solubility of water in 1-alkanol (x_2) as a function of temperature. It is calculated from the constraints fulfilled by chemical potentials at equilibrium:

$$\mu_1^w(x_1,\Theta) = \mu_1^a(x_2,\Theta), \quad (19a)$$

$$\mu_2^w(x_1,\Theta) = \mu_2^a(x_2,\Theta), \quad (19b)$$

where μ_1^w, μ_1^a, μ_2^w, and μ_2^a are the chemical potentials of the first and the second components in the water rich phase and the alkanol rich phase, respectively. Equations (19a) and (19b) contain one adjustable binary parameter, Θ, in the physical part of the EoSC. Otherwise, the chemical potentials are based on a model of association, which takes into account autoassociation of water, autoassociation of alkanols and coassociation between water and alkanols. The model of the association assumes that each active site of the donor type can interact with any active site of the acceptor type and that the equilibrium constant depends only on the type of the interacting sites. This assumption leads to a mixture of various pure and mixed associates. The equilibrium between them is described by three temperature dependent constants: K_{11}—the equilibrium constant of autoassociation of alkanols, K_{12}—the equilibrium constant of coassociation between alkanols and water, and K_{22}—the equilibrium constant of autoassociation of water. The temperature dependence of K_{22} was established in a previous article[166] using LLE data for alkane+water systems. The same equation was used in this work.

The model of autoassociation of alkanols was established using vapor–liquid equilibrium data for alkanol+alkane systems.[170] These data were originally correlated with EoSC using another model of association. Therefore they were recalculated with the model used in this work. All investigated

TABLE 2. Data for calculation of water solubility in 1-alkanols by means of Eq. (27) or (28), where the parameters $T_{2,\min}$, $\ln x_{2,\min}$, C_2, D_2, and α_2 are obtained from regression of the solubility data obtained from LLE calculations

Name	$T_{2,\min}$	$\ln x_{2,\min}$	C_2	D_2	α_2	T_{2c}
1-Butanol	270.0	−0.702	6.082	0.126	−30	398.0
2-Methyl-1-propanol	220.0	−0.968	4.136	0.140	−30	406.3
2,2-Dimethyl-1-propanol	94.8	−1.978	2.05			
2-Methyl-1-butanol	181.4	−1.450	3.39			
3-Methyl-1-butanol	194.5	−1.396	3.70			
1-Pentanol	280	0.349	3.293	0.207	−20	459.8
2-Ethyl-1-butanol	177.6	−2.020	4.35			
1-Hexanol	254.6	−1.277	5.780	0.120	−20	490.5
2-Methyl-1-pentanol	177.1	−1.955	4.23			
2,2-Dimethyl-1-butanol	177.1	−2.018	4.36			
1-Heptanol	258.3	−1.393	5.830	0.133	−40	517.7
2-Ethyl-1-hexanol	233.6	−2.068	6.55			
1-Octanol	277.2	−1.359	6.250	0.647	−50	545.0
1-Nonanol	284.5	−1.385	6.10			
1-Decanol	290.8	−1.399	6.11			
1-Undecanol	296.2	−1.411	5.92			
1-Dodecanol	301.2	−1.411	5.86			
1-Tetradecanol	308.4	−1.406	5.66			
1-Hexadecanol	311.6	−1.395	5.65			

1-alkanols were described with the same temperature dependent equilibrium constant. This does not mean that the degree of association of all these 1-alkanols is the same, because it depends also on the molar volumes of the alkanols. Temperature dependence of K_{11} is expressed by the van't Hoff equation:

$$K_{11} = K_{11}^0 \exp[(-\Delta H_{11}/R)(1/T - 1/T^0)], \tag{20}$$

where

$$\Delta H_{11}/R\ (\mathrm{K}) = 3000, \quad K_{11}^0\ (\mathrm{MPa}) = 0.620, \quad T^0\ (\mathrm{K}) = 303. \tag{21}$$

The excluded volumes of the alkanols in the chemical part of EoSC are shifted by some value (Δb) in respect to the excluded volume calculated from Eq. (15). This shift is calculated with

$$\Delta b = \lambda N_c \tag{22}$$

where $\lambda = -1.0\ \mathrm{cm}^3/\mathrm{mol}$ and N_c is number of carbon atoms of the alkanol.

The equilibrium constant of coassociation (K_{12}) was also approximated with the van't Hoff equation:

$$K_{12} = K_{12}^0 \exp[(-\Delta H_{12}/R)(1/T - 1/T^0)], \tag{23}$$

where for normal 1-alkanols

$$-\Delta H_{12}/R\ (\mathrm{K}) = (3000 - 3900/N_c),$$

$$K_{12}^0\ (\mathrm{MPa}) = 0.044, \quad T^0\ (\mathrm{K}) = 384; \tag{24}$$

for branched 1-alkanols

$$-\Delta H_{12}/R\ (\mathrm{K}) = (3000 - 3900/N_c^*),$$

$$K_{12}^0\ (\mathrm{MPa}) = 0.198, \quad T^0\ (\mathrm{K}) = 303. \tag{25}$$

Equations (24) and (25) contain 6 constants, which were optimized using the solubility of water in the alkanols. With these constants, the solubility of water as a function of temperature was calculated for 16 systems altogether containing 407 experimental points. After removing 57 points (the outliers) by the procedure described in the previous section, the average standard deviation of the experimental points was as follows:

$$s(\ln x_{2,\mathrm{exp}}) = 0.097. \tag{26}$$

Based on this estimation, the same criteria as those listed in previous section were adopted for the recommended data.

For the convenience of the reader the calculated mole fraction of water in 1-alkanols (x_2) are smoothed with an equation analogous to Eq. (8a):

$$\ln x_2 = \ln x_{2,\min} + C_2 f(T_{2,\min}/T), \tag{27}$$

where the function f is defined with Eq. (8b). If the experimental points were reported up to the critical point then an equation analogous to Eq. (18) was used:

$$\ln x_2 = \ln x_{2,\min} + C_2 f(T_{2,\min}/T) + D_2 \exp[\alpha_2(1 - T/T_{2c})]. \tag{28}$$

Parameters of Eq. (27) or (28) for the investigated 1-alkanols are given in Table 2.

4. Conclusions

The solubility of 1-alkanols in water can be calculated with Eq. (1) up to the boiling temperature of water or even

higher. The solubility of water in 1-alkanols can be calculated with EoSC in conjunction with Eq. (11). Empirical constants used in the calculations were obtained from regression of all available solubility data, which assures the good accuracy of the constants determination. Once these constants are established, no experimental solubility data are necessary for the calculation of the mutual solubility. The calculated solubility was treated as reference values for selecting the recommended data. This approach allows us to have confidence in the internal consistency and good quality of the recommended data.

5. Description of Tables Containing the Recommended Data

Each system is presented in separate table, which includes LLE data along the three phase equilibrium line and optionally the corresponding figures.

The tables contain data, which deviate from the calculated solubility by less than 10% or 20%. If more data at the same temperature fulfills the assumed limit, then only one selected experimental point was chosen and placed in the table. The selection was done taking into account the agreement with the recommended data at other temperatures and the agreement with the calculated (reference) solubility. The tables contain experimental mole fractions of the solute and the corresponding calculated values. Symbol x_1 denotes mole fraction of 1-alkanol in water-rich phase, x_2 denotes mole fraction of water in the 1-alkanol-rich phase. Values denoted by $x_{1,\mathrm{calc}}$ were calculated with Eq. (11) or (18). The data necessary for using these equations are given in Table 1. Values of $x_{2,\mathrm{calc}}$ were calculated with Eq. (27) or (28). Coefficients of these equations are given in Table 2. These coefficients were found in the following way: (1) LLE calculations were performed with EOSC using solubility of 1-alkanols predicted with Eq. (11) or (18) and (2) the calculated solubility of water was approximated with Eq. (27) or (28). See Tables 3–21.

TABLE 3. 1-Butanol–water

Components	References
(1) 1-Butanol; $C_4H_{10}O$; [71-36-3] (2) Water; H_2O; [7732-18-5]	[1]Y. Aoki and T. Moriyoshi, J. Chem. Thermodyn. **10**, 1173 (1978). [2]J. A. V. Butler, D. W. Thomson, and W. H. Maclennan, J. Chem. Soc. **1933**, 674 (1933). [3]R. De Santis, L. Marrelli, and P. N. Muscetta, J. Chem. Eng. Data **21**, 324 (1976). [4]L. Erichsen, Brennst.-Chem. **33**, 166 (1952). [5]C. F. Fu, C. L. King, Y. F. Chang, and C. X. Xeu, Hua Kung Hsueh Pao, **3**, 281 (1980). [6] H. Fühner, Ber. Dtsch. Chem. Ges. **57**, 510 (1924). [7]A. C. GomezMarigliano, M. B. Gramajo de Doz, and H. N. Solimo, Fluid Phase Equilib. **153**, 279 (1998). [8]M. Hayashi and T. Sasaki, Bull. Chem. Soc. Jpn. **29**, 857 (1956). [9]A. E. Hill and W. M. Malisoff, J. Am. Chem. Soc. **48**, 918 (1926). [10]D. C. Jones, J. Chem. Soc. **1929**, 799 (1929). [11]M-J. Lee, L-H. Tsai, G-B. Hong, and H-M. Lin, Fluid Phase Equilib. **216**, 219 (2004). [12]J. F. McCants, J. H. Jones, and W. H. Hopson, Ind. Eng. Chem. **45**, 454 (1953). [13]A. J. Müller, L. I. Pugsley, and J. B. Ferguson, J. Phys. Chem. **35**, 1314 (1931). [14]K. Ochi, M. Tada, and K. Koijma, Fluid Phase Equilib. **56**, 341 (1990). [15]O. Prochazka, J. Sushka, and J. Pick, Collect. Czech. Chem. Commun. **40**, 781 (1975). [16]L. A. Reber, W. M. McNabb, and W. A. Lucasse, J. Phys. Chem. **46**, 500 (1942). [17]F. Ruiz, M. I. Galan, D. Prats, and A. M. Ancheta, J. Chem. Eng. Data **29**, 143 (1984). [18]F. Ruiz, D. Prats, and V. Gomis, J. Chem. Eng. Data **29**, 147 (1984). [19]R. Stephenson and J. Stuart, J. Chem. Eng. Data **31**, 56 (1986).

Reference liquid–liquid equilibrium data

Water rich phase			Alcohol rich phase		
T (K)	$x_{1,exp}$	$x_{1,calc}$	T (K)	$x_{2,exp}$	$x_{2,calc}$
273.15	0.0275 (Ref. 6)	0.0276	268.15	0.494 (Ref. 10)	0.496
278.15	0.0250 (Ref. 9)	0.0250	273.15	0.497 (Ref. 10)	0.496
283.15	0.0230 (Ref. 4)	0.0229	286.15	0.500 (Ref. 10)	0.501
288.15	0.0213 (Ref. 9)	0.0213	289.10	0.502 (Ref. 17)	0.502
290.10	0.0210 (Ref. 17)	0.0207	290.10	0.502 (Ref. 17)	0.503
293.10	0.0200 (Ref. 17)	0.0200	291.10	0.504 (Ref. 17)	0.504
295.75	0.0193 (Ref. 2)	0.0194	292.10	0.505 (Ref. 17)	0.505
298.15	0.0189 (Ref. 9)	0.0189	293.15	0.507 (Ref. 3)	0.506
301.21	0.0182 (Ref. 2)	0.0184	296.55	0.511 (Ref. 2)	0.509
303.15	0.0180 (Ref. 8)	0.0181	298.10	0.510 (Ref. 18)	0.510
308.15	0.0175 (Ref. 9)	0.0174	300.60	0.514 (Ref. 2)	0.513
310.85	0.0170 (Ref. 12)	0.0172	302.97	0.514 (Ref. 10)	0.515
313.15	0.0170 (Ref. 3)	0.0170	303.95	0.516 (Ref. 19)	0.516
323.15	0.0165 (Ref. 9)	0.0164	308.15	0.523 (Ref. 9)	0.521
333.15	0.0166 (Ref. 9)	0.0164	310.85	0.525 (Ref. 12)	0.525
342.65	0.0171 (Ref. 1)	0.0168	313.25	0.528 (Ref. 19)	0.528
348.15	0.0174 (Ref. 13)	0.0173	323.15	0.544 (Ref. 4)	0.544
353.15	0.0180 (Ref. 11)	0.0179	331.65	0.561 (Ref. 10)	0.559
355.04	0.0180 (Ref. 14)	0.0181	333.15	0.562 (Ref. 4)	0.562
362.65	0.0193 (Ref. 1)	0.0196	343.15	0.583 (Ref. 11)	0.584
366.15	0.0208 (Ref. 11)	0.0205	348.15	0.594 (Ref. 13)	0.596
371.05	0.0227 (Ref. 9)	0.0221	353.25	0.608 (Ref. 19)	0.609
373.15	0.0232 (Ref. 4)	0.0229	363.15	0.639 (Ref. 11)	0.637
376.45	0.0245 (Ref. 14)	0.0245	366.15	0.647 (Ref. 5)	0.647
380.35	0.0270 (Ref. 15)	0.0271	372.45	0.672 (Ref. 1)	0.670
384.75	0.0310 (Ref. 15)	0.0311	378.15	0.695 (Ref. 13)	0.694
387.15	0.0340 (Ref. 15)	0.0340	382.95	0.719 (Ref. 1)	0.719
391.40	0.0412 (Ref. 16)	0.0415	388.15	0.751 (Ref. 11)	0.751
395.85	0.0536 (Ref. 1)	0.0544	392.95	0.791 (Ref. 15)	0.789
398.15	0.0642 (Ref. 7)	0.0648	395.85	0.817 (Ref. 1)	0.817

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TABLE 4. 2-Methyl-1-propanol–water

Components	References
(1) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1] (2) Water; H_2O; [7732-18-5]	[5]C. F. Fu, C. L. King, Y. F. Chang, and C. X. Xeu, Hua Kung Hsueh Pao **3**, 281 (1980). [19]R. Stephenson and J. Stuart, J. Chem. Eng. Data **31**, 56 (1986). [44]T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992). [48]R. V. Lyzlova, Zh. Prikl. Khim. (Leningrad) **52**, 545 (1979). [59]M. Ratouis and M. Dode, Bull. Soc. Chim. Fr. 3318 (1965). [73]W. Alexejew, Ann. Phys. Chem. **28**, 305 (1886). [74]P. Brun, C. R. Hebd. Seances Acad. Sci. **180**, 1745 (1925). [75]L. Janecke, Z. Phys. Chem., Abt. A **164**, 401 (1933). [76]A. Michels, Arch. Neerl. Sci. Exactes Nat., Ser. 3A **6**, 127 (1923). [77]T. Moriyoshi, Y. Aoki, and H. Kamiyama, J. Chem. Thermodyn. **9**, 495 (1977). [78]A. S. Mozzhukhin, L. A. Serafimov, V. A. Mitropolskaya, and T. S. Rudakovskaya, Khim. Tekhnol. Topl. Masel, **11**, 11 (1966).

Reference liquid–liquid equilibrium data

Water rich phase			Alcohol rich phase		
T (K)	$x_{1,\mathrm{exp}}$	$x_{1,\mathrm{calc}}$	T (K)	$x_{2,\mathrm{exp}}$	$x_{2,\mathrm{calc}}$
273.15	0.0320 (Ref. 74)	0.0328	267.25	0.405 (Ref. 76)	0.409
280.15	0.0275 (Ref. 76)	0.0280	270.25	0.411 (Ref. 76)	0.412
282.95	0.0264 (Ref. 19)	0.0265	274.15	0.415 (Ref. 76)	0.417
288.05	0.0241 (Ref. 76)	0.0242	280.25	0.422 (Ref. 76)	0.425
292.10	0.0230 (Ref. 76)	0.0228	286.05	0.435 (Ref. 76)	0.433
293.15	0.0220 (Ref. 78)	0.0224	291.35	0.441 (Ref. 76)	0.441
294.75	0.0219 (Ref. 76)	0.0219	297.05	0.450 (Ref. 76)	0.450
298.10	0.0210 (Ref. 44)	0.0210	303.75	0.461 (Ref. 19)	0.461
300.55	0.0207 (Ref. 76)	0.0205	308.85	0.469 (Ref. 76)	0.470
303.15	0.0202 (Ref. 59)	0.0200	311.85	0.479 (Ref. 76)	0.476
309.45	0.0193 (Ref. 76)	0.0190	314.15	0.482 (Ref. 76)	0.480
313.55	0.0188 (Ref. 19)	0.0185	323.25	0.496 (Ref. 19)	0.498
323.25	0.0182 (Ref. 19)	0.0179	333.35	0.516 (Ref. 19)	0.520
332.65	0.0174 (Ref. 77)	0.0178	336.95	0.525 (Ref. 76)	0.528
333.35	0.0181 (Ref. 19)	0.0178	341.45	0.540 (Ref. 76)	0.538
343.45	0.0178 (Ref. 19)	0.0183	343.45	0.542 (Ref. 19)	0.543
352.35	0.0191 (Ref. 77)	0.0192	353.65	0.566 (Ref. 19)	0.569
353.35	0.0193 (Ref. 76)	0.0194	358.15	0.576 (Ref. 76)	0.581
360.15	0.0207 (Ref. 76)	0.0205	360.05	0.589 (Ref. 76)	0.586
362.95	0.0191 (Ref. 5)	0.0211	363.85	0.599 (Ref. 19)	0.597
363.15	0.0210 (Ref. 48)	0.0212	367.75	0.613 (Ref. 76)	0.609
365.75	0.0219 (Ref. 76)	0.0218	372.15	0.619 (Ref. 77)	0.623
367.25	0.0230 (Ref. 76)	0.0222	382.05	0.662 (Ref. 77)	0.660
372.25	0.0241 (Ref. 76)	0.0238	387.65	0.687 (Ref. 76)	0.685
380.85	0.0280 (Ref. 75)	0.0277	390.35	0.696 (Ref. 76)	0.699
381.15	0.0280 (Ref. 75)	0.0279	393.85	0.716 (Ref. 76)	0.720
386.15	0.0315 (Ref. 73)	0.0314	396.85	0.743 (Ref. 77)	0.740
390.25	0.0354 (Ref. 76)	0.0354	399.65	0.758 (Ref. 73)	0.762
395.05	0.0412 (Ref. 76)	0.0422	402.25	0.785 (Ref. 76)	0.785
406.15	0.0813 (Ref. 75)	0.0795	404.95	0.815 (Ref. 76)	0.814

Other references:

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[42]T. M. Letcher, S. Ravindran, and S. E. Radloff, Fluid Phase Equilib. **69**, 251 (1991).
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TABLE 5. 2,2-Dimethyl-1-propanol–water

Components
(1) 2,2-Dimethyl-1-propanol; $C_5H_{12}O$; [75-84-3]
(2) Water; H_2O; [7732-18-5]

References
[59]M. Ratouis and M. Dode, Bull. Soc. Chim. Fr. 3318 (1965)
[88]P. M. Ginnings and R. Baum, J. Am. Chem. Soc. **59**, 1111 1937).
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Reference liquid–liquid equilibrium data

	Water rich phase		Alochol rich phase
T (K)	$x_{1,\mathrm{exp}}$	$x_{1,\mathrm{calc}}$	$x_{2,\mathrm{calc}}$
285.15	7.80×10^{-3} (Ref. 89)	8.17×10^{-3}	0.337
291.95	7.30×10^{-3} (Ref. 89)	7.38×10^{-3}	0.348
293.15	7.88×10^{-3} (Ref. 88)	7.27×10^{-3}	0.350
298.15	6.75×10^{-3} (Ref. 59)	6.84×10^{-3}	0.359
303.15	6.69×10^{-3} (Ref. 59)	6.51×10^{-3}	0.367
313.15	5.60×10^{-3} (Ref. 89)	6.04×10^{-3}	0.385
333.15	5.20×10^{-3} (Ref. 89)	5.70×10^{-3}	0.421
353.15	5.40×10^{-3} (Ref. 89)	5.95×10^{-3}	0.459

TABLE 6. Methyl-1-butanol–water

Components
(1) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]
(2) Water; H_2O; [7732-18-5]

References
[59]M. Ratouis and M. Dode, Bull. Soc. Chim. Fr., 3318 (1965).
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[89]R. Stephenson, J. Stuart, and M. Tabak, J. Chem. Eng. Data **29**, 287 (1984).

Reference liquid–liquid equilibrium data

Water rich phase			Alcohol rich phase		
T (K)	$x_{1,\mathrm{exp}}$	$x_{1,\mathrm{calc}}$	T (K)	$x_{2,\mathrm{exp}}$	$x_{2,\mathrm{calc}}$
273.65	8.30×10^{-3} (Ref. 89)	8.49×10^{-3}	292.75	0.307 (Ref. 89)	0.327
282.85	7.10×10^{-3} (Ref. 89)	7.10×10^{-3}	293.15	0.325 (Ref. 88)	0.328
292.75	5.90×10^{-3} (Ref. 89)	6.12×10^{-3}	298.15	0.331 (Ref. 88)	0.335
293.15	6.67×10^{-3} (Ref. 88)	6.09×10^{-3}	302.75	0.309 (Ref. 89)	0.342
298.15	6.21×10^{-3} (Ref. 88)	5.74×10^{-3}	303.15	0.333 (Ref. 88)	0.343
302.75	5.20×10^{-3} (Ref. 89)	5.49×10^{-3}	312.45	0.325 (Ref. 89)	0.357
303.15	5.45×10^{-3} (Ref. 59)	5.47×10^{-3}	322.75	0.340 (Ref. 89)	0.375
312.45	4.90×10^{-3} (Ref. 89)	5.11×10^{-3}	342.65	0.370 (Ref. 89)	0.411
322.75	4.60×10^{-3} (Ref. 89)	4.90×10^{-3}			
342.65	4.70×10^{-3} (Ref. 89)	4.91×10^{-3}			
352.85	4.80×10^{-3} (Ref. 89)	5.098×10^{-3}			
363.95	5.10×10^{-3} (Ref. 89)	5.42×10^{-3}			

Other references:
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TABLE 7. 3-Methyl-1-butanol–water

Components
(1) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]
(2) Water; H_2O; [7732-18-5]

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Reference liquid–liquid equilibrium data

Water rich phase			Alcohol rich phase		
T (K)	$x_{1,\mathrm{exp}}$	$x_{1,\mathrm{calc}}$	T (K)	$x_{2,\mathrm{exp}}$	$x_{2,\mathrm{calc}}$
273.15	7.90×10^{-3} (Ref. 89)	8.08×10^{-3}	273.15	0.326 (Ref. 74)	0.300
283.25	6.60×10^{-3} (Ref. 89)	6.64×10^{-3}	283.25	0.336 (Ref. 89)	0.312
288.15	6.36×10^{-3} (Ref. 93)	6.14×10^{-3}	288.15	0.335 (Ref. 93)	0.318
292.10	5.40×10^{-3} (Ref. 80)	5.82×10^{-3}	292.10	0.340 (Ref. 32)	0.324
292.95	5.50×10^{-3} (Ref. 89)	5.75×10^{-3}	292.95	0.343 (Ref. 89)	0.325
293.15	5.89×10^{-3} (Ref. 93)	5.74×10^{-3}	293.15	0.335 (Ref. 93)	0.325
298.15	5.57×10^{-3} (Ref. 88)	5.41×10^{-3}	298.15	0.330 (Ref. 90)	0.332
298.20	5.70×10^{-3} (Ref. 94)	5.41×10^{-3}	298.20	0.341 (Ref. 94)	0.332
303.15	5.27×10^{-3} (Ref. 88)	5.16×10^{-3}	303.15	0.337 (Ref. 63)	0.340
303.25	5.36×10^{-3} (Ref. 93)	5.15×10^{-3}	303.20	0.337 (Ref. 95)	0.340
303.35	4.80×10^{-3} (Ref. 89)	5.15×10^{-3}	303.35	0.359 (Ref. 89)	0.340
313.15	4.60×10^{-3} (Ref. 92)	4.81×10^{-3}	308.15	0.358 (Ref. 91)	0.347
332.95	4.60×10^{-3} (Ref. 89)	4.59×10^{-3}	313.15	0.364 (Ref. 89)	0.355
333.15	4.57×10^{-3} (Ref. 40)	4.59×10^{-3}	322.65	0.389 (Ref. 96)	0.370
343.15	4.40×10^{-3} (Ref. 89)	4.66×10^{-3}	323.05	0.390 (Ref. 89)	0.371
353.15	4.60×10^{-3} (Ref. 89)	4.84×10^{-3}	332.95	0.399 (Ref. 89)	0.388
363.15	4.70×10^{-3} (Ref. 89)	5.13×10^{-3}	333.15	0.400 (Ref. 40)	0.389
			343.15	0.420 (Ref. 89)	0.407
			353.15	0.433 (Ref. 89)	0.427
			363.15	0.453 (Ref. 89)	0.447

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TABLE 8. 1-Pentanol–water

Components
(1) 1-Pentanol; $C_5H_{12}O$; [71-41-0]
(2) Water; H_2O; [7732-18-5]

References

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Reference liquid-liquid equilibrium data

Water rich phase			Alcohol rich phase		
T (K)	$x_{1,\mathrm{exp}}$	$X_{1,\mathrm{calc}}$	T (K)	$x_{2,\mathrm{exp}}$	$x_{2,\mathrm{calc}}$
273.15	7.00×10^{-3} (Ref. 89)	6.78×10^{-3}	273.15	0.340 (Ref. 89)	0.351
283.15	5.50×10^{-3} (Ref. 4)	5.51×10^{-3}	283.15	0.339 (Ref. 111)	0.349
283.35	5.40×10^{-3} (Ref. 89)	5.49×10^{-3}	283.35	0.346 (Ref. 89)	0.349
288.20	4.80×10^{-3} (Ref. 72)	5.11×10^{-3}	285.15	0.357 (Ref. 109)	0.349
293.15	4.60×10^{-3} (Ref. 97)	4.72×10^{-3}	288.15	0.362 (Ref. 70)	0.350
293.35	4.70×10^{-3} (Ref. 89)	4.71×10^{-3}	292.10	0.348 (Ref. 80)	0.352
298.15	4.50×10^{-3} (Ref. 32)	4.44×10^{-3}	293.15	0.347 (Ref. 112)	0.353
303.15	4.21×10^{-3} (Ref. 88)	4.23×10^{-3}	293.35	0.358 (Ref. 89)	0.353
303.75	4.20×10^{-3} (Ref. 89)	4.21×10^{-3}	298.15	0.357 (Ref. 24)	0.356
310.20	3.90×10^{-3} (Ref. 105)	4.02×10^{-3}	298.70	0.355 (Ref. 110)	0.357
313.15	3.90×10^{-3} (Ref. 4)	3.94×10^{-3}	302.15	0.352 (Ref. 114)	0.359
313.35	3.90×10^{-3} (Ref. 89)	3.94×10^{-3}	303.15	0.369 (Ref. 70)	0.360
323.15	3.80×10^{-3} (Ref. 89)	3.80×10^{-3}	303.75	0.366 (Ref. 89)	0.361
333.15	3.60×10^{-3} (Ref. 4)	3.79×10^{-3}	305.15	0.352 (Ref. 113)	0.362
333.45	3.80×10^{-3} (Ref. 89)	3.79×10^{-3}	308.15	0.377 (Ref. 70)	0.365
343.15	4.00×10^{-3} (Ref. 89)	3.88×10^{-3}	309.15	0.357 (Ref. 113)	0.366
353.15	4.10×10^{-3} (Ref. 89)	4.08×10^{-3}	313.15	0.365 (Ref. 40)	0.371
358.15	4.20×10^{-3} (Ref. 106)	4.22×10^{-3}	313.35	0.379 (Ref. 89)	0.371
363.15	4.10×10^{-3} (Ref. 4)	4.39×10^{-3}	314.65	0.370 (Ref. 114)	0.372
363.85	4.60×10^{-3} (Ref. 89)	4.41×10^{-3}	323.15	0.384 (Ref. 106)	0.383
367.15	4.20×10^{-3} (Ref. 114)	4.55×10^{-3}	323.20	0.384 (Ref. 107)	0.383
368.15	4.20×10^{-3} (Ref. 106)	4.59×10^{-3}	329.15	0.389 (Ref. 114)	0.391
373.15	4.70×10^{-3} (Ref. 4)	4.83×10^{-3}	333.15	0.391 (Ref. 111)	0.397
383.15	5.40×10^{-3} (Ref. 4)	5.42×10^{-3}	339.15	0.409 (Ref. 114)	0.407
393.15	6.30×10^{-3} (Ref. 4)	6.24×10^{-3}	343.15	0.404 (Ref. 111)	0.414
403.15	7.50×10^{-3} (Ref. 4)	7.35×10^{-3}	346.65	0.422 (Ref. 114)	0.420
413.15	9.20×10^{-3} (Ref. 4)	8.91×10^{-3}	353.15	0.422 (Ref. 111)	0.432
423.15	1.14×10^{-2} (Ref. 4)	1.12×10^{-2}	358.15	0.400 (Ref. 106)	0.442
433.15	1.49×10^{-2} (Ref. 4)	1.49×10^{-2}	359.65	0.452 (Ref. 114)	0.445
443.15	2.11×10^{-2} (Ref. 4)	2.11×10^{-2}	363.15	0.450 (Ref. 4)	0.452
			363.85	0.463 (Ref. 89)	0.454
			368.15	0.435 (Ref. 106)	0.463
			368.45	0.519 (Ref. 108)	0.464
			368.95	0.421 (Ref. 104)	0.465
			373.15	0.480 (Ref. 4)	0.475
			383.15	0.511 (Ref. 4)	0.500

TABLE 8. 1-Pentanol–water—Continued

Components	References			
		393.15	0.544 (Ref. 4)	0.529
		403.15	0.578 (Ref. 4)	0.561
		413.15	0.615 (Ref. 4)	0.598
		423.15	0.655 (Ref. 4)	0.640
		433.15	0.697 (Ref. 4)	0.689
		443.15	0.745 (Ref. 4)	0.746

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TABLE 9. 2-Ethyl-1-butanol–water

Components	References
(1) 2-Ethyl-1-butanol; $C_6H_{14}O$; [97-95-0]	[19]R. Stephenson and J. Stuart, J. Chem. Eng. Data **31**, 56 (1986).
(2) Water; H_2O; [7732-18-5]	[59]M. Ratouis and M. Dode, Bull. Soc. Chim. Fr. 3318 (1965).

Reference liquid–liquid equilibrium data

Water rich phase			Alcohol rich phase		
T (K)	$x_{1,\mathrm{exp}}$	$x_{1,\mathrm{calc}}$	T (K)	$x_{2,\mathrm{exp}}$	$x_{2,\mathrm{exp}}$
293.35	1.63×10^{-3} (Ref. 19)	1.63×10^{-3}	273.15	0.185 (Ref. 19)	0.189
303.15	1.63×10^{-3} (Ref. 59)	1.50×10^{-3}	282.85	0.202 (Ref. 19)	0.199
304.05	1.47×10^{-3} (Ref. 19)	1.50×10^{-3}	293.35	0.217 (Ref. 19)	0.212
313.45	1.46×10^{-3} (Ref. 19)	1.43×10^{-3}	304.05	0.230 (Ref. 19)	0.225
323.15	1.40×10^{-3} (Ref. 19)	1.42×10^{-3}	313.45	0.246 (Ref. 19)	0.238
333.45	1.44×10^{-3} (Ref. 19)	1.44×10^{-3}	323.15	0.260 (Ref. 19)	0.253
343.35	1.42×10^{-3} (Ref. 19)	1.51×10^{-3}	333.45	0.274 (Ref. 19)	0.269
353.45	1.55×10^{-3} (Ref. 19)	1.62×10^{-3}	343.35	0.293 (Ref. 19)	0.286
363.65	1.67×10^{-3} (Ref. 19)	1.78×10^{-3}	353.45	0.297 (Ref. 19)	0.304
			363.65	0.318 (Ref. 19)	0.324

Other references:
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TABLE 10. 1-Hexanol–water

Components

(1) 1-Hexanol; $C_6H_{14}O$; [111-27-3]

(2) Water; H_2O; [7732-18-5]

References

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Reference liquid–liquid equilibrium data

Water rich phase			Alcohol rich phase		
T (K)	$x_{1,exp}$	$x_{1,calc}$	T (K)	$x_{2,exp}$	$x_{2,calc}$
273.15	1.40×10^{-3} (Ref. 4)	1.48×10^{-3}	273.15	0.283 (Ref. 89)	0.283
278.66	1.40×10^{-3} (Ref. 128)	1.33×10^{-3}	283.15	0.280 (Ref. 129)	0.288
280.00	1.36×10^{-3} (Ref. 128)	1.30×10^{-3}	283.35	0.289 (Ref. 89)	0.288
283.15	1.20×10^{-3} (Ref. 4)	1.24×10^{-3}	293.15	0.293 (Ref. 89)	0.295
284.15	1.25×10^{-3} (Ref. 128)	1.22×10^{-3}	298.15	0.288 (Ref. 24)	0.299
286.09	1.21×10^{-3} (Ref. 128)	1.19×10^{-3}	302.85	0.297 (Ref. 89)	0.303
287.83	1.18×10^{-3} (Ref. 128)	1.16×10^{-3}	303.15	0.299 (Ref. 126)	0.303
290.19	1.14×10^{-3} (Ref. 128)	1.13×10^{-3}	308.15	0.305 (Ref. 129)	0.308
293.15	1.10×10^{-3} (Ref. 4)	1.10×10^{-3}	312.95	0.312 (Ref. 89)	0.313
296.14	1.06×10^{-3} (Ref. 128)	1.06×10^{-3}	313.15	0.289 (Ref. 4)	0.313
298.15	1.06×10^{-3} (Ref. 37)	1.05×10^{-3}	323.15	0.318 (Ref. 89)	0.325
300.14	1.02×10^{-3} (Ref. 128)	1.03×10^{-3}	333.15	0.334 (Ref. 89)	0.338
302.85	1.00×10^{-3} (Ref. 89)	1.01×10^{-3}	343.15	0.354 (Ref. 4)	0.352
304.07	9.99×10^{-4} (Ref. 128)	1.01×10^{-3}	343.45	0.351 (Ref. 89)	0.353
306.24	9.85×10^{-4} (Ref. 128)	9.96×10^{-4}	353.15	0.377 (Ref. 4)	0.369
308.00	9.00×10^{-4} (Ref. 127)	9.89×10^{-4}	353.45	0.365 (Ref. 89)	0.369
312.95	9.00×10^{-4} (Ref. 89)	9.74×10^{-4}	363.15	0.398 (Ref. 4)	0.386
313.10	1.00×10^{-3} (Ref. 130)	9.74×10^{-4}	363.45	0.374 (Ref. 89)	0.387
318.00	9.00×10^{-4} (Ref. 127)	9.68×10^{-4}	373.15	0.419 (Ref. 4)	0.406
323.15	9.10×10^{-4} (Ref. 6)	9.70×10^{-4}	383.15	0.442 (Ref. 4)	0.426
333.15	9.40×10^{-4} (Ref. 6)	9.97×10^{-4}	393.15	0.465 (Ref. 4)	0.449
343.15	1.00×10^{-3} (Ref. 6)	1.05×10^{-3}	403.15	0.490 (Ref. 4)	0.474
353.15	1.10×10^{-3} (Ref. 6)	1.14×10^{-3}	413.15	0.516 (Ref. 4)	0.501
353.45	1.10×10^{-3} (Ref. 89)	1.14×10^{-3}	423.15	0.546 (Ref. 4)	0.530
363.15	1.21×10^{-3} (Ref. 6)	1.26×10^{-3}	433.15	0.576 (Ref. 4)	0.562
373.15	1.40×10^{-3} (Ref. 4)	1.42×10^{-3}	443.15	0.608 (Ref. 4)	0.597
383.15	1.60×10^{-3} (Ref. 4)	1.63×10^{-3}	453.15	0.647 (Ref. 4)	0.637
393.15	1.90×10^{-3} (Ref. 4)	1.91×10^{-3}	463.15	0.690 (Ref. 4)	0.682
403.15	2.10×10^{-3} (Ref. 4)	2.26×10^{-3}	473.15	0.740 (Ref. 4)	0.736
443.15	5.00×10^{-3} (Ref. 4)	5.25×10^{-3}	483.15	0.799 (Ref. 4)	0.803
453.15	6.60×10^{-3} (Ref. 4)	6.83×10^{-3}	493.15	0.876 (Ref. 4)	0.888
463.15	9.00×10^{-3} (Ref. 4)	9.18×10^{-3}			
473.15	1.28×10^{-2} (Ref. 4)	1.29×10^{-2}			
483.15	1.89×10^{-2} (Ref. 4)	1.93×10^{-2}			
493.15	3.42×10^{-2} (Ref. 4)	3.19×10^{-2}			

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TABLE 11. 2-Methyl-1-pentanol–water

Components
(1) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]
(2) Water; H_2O; [7732-18-5]

References
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[90] E. D. Jr. Crittenden and A. N. Hixon, Ind. Eng. Chem. **46**, 265 (1954).

Reference liquid–liquid equilibrium data

Water rich phase			Alcohol rich phase		
T (K)	$x_{1,\mathrm{exp}}$	$x_{1,\mathrm{calc}}$	T (K)	$x_{2,\mathrm{exp}}$	$x_{2,\mathrm{calc}}$
292.75	1.56×10^{-3} (Ref. 89)	1.42×10^{-3}	283.15	0.224 (Ref. 89)	0.211
298.15	1.44×10^{-3} (Ref. 59)	1.35×10^{-3}	292.45	0.227 (Ref. 89)	0.223
303.15	1.35×10^{-3} (Ref. 59)	1.31×10^{-3}	298.15	0.240 (Ref. 90)	0.230
303.95	1.40×10^{-3} (Ref. 89)	1.30×10^{-3}	304.05	0.240 (Ref. 89)	0.238
313.45	1.37×10^{-3} (Ref. 89)	1.25×10^{-3}	313.15	0.245 (Ref. 89)	0.251
323.15	1.33×10^{-3} (Ref. 89)	1.24×10^{-3}	323.15	0.264 (Ref. 89)	0.267
333.45	1.35×10^{-3} (Ref. 89)	1.27×10^{-3}	333.25	0.278 (Ref. 89)	0.283
343.25	1.37×10^{-3} (Ref. 89)	1.33×10^{-3}	343.35	0.289 (Ref. 89)	0.301
353.45	1.49×10^{-3} (Ref. 89)	1.43×10^{-3}	352.95	0.304 (Ref. 89)	0.318
363.85	1.64×10^{-3} (Ref. 89)	1.57×10^{-3}	363.65	0.306 (Ref. 89)	0.339

TABLE 12. 2,2-Dimethyl-1-butanol–water

Components
(1) 2,2-Dimethyl-1-butanol; $C_6H_{14}O$; [1185-33-7]
(2) Water; H_2O; [7732-18-5]

References
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Reference liquid–liquid equilibrium data

	Water rich phase		Alcohol rich phase
T (K)	$x_{1,\mathrm{exp}}$	$x_{1,\mathrm{calc}}$	$x_{2,\mathrm{calc}}$
293.15	1.46×10^{-3} (Ref. 88)	1.46×10^{-3}	0.213
298.15	1.35×10^{-3} (Ref. 88)	1.39×10^{-3}	0.220
303.15	1.26×10^{-3} (Ref. 88)	1.34×10^{-3}	0.226

Other references:
[59]M. Ratouis and M. Dode, Bull. Soc. Chim. Fr. 3318 (1965).

TABLE 13. 1-Heptanol–water

Components
(1) 1-Heptanol; $C_7H_{16}O$; [111-70-6]
(2) Water; H_2O; [7732-18-5]

References
[4]L. Erichsen, Brennst.-Chem. **33**, 166 (1952).
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Reference liquid–liquid equilibrium data

Water rich phase			Alcohol rich phase		
T (K)	$x_{1,exp}$	$x_{1,calc}$	T (K)	$x_{2,exp}$	$x_{2,calc}$
273.15	3.67×10^{-4} (Ref. 89)	3.43×10^{-4}	288.15	0.282 (Ref. 70)	0.257
283.69	3.10×10^{-4} (Ref. 128)	2.91×10^{-4}	293.15	0.243 (Ref. 4)	0.260
288.23	2.90×10^{-4} (Ref. 128)	2.76×10^{-4}	298.15	0.284 (Ref. 123)	0.263
291.09	2.78×10^{-4} (Ref. 128)	2.69×10^{-4}	303.15	0.261 (Ref. 4)	0.267
293.15	2.67×10^{-4} (Ref. 97)	2.64×10^{-4}	308.15	0.292 (Ref. 134)	0.271
295.05	2.66×10^{-4} (Ref. 128)	2.60×10^{-4}	313.15	0.282 (Ref. 4)	0.275
297.11	2.61×10^{-4} (Ref. 128)	2.57×10^{-4}	323.15	0.302 (Ref. 4)	0.285
299.19	2.56×10^{-4} (Ref. 128)	2.54×10^{-4}	473.15	0.661 (Ref. 4)	0.602
301.17	2.54×10^{-4} (Ref. 128)	2.52×10^{-4}	483.15	0.692 (Ref. 4)	0.640
303.15	2.50×10^{-4} (Ref. 2)	2.50×10^{-4}	493.15	0.727 (Ref. 4)	0.684
306.05	2.50×10^{-4} (Ref. 128)	2.48×10^{-4}	503.15	0.767 (Ref. 4)	0.741
308.05	2.49×10^{-4} (Ref. 128)	2.47×10^{-4}	513.15	0.821 (Ref. 4)	0.825
312.95	2.58×10^{-4} (Ref. 89)	2.47×10^{-4}	518.15	0.863 (Ref. 4)	0.886
323.25	2.51×10^{-4} (Ref. 89)	2.54×10^{-4}			
333.15	2.76×10^{-4} (Ref. 89)	2.69×10^{-4}			
343.25	3.17×10^{-4} (Ref. 89)	2.94×10^{-4}			
353.25	3.37×10^{-4} (Ref. 89)	3.29×10^{-4}			
363.65	3.78×10^{-4} (Ref. 89)	3.80×10^{-4}			
373.15	4.43×10^{-4} (Ref. 6)	4.41×10^{-4}			
383.15	5.21×10^{-4} (Ref. 6)	5.24×10^{-4}			
393.15	6.69×10^{-4} (Ref. 6)	6.34×10^{-4}			
403.15	8.02×10^{-4} (Ref. 6)	7.77×10^{-4}			
413.15	1.00×10^{-3} (Ref. 4)	9.65×10^{-4}			
423.15	1.20×10^{-3} (Ref. 4)	1.21×10^{-3}			
433.15	1.50×10^{-3} (Ref. 4)	1.54×10^{-3}			
443.15	1.90×10^{-3} (Ref. 4)	1.96×10^{-3}			
453.15	2.50×10^{-3} (Ref. 4)	2.53×10^{-3}			
463.15	3.20×10^{-3} (Ref. 4)	3.30×10^{-3}			
473.15	4.20×10^{-3} (Ref. 4)	4.33×10^{-3}			
483.15	5.60×10^{-3} (Ref. 4)	5.78×10^{-3}			
493.15	7.60×10^{-3} (Ref. 4)	7.89×10^{-3}			
503.15	1.10×10^{-2} (Ref. 4)	1.13×10^{-2}			
513.15	1.71×10^{-2} (Ref. 4)	1.77×10^{-2}			
518.15	2.45×10^{-2} (Ref. 4)	2.36×10^{-2}			

Other references:
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TABLE 14. 2-Ethyl-1-hexanol–water

Components

(1) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]

(2) Water; H_2O; [7732-18-5]

References

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Reference liquid–liquid equilibrium data

Water rich phase			Alcohol rich phase		
T (K)	$x_{1,exp}$	$x_{1,calc}$	T (K)	$x_{2,exp}$	$x_{2,calc}$
298.15	1.00×10^{-4} (Ref. 139)	9.78×10^{-5}	273.15	0.133 (Ref. 89)	0.136
323.35	1.02×10^{-4} (Ref. 89)	1.02×10^{-4}	282.95	0.142 (Ref. 89)	0.142
333.45	1.19×10^{-4} (Ref. 89)	1.11×10^{-4}	288.15	0.145 (Ref. 141)	0.145
353.25	1.50×10^{-4} (Ref. 89)	1.42×10^{-4}	293.15	0.151 (Ref. 89)	0.148
363.45	1.62×10^{-4} (Ref. 89)	1.67×10^{-4}	298.15	0.144 (Ref. 139)	0.151
			303.25	0.156 (Ref. 89)	0.155
			312.85	0.168 (Ref. 89)	0.163
			323.15	0.173 (Ref. 89)	0.172
			333.35	0.198 (Ref. 89)	0.183
			343.45	0.207 (Ref. 89)	0.194
			353.15	0.208 (Ref. 89)	0.206
			363.45	0.233 (Ref. 89)	0.220

Other references:

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TABLE 15. 1-Octanol–water

Components

(1) 1-Octanol; $C_8H_{18}O$; [111-87-5]

(2) Water; H_2O; [7732-18-5]

References

[4]L. Erichsen, Brennst.-Chem. **33**, 166 (1952).
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[40]O. A. Lavrova and T. M. Lesteva, Zh. Fiz. Khim. **50**, 1617 (1976).
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Reference liquid–liquid equilibrium data

Water rich phase			Alcohol rich phase		
T (K)	$x_{1,\mathrm{exp}}$	$x_{1,\mathrm{calc}}$	T (K)	$x_{2,\mathrm{exp}}$	$x_{2,\mathrm{calc}}$
288.15	7.30×10^{-5} (Ref. 72)	6.73×10^{-5}	288.15	0.262 (Ref. 70)	0.258
298.15	6.70×10^{-5} (Ref. 37)	6.37×10^{-5}	293.15	0.265 (Ref. 70)	0.259
298.20	6.78×10^{-5} (Ref. 148)	6.37×10^{-5}	298.15	0.260 (Ref. 20)	0.261
333.15	8.00×10^{-5} (Ref. 40)	7.42×10^{-5}	303.15	0.265 (Ref. 4)	0.263
428.20	5.40×10^{-4} (Ref. 147)	5.41×10^{-4}	308.15	0.271 (Ref. 70)	0.266
452.20	9.95×10^{-4} (Ref. 147)	1.08×10^{-3}	313.15	0.273 (Ref. 70)	0.269
			356.10	0.314 (Ref. 147)	0.308
			419.30	0.423 (Ref. 147)	0.410
			461.20	0.521 (Ref. 147)	0.511
			480.50	0.578 (Ref. 147)	0.569
			501.90	0.660 (Ref. 147)	0.648
			513.15	0.756 (Ref. 4)	0.705
			523.15	0.791 (Ref. 4)	0.786
			526.40	0.785 (Ref. 147)	0.825

Other references:

[2]J. A. V. Butler, D. W. Thomson, and W. H. Maclennan, J. Chem. Soc. **1933**, 674 (1933).
[89]R. Stephenson, J. Stuart, and M. Tabak, J. Chem. Eng. Data **29**, 287 (1984).
[90]E. D. Crittenden, Jr. and A. N. Hixon, Ind. Eng. Chem. **46**, 265 (1954).
[97]C. C. Addison, J. Chem. Soc. **98** (1945).
[120]J. C. Galan, J. M. M. Moreno, R. T. Valle, and A. R. Segado, An. Quim. Ser. A, **85**, 273 (1989).
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[155]I. K. Zhuravleva, E. F. Zhuravlev, and N. G. Lomakina, Zh. Fiz. Khim. **51**, 1700 (1977).

TABLE 16. 1-Nonanol–water

Components	References
(1) 1-Nonanol; $C_9H_{20}O$; [143-08-8]	[4]L. Erichsen, Brennst.-Chem. **33**, 166 (1952).
(2) Water; H_2O; [7732-18-5]	[19]R. Stephenson and J. Stuart, J. Chem. Eng. Data **31**, 56 (1986).
	[37]K. Kinoshita, H. Ishikawa, and K. Shinoda, Bull. Chem. Soc. Jpn. **31**, 1081 (1958).
	[70]S. Tokunaga, M. Manabe, and M. Koda, Mem. Niihama Technical College, Sci. Eng. **16**, 96 (1980).
	[72]R. Vochten and G. Petre, J. Colloid Interface Sci. **42**, 320 (1973).

Reference liquid–liquid equilibrium data

Water rich phase			Alcohol rich phase		
T (K)	$x_{1,exp}$	$x_{1,calc}$	T (K)	$x_{2,exp}$	$x_{2,calc}$
288.15	1.7×10^{-5} (Ref. 72)	1.66×10^{-5}	273.15	0.246 (Ref. 19)	0.252
298.15	1.7×10^{-5} (Ref. 37)	1.61×10^{-5}	282.95	0.236 (Ref. 19)	0.250
363.65	3.7×10^{-5} (Ref. 19)	3.64×10^{-5}	288.15	0.262 (Ref. 70)	0.251
			293.15	0.241 (Ref. 4)	0.251
			298.15	0.265 (Ref. 70)	0.252
			302.75	0.246 (Ref. 19)	0.253
			303.15	0.263 (Ref. 4)	0.253
			308.15	0.267 (Ref. 70)	0.255
			312.75	0.247 (Ref. 19)	0.257
			313.15	0.265 (Ref. 70)	0.257
			322.95	0.247 (Ref. 19)	0.263
			333.25	0.252 (Ref. 19)	0.269
			353.35	0.263 (Ref. 19)	0.286

Other references:
[69]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
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TABLE 17. 1-Decanol–water

Components	References
(1) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[19]R. Stephenson and J. Stuart, J. Chem. Eng. Data **31**, 56 (1986).
(2) Water; H_2O; [7732-18-5]	[37]K. Kinoshita, H. Ishikawa, and K. Shinoda, Bull. Chem. Soc. Jpn. **31**, 1081 (1958).
	[70]S. Tokunaga, M. Manabe, and M. Koda, Mem. Niihama Technical College, Sci. Eng. **16**, 96 (1980).
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	[158]C. C. Addison and S. K. Hutchinson, J. Chem. Soc, **1949**, 3387 (1949).

Reference liquid–liquid equilibrium data

Water rich phase			Alcohol rich phase		
T (K)	$x_{1,exp}$	$x_{1,calc}$	T (K)	$x_{2,exp}$	$x_{2,calc}$
293.15	4.00×10^{-6} (Ref. 158)	4.12×10^{-6}	283.65	0.240 (Ref. 155)	0.247
298.15	4.00×10^{-6} (Ref. 37)	4.13×10^{-6}	293.15	0.236 (Ref. 120)	0.247
			303.15	0.257 (Ref. 70)	0.248
			308.15	0.255 (Ref. 70)	0.250
			313.15	0.252 (Ref. 70)	0.251
			323.15	0.247 (Ref. 19)	0.255

Other references:
[4]L. Erichsen, Brennst.-Chem. **33**, 166 (1952).
[72]R. Vochten and G. Petre, J. Colloid Interface Sci. **42**, 320 (1973).
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TABLE 18. 1-Undecanol–water

Components
(1) 1-Undecanol; $C_{11}H_{24}O$; [112-42-5]
(2) Water; H_2O; [7732-18-5]

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Reference liquid–liquid equilibrium data

	Water rich phase	Alcohol rich phase	
T (K)	$x_{1,calc}$	$x_{2,exp}$	$x_{2,calc}$
288.15	1.05×10^{-6}	0.255 (Ref. 70)	0.244
292.95	1.05×10^{-6}	0.241 (Ref. 19)	0.244
293.15	1.05×10^{-6}	0.252 (Ref. 70)	0.244
298.15	1.07×10^{-6}	0.254 (Ref. 70)	0.244
303.05	1.10×10^{-6}	0.234 (Ref. 19)	0.244
303.15	1.10×10^{-6}	0.251 (Ref. 70)	0.244
308.15	1.15×10^{-6}	0.250 (Ref. 70)	0.245
313.15	1.21×10^{-6}	0.245 (Ref. 70)	0.246
313.45	1.22×10^{-6}	0.234 (Ref. 19)	0.246
323.15	1.40×10^{-6}	0.230 (Ref. 19)	0.249
333.25	1.69×10^{-6}	0.234 (Ref. 19)	0.254
343.35	2.12×10^{-6}	0.242 (Ref. 19)	0.259
353.25	2.73×10^{-6}	0.250 (Ref. 19)	0.266
363.65	3.66×10^{-6}	0.250 (Ref. 19)	0.274

TABLE 19. 1-Dodecanol–water

Components
(1) 1-Dodecanol; $C_{12}H_{26}O$; [27342-88-7]
(2) Water; H_2O; [7732-18-5]

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Reference liquid–liquid equilibrium data

Water rich phase			Alcohol rich phase		
T (K)	$x_{1,exp}$	$x_{1,calc}$	T (K)	$x_{2,exp}$	$x_{2,calc}$
307.15	2.80×10^{-7} (Ref. 161)	3.03×10^{-7}	302.7	0.234 (Ref. 19)	0.244
322.15	3.50×10^{-7} (Ref. 161)	3.84×10^{-7}	303.2	0.248 (Ref. 70)	0.244
			308.2	0.246 (Ref. 70)	0.244
			313.2	0.244 (Ref. 70)	0.245
			323.4	0.222 (Ref. 19)	0.248
			333.7	0.239 (Ref. 19)	0.251
			343.7	0.223 (Ref. 19)	0.256
			353.5	0.235 (Ref. 19)	0.262
			364.0	0.240 (Ref. 19)	0.270

Other references:
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TABLE 20. 1-Tetradecanol–water

Components
(1) 1-Tetradecanol; $C_{14}H_{30}O$; [112-72-1]
(2) Water; H_2O; [7732-18-5]

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Reference liquid–liquid equilibrium data

T (K)	Water rich phase		Alcohol rich phase
	$x_{1,exp}$	$x_{1,calc}$	$x_{2,calc}$
298.15	2.60×10^{-8} (Ref. 162)	1.93×10^{-8}	0.246
305.15	2.20×10^{-8} (Ref. 164)	2.12×10^{-8}	0.245

TABLE 21. 1-Hexadecanol–water

Components	References
(1) 1-Hexadecanol; $C_{16}H_{34}O$; [36653-82-4] (2) Water; H_2O; [7732-18-5]	[161] F. P. Krause and W. Lange, J. Phys. Chem. **69**, 3171 (1965).

Reference liquid–liquid equilibrium data

	Water rich phase		Alcohol rich phase
T (K)	$x_{1,calc}$	$x_{1,calc}$	$x_{2,calc}$
328.15	2.30×10^{-9} (Ref. 161)	2.98×10^{-9}	0.250

Other references:
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6. References

Editor's Note—For past articles in this series, each binary system was presented with references for a particular system given with the corresponding tabular data (with each set of references beginning with the number one). However, starting with this article (Part 4), all references have been collected together at the end of the article as well. Thus, the references are numbered sequentially in the reference section, but appear as well with each binary system, with the same numbering.

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