

Recommended Liquid–Liquid Equilibrium Data. Part 1. Binary Alkane–Water Systems

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The recommended liquid–liquid equilibrium (LLE) data for 32 binary *n*-alkane, isoalkane, and cycloalkane–water systems have been obtained after critical evaluation of all data (345 data sets) reported in the open literature up to the end of 2002. The evaluation of the alkane solubility data was based on a generalized equation, which allows prediction of the alkane solubility as a function of temperature. Using the predicted alkane solubilities the concentration of water in the alkane rich phase was calculated. The LLE calculations were performed with the equation of state appended with a chemical term (EoS_C) proposed by Góral. The experimental solubilities of water in various alkanes were compared to each other and to the calculated values. The recommended data are presented in the form of individual pages containing tables, all the references, and optionally figures. © 2004 American Institute of Physics. [DOI: 10.1063/1.1643922]

Key words: alkane; binary systems; liquid–liquid equilibria; predicted data; recommended data; water.

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1. Introduction

The objective of this paper is to provide selected and critically evaluated liquid–liquid equilibrium (LLE) data for bi-

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TABLE 1. Data for calculation of solubilities of alkanes in water by means of Eq. (11)

CAS	Name	T_c (K)	P_c (kPa)	b (cm ³)	$\ln x_{\min}$	T_{\min}
109-66-0	pentane, C ₅ H ₁₂	470	3365	100.5	-11.50	306
110-54-3	hexane, C ₆ H ₁₄	508	3012	121.4	-13.04	306
142-82-5	heptane, C ₇ H ₁₆	540	2736	142.3	-14.58	306
111-65-9	octane, C ₈ H ₁₈	569	2487	164.8	-16.24	306
111-84-2	nonane, C ₉ H ₂₀	595	2280	187.9	-17.95	306
124-18-5	decane, C ₁₀ H ₂₂	618	2100	211.9	-19.72	306
1120-21-4	undecane, C ₁₁ H ₂₄	639	1930	238.5	-21.68	306
78-78-4	2-methylbutane, C ₅ H ₁₂	460	3381	98.1	-11.32	306
75-83-2	2,2-dimethylbutane, C ₆ H ₁₄	489	3080	114.3	-12.52	306
79-29-8	2,3-dimethylbutane, C ₆ H ₁₄	500	3130	115.1	-12.57	306
107-83-5	2-methylpentane, C ₆ H ₁₄	498	3010	119.1	-12.87	306
96-14-0	3-methylpentane, C ₆ H ₁₄	504	3120	116.5	-12.68	306
590-35-2	2,2-dimethylpentane, C ₇ H ₁₆	520	2770	135.3	-14.07	306
565-59-3	2,3-dimethylpentane, C ₇ H ₁₆	537	2910	133.0	-13.90	306
108-08-7	2,4-dimethylpentane, C ₇ H ₁₆	520	2740	136.6	-14.16	306
562-49-2	3,3-dimethylpentane, C ₇ H ₁₆	536	2950	131.0	-13.75	306
591-76-4	2-methylhexane, C ₇ H ₁₆	530	2730	139.9	-14.40	306
589-34-4	3-methylhexane, C ₇ H ₁₆	535	2810	137.2	-14.21	306
589-81-1	3-methylheptane, C ₈ H ₁₈	564	2550	159.2	-15.83	306
540-84-1	2,2,4-trimethylpentane, C ₈ H ₁₈	544	2570	152.5	-15.33	306
565-75-3	2,3,4-trimethylpentane, C ₈ H ₁₈	566	2730	149.4	-15.11	306
3522-94-9	2,2,5-trimethylhexane, C ₉ H ₂₀	569	2370	173.0	-16.85	306
287-92-3	cyclopentane, C ₅ H ₁₀	512	4508	81.8	-10.12	298
110-82-7	cyclohexane, C ₆ H ₁₂	554	4073	97.9	-11.31	298
96-37-7	methylcyclopentane, C ₆ H ₁₂	533	3784	101.4	-11.56	298
291-64-5	cycloheptane, C ₇ H ₁₄	604	3840	113.4	-12.45	298
108-87-2	methylcyclohexane, C ₇ H ₁₄	572	3471	118.8	-12.85	298
292-64-8	cyclooctane, C ₈ H ₁₆	647	3570	130.6	-13.72	298
2207-01-4	1,2-dimethylcyclohexane, C ₈ H ₁₆	601	3170	136.6	-14.16	298
1678-91-7	ethylcyclohexane, C ₈ H ₁₆	602	3170	136.9	-14.18	298
1678-93-9	butylcyclohexane, C ₁₀ H ₂₀	648	2450	190.6	-18.15	298
3741-00-2	pentylcyclopentane, C ₁₀ H ₂₀	644	2450	189.3	-18.05	298

nary *n*-alkane, isoalkane, and cycloalkane–water systems, taken from the open literature up to the end of 2002 and mostly completed with predicted data.

Solubility data for hydrocarbon–water systems were the object of the IUPAC Commission on Solubility Data and presented as Volumes 37 and 38 of the IUPAC Solubility Data Series, edited by Shaw.^{1,2} This work takes into account new data, which were published since that time. The critical evaluation procedures were based on the correlating equations developed by Góral presented by Mączyński *et al.*³ Recommended data were prepared for 32 hydrocarbons on the bases of 345 data sets for 42 hydrocarbons obtained from 82 references.

2. Solubility of Alkanes in Water

When a molecule of alkane is dissolved in water, the number of hydrogen bonds broken and distorted depends very much on the size of the cavity in the water needed to accommodate the dissolved molecule. It is assumed here that the size of the cavity is proportional to the excluded volume (b) used in equations of state of van der Waals type. In this work Redlich–Kwong Equation of State (RK EoS) is used, where b is calculated from critical temperature (T_c) and critical pressure (P_c): given in Table 1

$$b = 0.08664RT_c/P_c. \quad (1)$$

The solubility of alkanes has a minimum at room temperature. It was found that mole fraction of the alkane at the minimum (x_{\min}) depends linearly on b

$$\ln x_{\min} = c_1 + c_2 b. \quad (2)$$

The coefficients c_1 and c_2 were determined using solubility data in range 292–313 K. At these temperatures (around the minimum) change of the solubility due to temperature is negligible compared to experimental errors. The mole fractions (x) reported for this region were treated as experimental estimations of x_{\min} . Altogether 169 points for 29 alkanes including *n*-alkanes, isoalkanes, and cycloalkanes were taken into account. For each alkane the following procedure was applied: At first $\ln x_{\min}$ was calculated as the arithmetic mean of all experimental values of $\ln x$ reported for given mixture within the temperature interval 292–313 K. The points deviating from the arithmetic mean of more than 2 standard errors were rejected from further calculations. Then the data were examined once more using the same procedure but with corrected arithmetic mean and new estimation of the standard error. The procedure was repeated until no outlying points were found. The remaining 134 points were regressed

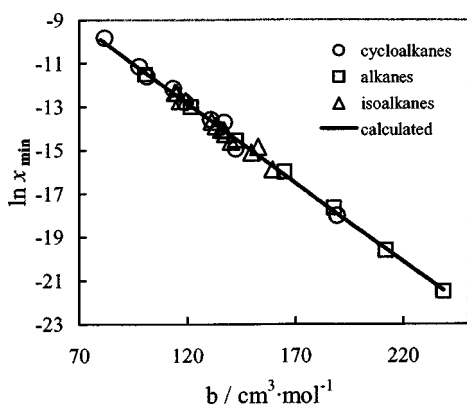


FIG. 1. $\ln x_{\min}$ versus excluded volume of the corresponding alkane (b).

with Eq. (2), which gave $c_1 = -4.08$ and $c_2 = -0.0730 \text{ mol cm}^{-3}$. Standard error, $s(\ln x_{\min})$, resulting from Eq. (2) can be estimated with

$$s(\ln x_{\min}) = (D_{11} + 2D_{12}b + D_{22}b^2)^{0.5}, \quad (3)$$

where D_{11} , D_{12} , D_{22} are elements of the variance-covariance matrix yielded by the method of least squares: $D_{11} = 9.9 \times 10^{-3}$, $D_{12} = -6.9 \times 10^{-5} \text{ mol cm}^{-3}$, and $D_{22} = 5.2 \times 10^{-7} (\text{mol cm}^{-3})^2$. Validity of Eq. (2) is illustrated in Fig. 1.

Each point in Fig. 1 is a mean value of solubility data in range 292–313 K using the following number of the experimental points: cyclopentane (6), cyclohexane (16), methylcyclopentane (3), cycloheptane (2), methylcyclohexane (7), cyclooctane (1), ethylcyclohexane (1), propylcyclopentane (1), pentylcyclopentane (1), pentane (11), hexane (17), heptane (13), octane (13), nonane (4), decane (8), undecane (2), 2,2-dimethylbutane (3), 2,3-dimethylbutane (3), 3-methylpentane (4), 2-methylpentane (5), 3,3-dimethylpentane (2), 2,3-dimethylpentane (1), 2,2-dimethylpentane (1), 2,4-dimethylpentane (4), 3-methylhexane (2), 2-methylhexane (1), 2,3,4-trimethylpentane (2), 2,2,4-trimethylpentane (5), and 3-methylheptane (1). The alkanes within each group are listed in increasing order of b .

Equation (2) is useful for identification of outlying experimental data not only at the minimum but also at other temperatures, because the experimental points at other temperatures should lie on a curve going through $\ln x_{\min}$ predicted with Eq. (2).

The mole fraction of an alkane in water (x) at temperature (T) along the three phase equilibrium line can be obtained by integration of equation:

$$[\partial \ln x / \partial (1/T)]_P \cong -\Delta_{\text{sln}}h/R, \quad (4)$$

where $\Delta_{\text{sln}}h$ is the heat of solution of the alkane, which is equal to the difference between the partial enthalpy of the alkane at infinite dilution and the molar enthalpy of the pure alkane. Activity coefficient was omitted in Eq. (4), because $x < 0.001$ in the whole temperature range. $\Delta_{\text{sln}}h$ includes a positive heat of cavity formation and a negative heat of hydrophobic interaction between the hydrocarbon and water. At

some temperature, T_{\min} , these two effects cancel each other giving $\Delta_{\text{sln}}h=0$ which, according to Eq. (4), corresponds to the minimum solubility. Gill *et al.*⁴ have measured $\Delta_{\text{sln}}h$ as a function of temperature. The measurements were made over a narrow temperature range, but they suggest that $\Delta_{\text{sln}}h$ is linearly dependent on temperature, which implies that heat capacity of solution ($\Delta_{\text{sln}}C_P$) is constant. In this case $\Delta_{\text{sln}}h$ can be written as follows:

$$\Delta_{\text{sln}}h = \Delta_{\text{sln}}C_P(T - T_{\min}). \quad (5)$$

Integration of Eq. (4) with $\Delta_{\text{sln}}h$ as expressed with Eq. (5) yields

$$\ln x = \ln x_{\min} + (\Delta_{\text{sln}}C_P/R)[1/T_r + \ln T_r - 1], \quad (6)$$

where $T_r = T/T_{\min}$. It is uncertain to what extent Eq. (5) is justified but the resulting Eq. (6) is commonly used for the description of solubility of hydrocarbons in water. Economou *et al.*⁵ claim that Eq. (6) is very satisfactory up to the three phase critical temperature (T_{3c}).

The minimum of the solubility curve is rather flat, whose obstacles determine T_{\min} . It can be varied by about 10 K without affecting the accuracy of the approximation of the solubility data with Eq. (6). In this situation an average value $T_{\min} = 306 \text{ K}$ was adopted for n -alkanes and isoalkanes. For the cyclohexane/water mixture the calorimetric measurements yielded $T_{\min} = 298 \text{ K}$. This temperature works well for all cycloalkanes investigated in this work and was adopted for cycloalkane/water mixtures.

Equation (6) can be linearized using the notation: $Y = \ln x$, $Y_0 = \ln x_{\min}$, and $X = [1/T_r + \ln T_r - 1]$, which gives

$$Y = Y_0 + (\Delta_{\text{sln}}C_P/R)X. \quad (7)$$

The experimental points for the given alkane should lie on a straight line defined by Eq. (7), where Y_0 is determined by Eq. (2). This feature was used for identification of the outlying points. The example is shown in Fig. 2. The black circle in Fig. 2 indicates Y_0 determined by Eq. (2). It agrees with data of Heidman *et al.*⁶ The second set of points also lie on a straight line but the dashed line does not go through the black circle and consequently it is not consistent with Eq. (2). This deviation between the black point and the points approximated with the dashed line was ascribed to error of the experimental points.

The positively evaluated experimental points were regressed with Eq. (7) (solid line in Fig. 2) yielding the value of $(\Delta_{\text{sln}}C_P/R)$. Plots such as those shown in Fig. 2 were done for ten mixtures. Other systems reported in the literature were not suitable for determination of $(\Delta_{\text{sln}}C_P/R)$, because they were investigated only in the vicinity of T_{\min} , where $X \approx 0$ or they are too scattered. The adjusted values of $(\Delta_{\text{sln}}C_P/R)$ are plotted in Fig. 3 for the following cycloalkanes, n -alkanes, and isoalkanes (listed in increasing order of b within each group): cyclohexane, methylcyclohexane, ethylcyclohexane, pentane, hexane, heptane, octane, 2,3-dimethylbutane, 2-methylpentane, and 3,3-dimethylpentane.

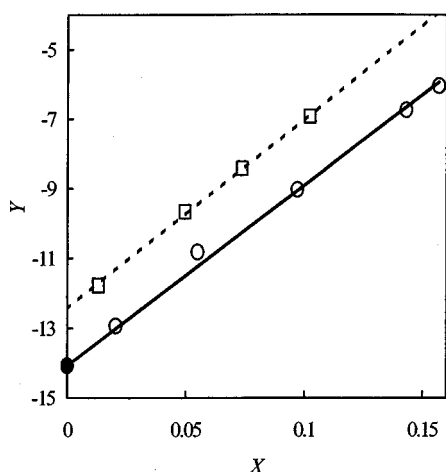


FIG. 2. Solubility of ethylcyclohexane in water: (●) calculated with Eq. (2); (□) data of Guseva and Parnov⁷; (○) data of Heidman *et al.*⁶; approximated with Eq. (7).

The approximating line in Fig. 3 fulfills the relation

$$(\Delta_{\text{sln}}C_p/R) = c_3b. \quad (8)$$

In order to determine c_3 Eq. (8) was introduced into Eq. (7), which was rearranged to form

$$\Delta Y = c_3Z, \quad (9)$$

where

$$\Delta Y = Y - Y_0 \quad \text{and} \quad Z = b[1/T_r + \ln T_r - 1].$$

Equation (9) allows for simultaneous description of solubility data for various alkanes. These data were evaluated using plots like that shown in Fig. 2. Altogether 52 points corresponding to ten mixtures were selected. This set does not include points, which were measured in the vicinity of T_{min} , because such points fulfill Eq. (9) by definition. Simultaneous regression with Eq. (9) gave the following estimations:

$$c_3 = 0.376 \text{ mol cm}^{-3}, \quad (10a)$$

$$s(\Delta Y) = Z(G_{11})^{0.5}, \quad (10b)$$

$$G_{11} = 6.6 \times 10^{-6} (\text{mol cm}^{-3})^2, \quad (10c)$$

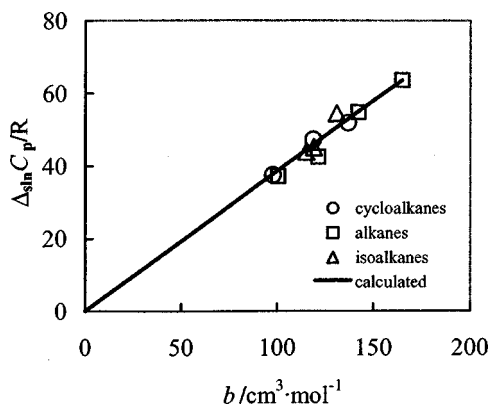


FIG. 3. $(\Delta_{\text{sln}}C_p/R)$, obtained from experimental data by means of Eq. (7) versus excluded volume (b).

where $s(\Delta Y)$ is the standard error of ΔY resulting from Eq. (9) and G_{11} is the variance of c_3 obtained from the least squares method. Summarizing the obtained results one can write Eq. (6) in the following form:

$$\ln x = \ln x_{\text{min}} + c_3b[T_{\text{min}}/T + \ln(T/T_{\text{min}}) - 1], \quad (11)$$

where $\ln x_{\text{min}}$ is calculated with Eq. (2). Parameters of Eq. (11) for alkanes investigated in this work are given in Table 1. For other alkanes $\ln x_{\text{min}}$ and b can be estimated from critical parameters by means of Eqs. (1) and (2).

Taking into account Eqs. (3) and (10b) one obtains the formula for standard error of $\ln x$ resulting from Eq. (11), denoted here by $s(\ln x)$:

$$s(\ln x) = \{D_{11} + 2D_{12}b_i + D_{22}b^2 + G_{11}b^2 \times [T_{\text{min}}/T + \ln(T/T_{\text{min}}) - 1]^2\}^{0.5}. \quad (12)$$

Coefficients of Eq. (12) are given above in the text.

The verification procedure for solubility of alkanes in water was based on Eq. (11). Accuracy of this equation can be estimated with Eq. (12). For example, if one assumes $b = 100 \text{ cm}^3 \text{ mol}^{-1}$ then Eq. (12) gives $s(\ln x) = 0.04$ at 300 K and $s(\ln x) = 0.05$ at 500 K. For $b = 200 \text{ cm}^3 \text{ mol}^{-1}$ the corresponding values of $s(\ln x)$ are 0.06 and 0.08, respectively. A standard error of the experimental data was estimated using the set of 134 selected experimental points, which were regressed with Eq. (2). The regression gave the standard error of individual experimental value of $\ln x$ equal to 0.27. Moreover some data exhibit systematic errors, as for example the data shown in Fig. 2. Therefore discrepancy between Eq. (11) and a particular experimental point should be rather ascribed to the error of the data.

Equations (2) and (11) are not valid for n -alkanes higher than undecane. Their solubility is bigger than those predicted by Eq. (11). This phenomena is discussed by Tsionopoulos.⁸

3. Solubility of Water in Alkanes

Solubility of water in hydrocarbons can be described by Eq. (13):

$$[\partial \ln(x_w \gamma_w) / \partial (1/T)]_P \cong -\Delta_{\text{sln}}h_w/R, \quad (13)$$

where γ_w denotes activity coefficient of water standardized in respect to infinite dilution, e.g., $\gamma_w = 1$, when concentration of water is sufficiently low. $\Delta_{\text{sln}}h_w$ denotes the change in enthalpy when 1 mole of water is transferred to the infinitely diluted solution. This process causes complete breaking of the hydrogen bonds between water molecules and their replacement by much weaker van der Waals interactions between water and the hydrocarbon molecules. Thus $\Delta_{\text{sln}}h_w$ depends mainly on the enthalpy of the hydrogen bonds and is weakly dependent on alkane. Equation (13) is analogous to Eq. (4) but due to the big value of $\Delta_{\text{sln}}h_w$ the solubility of water increases quickly with temperature achieving such big values that γ_w must be taken into account, when one integrates Eq. (13). Therefore an approach based on integration of Eq. (13) is not used here.

In this work the alkane solubilities predicted with Eq. (11) were used for the calculation of water concentration in the second liquid phase. These calculations use LLE.

The equilibria between vapor and the alkane saturated with water were successfully correlated by the modification of the Redlich-Kwong equation proposed by Zudkevitch and Joffe.⁹ A similar approach was used by Tsonopoulos and Wilson.¹⁰ However, these simple EoSs fail for the water-rich phase.

Another approach is to use equations which account for hydrogen bonding. In this work a method of correlation of phase equilibrium developed by Góral¹¹ is used. This method (EoS_C) is based on the RK EoS appended with a term, which accounts for hydrogen bonding. EoS_C was successfully used for correlation and prediction of vapor-liquid equilibrium (VLE) and LLE in hydrogen bond forming binary and multicomponent systems,¹¹ for correlation and verification of selected VLE data on alcohols and hydrocarbons,¹²⁻¹⁴ and for simultaneous correlation and prediction of VLE and LLE data in a hydrogen bonding quaternary system.¹⁵

The calculations of the phase equilibria were performed using general constraints:

$$\mu_i^{(1)}(x_i, \Theta) = \mu_i^{(2)}(x_w, \Theta), \quad (14a)$$

$$\mu_w^{(1)}(x_i, \Theta) = \mu_w^{(2)}(x_w, \Theta), \quad (14b)$$

where $\mu_i^{(1)}$, $\mu_i^{(2)}$, $\mu_w^{(1)}$, and $\mu_w^{(2)}$ are the chemical potentials of i th hydrocarbon and water in the coexisting phases. The chemical potentials yielded by EoS_C depend on one adjustable parameter Θ defined by Eq. (18). Because the mole fraction of alkane (x_i) in the water rich phase is known from Eq. (11) then two unknown quantities, Θ and mole fraction of water (x_w) in the second phase, can be found by solving the set of two equations (14a) and (14b).

In the EoS_C chemical potential is separated into physical and chemical contributions. To calculate the physical contribution the RK EoS was used. This yields the following formula for change of the chemical potential of the k th component with respect to the standard state defined as a perfect gas at 1 kPa at the same temperature:

$$\Delta\mu_k = RT \ln[x_k RT / (V - b) P^*] - (na/b)' \ln(1 + b/V) + (b_k/b)(PV - RT), \quad (15)$$

where P^* is standard pressure, V is molar volume determined with the RK EoS at temperature T , pressure P , and mole fraction x_k using parameters b and a calculated with the classical mixing rules

$$b = x_i b_i + x_j b_j, \quad (16)$$

$$a = x_i^2 a_{ii} + 2x_i x_j a_{ij} + x_j^2 a_{jj}, \quad (17)$$

where a_{ij} is related to the binary adjustable parameter Θ_{ij} by the equation:

$$a_{ij} = (a_{ii} a_{jj})^{0.5} (1 - \Theta_{ij}). \quad (18)$$

$(na/b)'$ in Eq. (15) denotes the differential of (na/b) where n is the total number of moles and a , b are expressed with

Eqs. (16) and (17). Differentiation is performed with respect to the number of moles of the k th component. Equation (15) is also applicable for pure components provided that the following constraints are used: $x_k = 1$, $a = a_{kk}$; and $b = b_k$. In the EoS_C method the equation of state of the pure hydrogen bonding component is not modified. Pure water is treated in the same way as a hydrocarbon. The excluded volume of a pure substance is assumed to be temperature independent and is calculated from the relevant critical parameters T_c and P_c using the standard formula for RK EoS given previously by Eq. (1). For alkanes a was calculated from the equation given by Soave¹⁶

$$a(T) = a(T_c) \{1 - m[(T/T_c)^{0.5} - 1]\}^2, \quad (19)$$

where $a(T_c)$ is calculated from critical temperature (T_c) and critical pressure (P_c):

$$a(T_c) = 0.42747(T_c^2/P_c). \quad (20)$$

Coefficient m in Eq. (19) is temperature independent but it depends on alkane. m was determined via Eq. (19) from the value of a at $T = 0.7T_c$. This value of a was found from adjustment to the saturated vapor pressure of the alkane in the following way: at first liquid and vapor molar volumes, under the vapor pressure, were calculated from the RK EoS using a starting value of a . These volumes were introduced into Eq. (15) to calculate chemical potentials of the pure component in the liquid and vapor phases. At equilibrium the chemical potentials in both phases must be equal. If not, the value of a was improved in the next iterations until a satisfactory value of a was obtained.

For water Eq. (19) was modified. The following resulting equation used in RK EoS reproduces well the temperature dependence of the saturated vapor pressure of water:

$$a(T) = a(T_c) \{1 - 0.699[(T/T_c)^{0.74} - 1]\}^2. \quad (21)$$

In mixtures Eq. (15) is supplemented with the chemical term $F_{k,\text{chem}}^E$, which accounts for the change in hydrogen bonding in the mixture with respect to the pure component. This gives

$$F_{k,\text{chem}}^E = F_{k,\text{chem}} - F_{k,\text{chem}}^\circ + \Delta_k, \quad (22)$$

where $F_{k,\text{chem}}$ and $F_{k,\text{chem}}^\circ$ correspond to the k th substance in the mixture and in the pure state, respectively. The expression for $F_{k,\text{chem}}$ is as follows:

$$F_{k,\text{chem}} = RT \ln \beta_k - (V_k - b_k) P_{\text{chem}}, \quad (23)$$

where β_k is the fraction of free, nonhydrogen bonded molecules of the bonding substance (here water) at chemical equilibrium with hydrogen bonded clusters. For the nonassociating component the constraint: $\beta_k = 1$ must be used in Eq. (23). P_{chem} is change of vapor pressure due to the hydrogen bonding. To use Eq. (23) one must determine the dependence of β_k and P_{chem} on concentration. General formulas were described by Góral.¹⁷ These formulas applied to the systems investigated here (water and nonhydrogen bonding second component) reduce to the following equations:

$$\beta_k = X^4, \quad (24)$$

$$P_{\text{chem}} = (X - 1)C, \quad (25)$$

where X is a fraction of free hydrogen atoms of water (not engaged in hydrogen bonds). C depends on the mole fraction of water (x_w) and alkane (x_i) in the following way:

$$C = 2RTx_w/[x_w(V_w - b_w) + x_i(V_i - b_i)], \quad (26)$$

in which V_w and V_i are molar volumes of pure water and i th alkane. They are calculated with the RK EoS under the vapor pressure of the mixture. b_w and b_i are excluded volumes used in RK EoS. X is calculated by solving the equation

$$X = 1/(1 + KXC), \quad (27)$$

where K is the equilibrium constant of self-association of water. For pure water $F_{k,\text{chem}}^0$ is calculated with the same equations as $F_{k,\text{chem}}$, but using the constraint $x_k = 1$. For hydrocarbons $F_{k,\text{chem}}^0$ is zero by definition. The term Δ_k in Eq. (22) is a small correction, which does not contain any adjustable parameters and was defined by Góral.¹¹

Equations (24)–(27) are valid for the continuous association model in which a hydrogen bonded cluster of water molecules possessing unshared electron pairs or nonhydrogen bonded hydrogen atoms can grow by hydrogen bonding to adjacent molecules of water. The kind and concentration of the hydrogen bonded clusters depends on the chemical equilibrium in the mixture. It is assumed that formation of each hydrogen bond in water is described by the same association constant K . In this work the temperature dependence of K was obtained by integration of the van't Hoff equation, which yields the following expression:

$$K = K_0 \exp\left[-\frac{\Delta H^0}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right] \exp\left\{-\frac{\Delta C_p}{R}\right. \\ \left. \times \left[\frac{T_0}{T} - 1 + \ln\left(\frac{T}{T_0}\right)\right]\right\}, \quad (28)$$

where K_0 is the equilibrium constant at the reference temperature $T_0 = 303.15$ K, ΔH^0 is the molar enthalpy of hydrogen bond formation, and ΔC_p is the corresponding heat capacity. The following values of these quantities were adopted:

$$K_0 = 0.100 \text{ MPa}^{-1}, \quad (29a)$$

$$(-\Delta H^0/R) = 2200 \text{ K}, \quad (29b)$$

$$(-\Delta C_p/R) = 3, \quad (29c)$$

where ΔH^0 was estimated from $\Delta_{\text{sln}}h_w$, used in Eq. (13). As was noted above, the main contribution to Δh_w results from breaking about 2 moles of hydrogen bonds, hence it was assumed:

$$-\Delta H^0 \approx \Delta_{\text{sln}}h_w/2. \quad (30)$$

These solubility data yielded $(\Delta_{\text{sln}}h_w/R)/2 \approx 2200$ K, which agrees with the assumed value of $-\Delta H^0/R$. Nilsson¹⁸ has obtained a similar value from the calorimetric measurements. $(-\Delta C_p/R)$ in Eq. (28) was treated as an adjustable parameter, which should be nearly zero as is suggested by the Nilsson's calorimetric measurements. K_0 was adjusted to the LLE data. The numerical values, listed in Eqs. (29a)–(29c) were used in all LLE calculations.

The excluded volume of water (b_w) used in the chemical part [Eqs. (23) and (26)] is shifted with respect to b_w , calculated with Eq. (1) and used in the physical part. This shift $\Delta b_w = -6.5 \text{ cm}^3 \text{ mol}^{-1}$ is used in all mixtures of water. For hydrocarbons $\Delta b_i = 0$.

The input information for the described LLE calculations is solubility of alkane in water, calculated with Eq. (11). Using the alkane solubilities the concentration of water in the alkane rich phase was calculated. The solubility of water was used only at the beginning of this investigation to fix the parameters used in the model of water (K_0 , ΔH^0 , ΔC_p , and Δb).

Altogether solubility of water in 32 selected alkanes was calculated. These systems include n -alkanes, isoalkanes, as well as cycloalkanes. For 11 systems only alkane solubilities were reported. For the other 21 systems the calculated water solubilities were compared with experimental solubilities at 298 K. This temperature was chosen because many systems were measured only in the vicinity of this temperature. The experimental mean value of the water solubility at 298 K was obtained from regression of the experimental data. The approximating equation was derived from Eq. (15) appended with the association term, which gives

$$\mu_k = \mu_i^* + RT \ln[x_k RT/\nu P^*] + \mu_{k,\text{resid.}} + \mu_{k,\text{chem}}, \quad (31)$$

where RT/ν is a shortened notation for the repulsive term, $RT/(V-b)$, in RK EoS, $\mu_{k,\text{resid.}}$ results from the attraction term in EoS, and $\mu_{k,\text{chem}}$ results from association. At equilibrium the chemical potential of the k th component in both coexisting phases must be equal. When Eq. (31) is applied to water this constraint gives the following equation for mole fraction of water in the i th alkane (x_w):

$$\ln[x_w \nu_w/\nu_i] = -[\Delta \mu_{w,\text{resid.}} + \Delta \mu_{w,\text{chem}}]/RT, \quad (32)$$

where it was assumed that in the water rich phase ν can be replaced by a corresponding value of pure water (ν_w) and analogously for the alkane rich phase at low temperature $x_i \approx 1$, $\nu \approx \nu_i$. Further rearrangement gives

$$\ln[x_w \nu_w/\nu_i] = A_i - B_i/T. \quad (33)$$

This equation is valid at low temperatures where solubilities in both phases are small. Parameters A_i and B_i were adjusted to experimental solubilities of water in the i th alkane below 323 K. It appears that values of A_i and B_i have similar values for various alkanes, which is useful for evaluation of the water solubility data. Values of $\ln[x_w \nu_w/\nu_i]$ at temperature 293 K obtained from regression of experimental data were compared with the values predicted with EoS in Fig. 4.

The four points shown in the upper left corner of Fig. 4 are too high with respect to the calculated points as well as with respect to other cyclohexanes. These points correspond to solubility of water in cyclopentane, methylcyclopentane, methylcyclohexane, and ethylcyclopentane reported by Englin *et al.*¹⁹ It should be noted that solubility of water in cyclohexane and ethylcyclohexane, investigated by 15 different laboratories, agree with the calculated values. This suggests

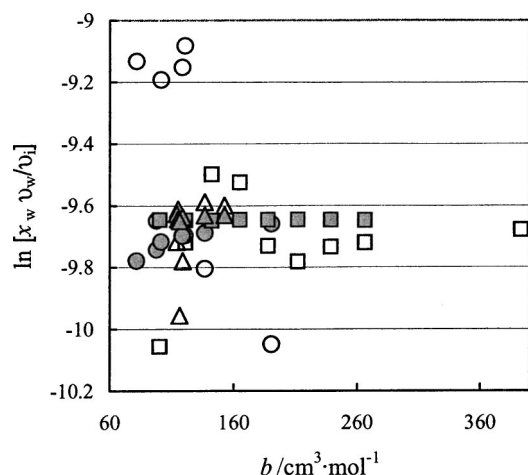


FIG. 4. $\ln[x_w v_w / v_i]$ at 298 K versus excluded volume of the alkane (b) for cycloalkanes (○); n -alkanes (□); and isoalkanes (△). The shadow points correspond to solubilities predicted with EoS.

systematic error of the mentioned data of Englin *et al.*¹⁹ On the other hand the point corresponding to butylcyclohexane is too low, but it was extrapolated from a single experimental point measured at 311 K. With the exception of two points, relatively small deviations are observed for n -alkanes and isoalkanes. Each of the deviating points correspond to data reported by only one source.

Apart from the cases mentioned the differences between experimental and calculated values are lower than 20% of x_w , which corresponds to absolute error of x_w lower than 0.0001. It seems that the deviations result mainly from error of the experimental data, because within the same class of mixtures both positive and negative deviations are observed in Fig. 4.

The experimental solubilities at other temperatures are compared to the predicted solubility curves in the sheets corresponding to the particular mixtures. The plots are given for mixtures investigated in a sufficiently large temperature interval. These plots show good agreement between experimental and predicted data.

For convenience of the reader the solubility curves predicted with EoS were approximated with the following equation proposed by Economou *et al.*:⁵

$$\ln x_w = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r), \quad (34)$$

where originally $T_r = T/T_{3c}$. In most cases three phase critical temperature (T_{3c}) is not known and instead of T_{3c} some adjustable temperature $T^0 \geq T_{3c}$ is used in Eq. (34). Parameters of Eq. (34) are given in Table 2 for alkanes investigated in this work. This equation approximates well the solubilities produced by EoS. However, one must take into account that the solubilities, yielded by EoS, are less accurate in the vicinity of T_{3c} . Only few systems are measured in the whole temperature range. In these systems EoS approximates well the experimental data but generally no definite conclusions

can be drawn. We believe that Eq. (34) with the parameters given in Table 2 can be used up to temperatures about 40 K below T^0 .

4. Conclusions

Solubility of alkanes in water can be calculated with good accuracy with Eq. (11). Solubility of water in alkanes can be calculated with EoS in conjunction with Eq. (11). To apply the presented equations no experimental solubility data are necessary. This method of prediction was tested using all available solubility data for the alkane-water systems. The presented tests and good agreement between the calculated solubilities and the recommended data convince us of the accuracy of the calculations as well as internal consistency and good quality of the recommended data. As was mentioned previously, Eq. (11) must not be applied to C_{11}^+ normal alkanes.

5. Description of Tables Containing the Recommended Data

Each system in Table 3 is presented separately, which includes a table of LLE data along the three phase equilibrium line and optionally the corresponding figures.

The tables contain data which differ from the calculated values by less than 30% with respect to the mole fraction of the solute compound. This criterion discarded 245 out of a total number of 568 experimental points investigated in this work. If more data at the same temperature fulfills this criterion then only one 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 solubility. The tables contain experimental mole fractions of the solute component and the corresponding calculated values. Symbol x_1 denotes the mole fraction of the alkane in the water-rich phase, and x_2 denotes mole fraction of water in the alkane-rich phase. Values denoted by $x_{1,calc}$ were calculated with Eq. (11). Coefficients of this equation are given in Table 1. Values of $x_{2,calc}$ were calculated with Eq. (34). Coefficients of this equation are given in Table 2. These coefficients were found in the following way: at first LLE calculations were performed with EoS using solubility of alkane predicted with Eq. (11). Next the calculated solubilities of water were approximated with Eq. (34).

Additionally, for mixtures investigated at a sufficiently large temperature interval the figures are given. One type of figure shows solubility of alkanes in water. In these figures temperature (T) is plotted versus x_1 . The figures where T is plotted versus x_2 show solubility of water in the corresponding alkane.

TABLE 2. Data for calculation of solubilities of water in alkanes by means of Eq. (34)

CAS	Name	d_1	d_2	d_3	d_4	T^0
109-66-0	pentane, C ₅ H ₁₂	-1.591	-6.577	-0.064	-5.526	467.5
110-54-3	hexane, C ₆ H ₁₄	-1.118	-6.113	-0.144	-5.049	499.8
142-82-5	heptane, C ₇ H ₁₆	-0.633	-6.177	-0.846	-3.372	524.2
111-65-9	octane, C ₈ H ₁₈	-0.456	-5.460	-0.260	-4.467	553.8
111-84-2	nonane, C ₉ H ₂₀	-0.240	-5.636	-1.029	-3.056	558.8
124-18-5	decane, C ₁₀ H ₂₂	-0.087	-5.338	-0.910	-3.269	577.2
1120-21-4	undecane, C ₁₁ H ₂₄	-0.104	-5.430	-0.984	-2.656	582.6
78-78-4	2-methylbutane, C ₅ H ₁₂	-1.706	-6.782	-0.047	-5.509	458.7
75-83-2	2,2-dimethylbutane, C ₆ H ₁₄	-1.299	-6.468	-0.056	-5.005	484.4
79-29-8	2,3-dimethylbutane, C ₆ H ₁₄	-1.219	-6.291	-0.091	-4.950	493.7
107-83-5	2-methylpentane, C ₆ H ₁₄	-1.207	-6.227	-0.065	-5.204	491.7
96-14-0	3-methylpentane, C ₆ H ₁₄	-1.169	-6.213	-0.158	-4.918	497.4
590-35-2	2,2-dimethylpentane, C ₇ H ₁₆	-0.979	-6.097	-0.080	-4.698	509.8
565-59-3	2,3-dimethylpentane, C ₇ H ₁₆	-0.810	-6.176	-0.538	-3.671	522.1
108-08-7	2,4-dimethylpentane, C ₇ H ₁₆	-0.974	-6.061	-0.081	-4.808	509.3
562-49-2	3,3-dimethylpentane, C ₇ H ₁₆	-0.879	-6.176	-0.367	-3.816	521.4
591-76-4	2-methylhexane, C ₇ H ₁₆	-0.806	-6.122	-0.457	-4.092	517.0
589-34-4	3-methylhexane, C ₇ H ₁₆	-0.789	-6.140	-0.530	-3.835	520.6
589-81-1	3-methylheptane, C ₈ H ₁₈	-0.509	-5.789	-0.714	-3.681	539.9
540-84-1	2,2,4-trimethylpentane, C ₈ H ₁₈	-0.499	-6.314	-0.954	-2.859	526.7
565-75-3	2,3,4-trimethylpentane, C ₈ H ₁₈	-0.466	-5.950	-0.968	-3.034	541.6
3522-94-9	2,2,5-trimethylhexane, C ₉ H ₂₀	-0.486	-5.745	-0.518	-3.776	543.4
287-92-3	cyclopentane, C ₅ H ₁₀	-1.397	-6.191	-0.339	-4.792	503.1
110-82-7	cyclohexane, C ₆ H ₁₂	-0.963	-6.267	-0.710	-3.111	533.3
96-37-7	methylcyclopentane, C ₆ H ₁₂	-1.054	-6.303	-0.450	-3.846	518.9
291-64-5	cycloheptane, C ₇ H ₁₄	0.158	-6.158	-2.940	-0.450	564.3
108-87-2	methylcyclohexane, C ₇ H ₁₄	-0.203	-6.277	-1.935	-1.695	545.3
292-64-8	cyclooctane, C ₈ H ₁₆	0.050	-5.445	-2.013	-2.032	586.6
2207-01-4	1,2-dimethylcyclohexane, C ₈ H ₁₆	-0.028	-5.810	-1.851	-2.191	562.4
1678-91-7	ethylcyclohexane, C ₈ H ₁₆	-0.006	-5.839	-1.937	-2.037	563.2
1678-93-9	butylcyclohexane, C ₁₀ H ₂₀	0.178	-5.506	-1.566	-2.253	587.2
3741-00-2	pentylcyclopentane, C ₁₀ H ₂₀	0.018	-5.412	-1.207	-2.827	585.0

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3. Recommended LLE data for alkane-water systems

Table 3.1. Pentane-water

Components

Pentane; C₅H₁₂; [109-66-0]
 Water; H₂O; [7732-18-5]

References

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Reference liquid-liquid equilibrium data

Water rich phase			Hydrocarbon rich phase		
<i>T</i> (K)	<i>x</i> _{1,exp}	<i>x</i> _{1,calc}	<i>T</i> (K)	<i>x</i> _{2,exp}	<i>x</i> _{2,calc}
273.2	1.64 × 10 ⁻⁵ (Ref. 4)	1.4 × 10 ⁻⁵	298.0	4.81 × 10 ⁻⁴ (Ref. 1)	6.2 × 10 ⁻⁴
277.2	1.02 × 10 ⁻⁵ (Ref. 3)	1.3 × 10 ⁻⁵			
283.2	1.07 × 10 ⁻⁵ (Ref. 3)	1.2 × 10 ⁻⁵			
288.2	1.07 × 10 ⁻⁵ (Ref. 2)	1.2 × 10 ⁻⁵			
293.2	1.03 × 10 ⁻⁵ (Ref. 2)	1.1 × 10 ⁻⁵			
298.2	1.19 × 10 ⁻⁵ (Ref. 4)	1.1 × 10 ⁻⁵			
303.2	1.01 × 10 ⁻⁵ (Ref. 3)	1.1 × 10 ⁻⁵			
308.2	1.01 × 10 ⁻⁵ (Ref. 2)	1.1 × 10 ⁻⁵			
313.3	9.90 × 10 ⁻⁶ (Ref. 5)	1.1 × 10 ⁻⁵			
328.9	1.04 × 10 ⁻⁵ (Ref. 5)	1.2 × 10 ⁻⁵			
372.3	1.73 × 10 ⁻⁵ (Ref. 5)	2.2 × 10 ⁻⁵			
394.5	2.74 × 10 ⁻⁵ (Ref. 5)	3.4 × 10 ⁻⁵			
410.5	5.01 × 10 ⁻⁵ (Ref. 5)	4.8 × 10 ⁻⁵			
422.7	7.43 × 10 ⁻⁵ (Ref. 5)	6.5 × 10 ⁻⁵			

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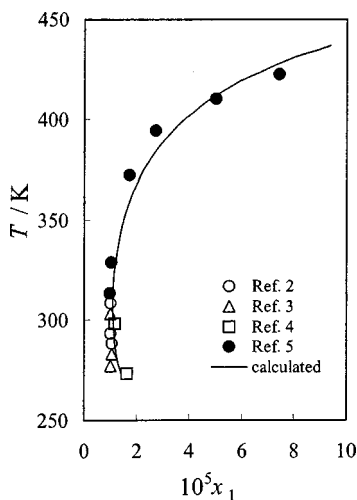


Table 3.2. Hexane–water

Components			References		
Hexane; C ₆ H ₁₄ ; [110-54-3]			¹ S. D. Burd, Jr. and W. G. Braun, Proc. Am. Pet. Inst., Div. Refin. 48 , 464 (1968).		
Water; H ₂ O; [7732-18-5]			² B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel 10 , 42 (1965).		
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Reference liquid–liquid equilibrium data					
Water rich phase			Hydrocarbon rich phase		
T (K)	x _{1,exp}	x _{1,calc}	T (K)	x _{2,exp}	x _{2,calc}
273.2	3.44 × 10 ⁻⁶ (Ref. 6)	3.3 × 10 ⁻⁶	273.2	1.34 × 10 ⁻⁴ (Ref. 6)	1.9 × 10 ⁻⁴
277.2	3.42 × 10 ⁻⁶ (Ref. 5)	3.0 × 10 ⁻⁶	293.2	4.83 × 10 ⁻⁴ (Ref. 2)	4.9 × 10 ⁻⁴
287.2	3.17 × 10 ⁻⁶ (Ref. 5)	2.6 × 10 ⁻⁶	298.2	5.10 × 10 ⁻⁴ (Ref. 8)	6.1 × 10 ⁻⁴
288.2	2.24 × 10 ⁻⁶ (Ref. 3)	2.6 × 10 ⁻⁶	303.2	8.56 × 10 ⁻⁴ (Ref. 2)	7.6 × 10 ⁻⁴
293.2	2.15 × 10 ⁻⁶ (Ref. 3)	2.5 × 10 ⁻⁶	313.2	1.17 × 10 ⁻³ (Ref. 9)	1.2 × 10 ⁻³
298.2	2.50 × 10 ⁻⁶ (Ref. 4)	2.4 × 10 ⁻⁶	354.8	6.70 × 10 ⁻³ (Ref. 1)	5.6 × 10 ⁻³
303.2	2.09 × 10 ⁻⁶ (Ref. 3)	2.4 × 10 ⁻⁶	366.5	1.00 × 10 ⁻² (Ref. 1)	8.4 × 10 ⁻³
308.2	2.11 × 10 ⁻⁶ (Ref. 3)	2.4 × 10 ⁻⁶	379.3	1.51 × 10 ⁻² (Ref. 1)	1.3 × 10 ⁻²
313.3	2.11 × 10 ⁻⁶ (Ref. 7)	2.4 × 10 ⁻⁶	394.3	2.30 × 10 ⁻² (Ref. 1)	2.0 × 10 ⁻²
328.9	2.76 × 10 ⁻⁶ (Ref. 7)	2.7 × 10 ⁻⁶	400.4	2.72 × 10 ⁻² (Ref. 1)	2.4 × 10 ⁻²
342.9	3.18 × 10 ⁻⁶ (Ref. 7)	3.2 × 10 ⁻⁶	417.6	4.21 × 10 ⁻² (Ref. 1)	3.9 × 10 ⁻²
372.3	4.68 × 10 ⁻⁶ (Ref. 7)	5.5 × 10 ⁻⁶	422.0	4.74 × 10 ⁻² (Ref. 1)	4.5 × 10 ⁻²
387.6	6.10 × 10 ⁻⁶ (Ref. 7)	7.8 × 10 ⁻⁶	431.5	5.75 × 10 ⁻² (Ref. 1)	5.8 × 10 ⁻²
394.5	7.86 × 10 ⁻⁶ (Ref. 7)	9.3 × 10 ⁻⁶	442.6	7.30 × 10 ⁻² (Ref. 1)	7.8 × 10 ⁻²
410.5	1.19 × 10 ⁻⁵ (Ref. 7)	1.4 × 10 ⁻⁵	449.8	8.44 × 10 ⁻² (Ref. 1)	9.3 × 10 ⁻²
425.0	2.32 × 10 ⁻⁵ (Ref. 7)	2.2 × 10 ⁻⁵	452.6	9.02 × 10 ⁻² (Ref. 1)	1.0 × 10 ⁻¹
			460.4	1.032 × 10 ⁻¹ (Ref. 1)	1.2 × 10 ⁻¹
			468.2	1.294 × 10 ⁻¹ (Ref. 1)	1.5 × 10 ⁻¹

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- ³⁵G. Sultanov and V. E. Skripka, Zh. Fiz. Khim. **47**, 1035 (1973).
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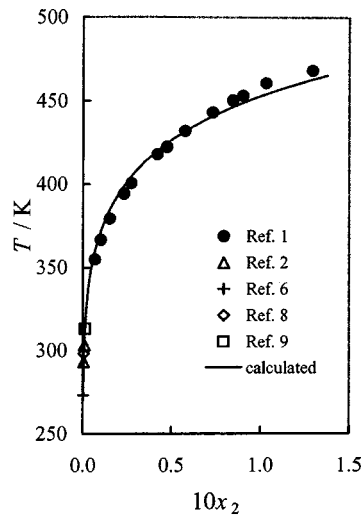
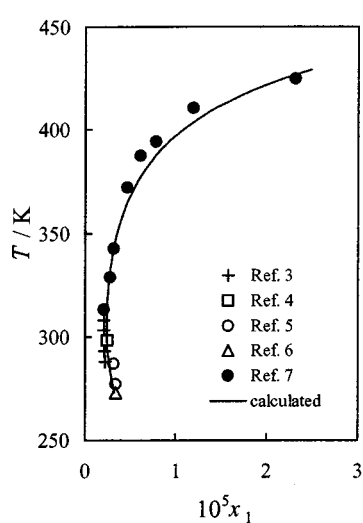


Table 3.3. Heptane–water

Components			References		
Heptane;			¹ H.-J. Bittrich, H. Gedan, and G. Feix, <i>Z. Phys. Chem. (Leipzig)</i> 260 , 1009 (1979).		
C ₇ H ₁₆ ; [142-82-5]			² L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, <i>Zh. Fiz. Khim.</i> 50 , 1344 (1976).		
Water; H ₂ O; [7732-18-5]			³ B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, <i>Khim. Tekhnol. Topl. Masel</i> 10 , 42 (1965).		
			⁴ J. A. Jonsson, J. Vejrosta, and J. Novak, <i>Fluid Phase Equilib.</i> 9 , 79 (1982).		
			⁵ C. McAuliffe, <i>J. Phys. Chem.</i> 70 , 1267 (1966).		
			⁶ H. D. Nelson and C. L. De Ligny, <i>Recl. Trav. Chim. Pays-Bas Belg.</i> 87 , 528 (1968).		
			⁷ J. Polak and B. C. Y. Lu, <i>Can. J. Chem.</i> 51 , 4018 (1973).		
			⁸ L. C. Price, <i>Am. Assoc. Pet. Geol. Bull.</i> 60 , 213 (1976).		

Reference liquid–liquid equilibrium data					
Water rich phase			Hydrocarbon rich phase		
T (K)	x _{1,exp}	x _{1,calc}	T (K)	x _{2,exp}	x _{2,calc}
273.2	7.88 × 10 ⁻⁷ (Ref. 7)	7.5 × 10 ⁻⁷	273.15	1.50 × 10 ⁻⁴ (Ref. 3)	1.9 × 10 ⁻⁴
288.2	4.80 × 10 ⁻⁷ (Ref. 4)	5.8 × 10 ⁻⁷	283.15	3.00 × 10 ⁻⁴ (Ref. 3)	3.0 × 10 ⁻⁴
293.2	4.62 × 10 ⁻⁷ (Ref. 4)	5.5 × 10 ⁻⁷	293.15	5.00 × 10 ⁻⁴ (Ref. 2)	4.8 × 10 ⁻⁴
298.2	5.30 × 10 ⁻⁷ (Ref. 5)	5.3 × 10 ⁻⁷	298.15	6.70 × 10 ⁻⁴ (Ref. 1)	6.0 × 10 ⁻⁴
303.2	4.47 × 10 ⁻⁷ (Ref. 4)	5.2 × 10 ⁻⁷	303.15	9.57 × 10 ⁻⁴ (Ref. 3)	7.5 × 10 ⁻⁴
308.2	4.53 × 10 ⁻⁷ (Ref. 4)	5.2 × 10 ⁻⁷	313.15	8.70 × 10 ⁻⁴ (Ref. 1)	1.1 × 10 ⁻³
313.3	5.00 × 10 ⁻⁷ (Ref. 8)	5.3 × 10 ⁻⁷			
318.2	4.32 × 10 ⁻⁷ (Ref. 6)	5.4 × 10 ⁻⁷			
328.9	5.60 × 10 ⁻⁷ (Ref. 8)	6.0 × 10 ⁻⁷			
372.3	1.01 × 10 ⁻⁶ (Ref. 8)	1.4 × 10 ⁻⁷			
391.2	2.05 × 10 ⁻⁶ (Ref. 8)	2.3 × 10 ⁻⁷			
409.8	4.91 × 10 ⁻⁶ (Ref. 8)	4.1 × 10 ⁻⁷			
423.6	7.86 × 10 ⁻⁶ (Ref. 8)	6.6 × 10 ⁻⁶			

Other references:

- ⁹C. Black, G. G. Joris, and H. S. Taylor, *J. Chem. Phys.* **16**, 537 (1948).
¹⁰H. S. Booth and H. E. Everson, *Ind. Eng. Chem.* **40**, 1941 (1948).
¹¹J. F. Connolly, *J. Chem. Eng. Data* **11**, 13 (1966).
¹²R. Durand, *C. R. Acad. Sci.* **226**, 409 (1948).
¹³H. Fuehner, *Ber. Dtsch. Chem. Ges.* **57**, 510 (1924).
¹⁴N. A. Ghanem, M. Marek, and J. Exner, *Int. J. Appl. Radiat. Isot.* **21**, 239 (1970).
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¹⁹E. S. Rudakov and A. I. Lutsyk, *Zh. Fiz. Khim.* **53**, 1298 (1979).
²⁰P. Schatzberg, *J. Phys. Chem.* **67**, 776 (1963).
²¹Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, *J. Chem. Eng. Data* **27**, 451 (1982).
²²Ya. D. Zel'venskii, A. A. Efremov, and G. M. Larin, *Khim. Tekhnol. Topl. Masel* **10**, 3 (1965).

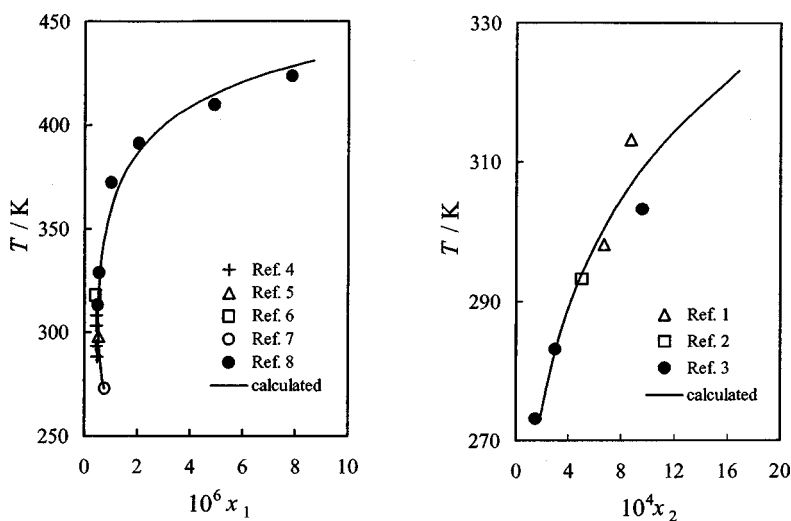


Table 3.4. Octane-water

Components			References		
Octane; C ₈ H ₁₈ ; [111-65-9]			¹ L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. 50 , 1344 (1976).		
Water; H ₂ O; [7732-18-5]			² B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel 10 , 42 (1965).		
			³ J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M. Wilson, AIChE J. 31 , 376 (1985).		
			⁴ J. A. Jonsson, J. Vejrosta, and J. Novak, Fluid Phase Equilib. 9 , 279 (1982).		
			⁵ C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).		
			⁶ J. Polak and B. C. Y. Lu, Can. J. Chem. 51 , 4018 (1973).		
			⁷ L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).		
Reference liquid-liquid equilibrium data					
Water rich phase			Hydrocarbon rich phase		
T (K)	x _{1,exp}	x _{1,calc}	T (K)	x _{2,exp}	x _{2,calc}
288.2	1.03 × 10 ⁻⁷ (Ref. 4)	1.1 × 10 ⁻⁷	273.15	1.46 × 10 ⁻⁴ (Ref. 6)	2.0 × 10 ⁻⁴
293.2	9.90 × 10 ⁻⁸ (Ref. 4)	1.1 × 10 ⁻⁷	283.15	3.24 × 10 ⁻⁴ (Ref. 2)	3.2 × 10 ⁻⁴
298.2	1.04 × 10 ⁻⁷ (Ref. 5)	1.0 × 10 ⁻⁷	293.15	4.30 × 10 ⁻⁴ (Ref. 1)	4.9 × 10 ⁻⁴
303.2	9.60 × 10 ⁻⁸ (Ref. 4)	1.0 × 10 ⁻⁷	298.15	5.01 × 10 ⁻⁴ (Ref. 6)	6.1 × 10 ⁻⁴
308.2	9.80 × 10 ⁻⁸ (Ref. 4)	1.0 × 10 ⁻⁷	310.90	1.00 × 10 ⁻³ (Ref. 3)	1.0 × 10 ⁻³
310.9	1.20 × 10 ⁻⁷ (Ref. 3)	1.0 × 10 ⁻⁷	366.50	6.20 × 10 ⁻³ (Ref. 3)	7.2 × 10 ⁻³
313.3	8.26 × 10 ⁻⁸ (Ref. 7)	1.0 × 10 ⁻⁷	422.00	3.94 × 10 ⁻² (Ref. 3)	3.4 × 10 ⁻²
342.9	1.43 × 10 ⁻⁷ (Ref. 7)	1.5 × 10 ⁻⁷	477.60	1.26 × 10 ⁻¹ (Ref. 3)	1.3 × 10 ⁻¹
394.5	7.29 × 10 ⁻⁷ (Ref. 7)	6.3 × 10 ⁻⁷	533.10	3.87 × 10 ⁻¹ (Ref. 3)	4.0 × 10 ⁻¹
409.8	1.34 × 10 ⁻⁶ (Ref. 7)	1.1 × 10 ⁻⁶	539.10	5.27 × 10 ⁻¹ (Ref. 3)	4.5 × 10 ⁻¹
422.7	1.86 × 10 ⁻⁶ (Ref. 7)	1.9 × 10 ⁻⁶	550.40	5.49 × 10 ⁻¹ (Ref. 3)	5.7 × 10 ⁻¹
536.1	3.50 × 10 ⁻⁴ (Ref. 3)	3.5 × 10 ⁻⁴			
552.8	6.00 × 10 ⁻⁴ (Ref. 3)	8.0 × 10 ⁻⁴			

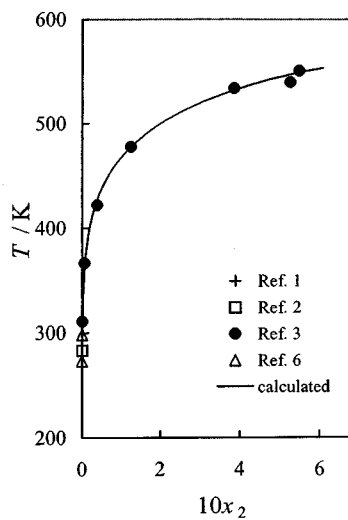
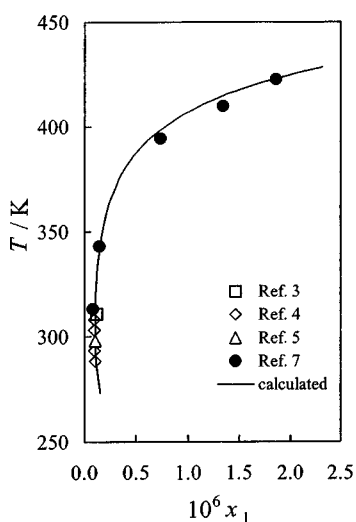
Other references:⁸E. G. Baker, Geochim. Cosmochim. Acta **19**, 309 (1960).⁹C. Black, G. G. Joris, and H. S. Taylor, J. Chem. Phys. **16**, 537 (1948).¹⁰H. Fuehner, Ber. Dtsch. Chem. Ges. **57**, 510 (1924).¹¹P. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).¹²D. J. Miller and S. B. Hawthorne, J. Chem. Eng. Data **45**, 78 (2000).¹³H. D. Nelson and C. L. De Ligny, Recl. Trav. Chim. Pays-Bas Belg. **87**, 528 (1968).¹⁴V. G. Skripka, Tr. Vses. Neftegazov. Nauch.-Issled. Inst. **61**, 139 (1976).¹⁵Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Table 3.5. Nonane–water

Components			References		
Nonane; C ₉ H ₂₀ ; [111-84-2]			¹ L. C. Price, <i>Am. Assoc. Pet. Geol. Bull.</i> 60 , 213 (1976).		
Water; H ₂ O; [7732-18-5]			² P. Schatzberg, <i>J. Phys. Chem.</i> 67 , 776 (1963).		
Reference liquid–liquid equilibrium data					
Water rich phase			Hydrocarbon rich phase		
<i>T</i> (K)	<i>x</i> _{1,exp}	<i>x</i> _{1,calc}	<i>T</i> (K)	<i>x</i> _{2,exp}	<i>x</i> _{2,calc}
298.2	1.71 × 10 ⁻⁸ (Ref. 1)	1.9 × 10 ⁻⁸	298.2	5.6 × 10 ⁻⁴ (Ref. 2)	6.2 × 10 ⁻⁴
372.3	5.90 × 10 ⁻⁸ (Ref. 1)	6.7 × 10 ⁻⁸			

Other references:

³V. G. Benkovski, M. H. Nauruzov, and T. M. Bogoslovskaya, *Tr. Inst. Khim. Nefti Prir. Solei, Akad. Nauk Kaz. SSR* **2**, 25 (1970).

⁴J. A. Jonsson, J. Vejrosta, and J. Novak, *Fluid Phase Equilib.* **9**, 279 (1982).

⁵P. Ya. Krasnoshchekova and M. Ya. Gubergits, *Neftekhimiya* **13**, 885 (1973).

⁶C. McAuliffe, *Science* **163**, 478 (1969).

Table 3.6. Decane-water

Components			References			
Decane; C ₁₀ H ₂₂ ; [124-18-5]			¹ A. Becke and G. Quitzsch, Chem. Tech. (Leipzig) 29 , 49 (1977).			
Water; H ₂ O; [7732-18-5]			² I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. 43 , 535 (1997).			
			³ F. Franks, Nature (London) 210 , 87 (1966).			
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			⁵ P. Schatzberg, J. Phys. Chem. 67 , 776 (1963).			
Reference liquid-liquid equilibrium data						
Water rich phase			Hydrocarbon rich phase			
T (K)	x _{1,exp}	x _{1,calc}	T (K)	P (kPa)	x _{2,exp}	x _{2,calc}
293.2	2.50 × 10 ⁻⁹ (Ref. 1)	3.5 × 10 ⁻⁹	298.2		5.70 × 10 ⁻⁴ (Ref. 5)	6.3 × 10 ⁻⁴
298.2	2.50 × 10 ⁻⁹ (Ref. 3)	3.3 × 10 ⁻⁹	313.2		1.07 × 10 ⁻³ (Ref. 5)	1.1 × 10 ⁻³
			374.2	124	8.42 × 10 ⁻³ (Ref. 2)	8.4 × 10 ⁻³
			423.2	520	2.80 × 10 ⁻² (Ref. 4)	3.1 × 10 ⁻²
			424.7	531	3.76 × 10 ⁻² (Ref. 2)	3.2 × 10 ⁻²
			473.2	1790	9.50 × 10 ⁻² (Ref. 4)	9.4 × 10 ⁻²
			475.2	1779	1.18 × 10 ⁻¹ (Ref. 2)	9.8 × 10 ⁻²
			498.2	2900	1.62 × 10 ⁻¹ (Ref. 4)	1.6 × 10 ⁻¹
			523.2	4630	2.48 × 10 ⁻¹ (Ref. 4)	2.6 × 10 ⁻¹
			548.2	7180	4.03 × 10 ⁻¹ (Ref. 4)	4.2 × 10 ⁻¹
			558.2	8230	5.04 × 10 ⁻¹ (Ref. 4)	5.1 × 10 ⁻¹
			563.2	9360	6.06 × 10 ⁻¹ (Ref. 4)	5.7 × 10 ⁻¹

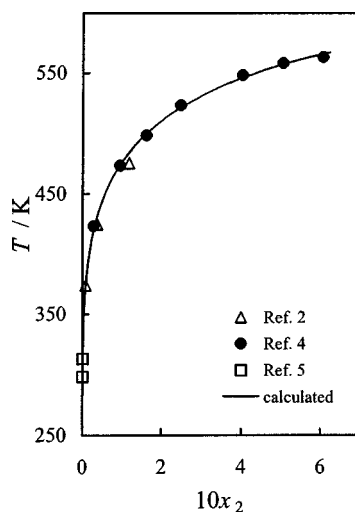
Other references:⁶E. G. Baker, Amer. Chem. Soc., Div. Petrol. Chem., Prepr. **3**, No4, C-61 (1958).⁷E. G. Baker, Science **129**, 871 (1959).⁸S. Hellinger and S. I. Sandler, J. Chem. Eng. Data **40**, 321 (1995).⁹P. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).¹⁰D. Mackay, W. J. Shiu, and A. W. Wolkoff, ASTM Spec. Tech. Pub. **573**, 251 (1975).¹¹C. McAuliffe, Science **163**, 478 (1969).¹²V. G. Skripka, Tr. Vses. Neftegazov. Nauch.-Issled. Inst. **61**, 139 (1976).¹³Q. Wang and K.-C. Chao, Fluid Phase Equilib. **59**, 207 (1990).

Table 3.7. Undecane–water

Components			References		
Undecane; C ₁₁ H ₂₄ ; [1120-21-4]			¹ C. McAuliffe, <i>Science</i> 163 , 478 (1969).		
Water; H ₂ O; [7732-18-5]			² P. Schatzberg, <i>J. Phys. Chem.</i> 67 , 776 (1963).		
Reference liquid–liquid equilibrium data					
Water rich phase			Hydrocarbon rich phase		
<i>T</i> (K)	<i>x</i> _{1,exp}	<i>x</i> _{1,calc}	<i>T</i> (K)	<i>x</i> _{2,exp}	<i>x</i> _{2,calc}
298.2	5.07 × 10 ⁻¹⁰ (Ref. 1)	4.8 × 10 ⁻¹⁰	298.2	6.0 × 10 ⁻⁴ (Ref. 2)	6.4 × 10 ⁻⁴
			313.2	1.13 × 10 ⁻³ (Ref. 2)	1.2 × 10 ⁻⁴

Other references:³P. Ya. Krasnoshchekova and M. Ya. Gubergits, *Neftekhimiya* **13**, 885 (1973).

Table 3.8. 2-Methylbutane–water

Components			References		
2-Methylbutane; C ₅ H ₁₂ ; [78-78-4]			¹ C. Black, G. G. Joris, and H. S. Taylor, <i>J. Chem. Phys.</i> 16 , 537 (1948).		
Water; H ₂ O; [7732-18-5]			² B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, <i>Khim. Tekhnol. Topl. Masel</i> 10 , 42 (1965).		
			³ S. P. Pavlova, S. Yu. Pavlov, L. A. Serafimov, and L. S. Kofman, <i>Prom-st. Sint. Kauch.</i> 3 , 18 (1966).		
			⁴ J. Polak and B. C. Y. Lu, <i>Can. J. Chem.</i> 51 , 4018 (1973).		
Reference liquid–liquid equilibrium data					
Water rich phase			Hydrocarbon rich phase		
<i>T</i> (K)	<i>x</i> _{1,exp}	<i>x</i> _{1,calc}	<i>T</i> (K)	<i>x</i> _{2,exp}	<i>x</i> _{2,calc}
273.2	1.81 × 10 ⁻⁵ (Ref. 4)	1.7 × 10 ⁻⁵	283.2	2.37 × 10 ⁻⁴ (Ref. 2)	3.2 × 10 ⁻⁴
293.2	1.17 × 10 ⁻⁵ (Ref. 3)	1.4 × 10 ⁻⁵	293.2	4.49 × 10 ⁻⁴ (Ref. 2)	5.2 × 10 ⁻⁴
298.2	1.24 × 10 ⁻⁵ (Ref. 4)	1.3 × 10 ⁻⁵	293.7	4.02 × 10 ⁻⁴ (Ref. 1)	5.4 × 10 ⁻⁴
313.2	1.44 × 10 ⁻⁵ (Ref. 3)	1.3 × 10 ⁻⁵	313.2	1.03 × 10 ⁻³ (Ref. 3)	1.3 × 10 ⁻³
323.2	1.75 × 10 ⁻⁵ (Ref. 3)	1.4 × 10 ⁻⁵	333.2	2.34 × 10 ⁻³ (Ref. 3)	3.0 × 10 ⁻³

Other references:⁵C. McAuliffe, *J. Phys. Chem.* **70**, 1267 (1966).⁶L. C. Price, *Am. Assoc. Pet. Geol. Bull.* **60**, 213 (1976).

Table 3.9. 2,2-Dimethylbutane–water

Components			References		
2,2-Dimethylbutane; C ₆ H ₁₄ ; [75-83-2]			¹ C. McAuliffe, <i>J. Phys. Chem.</i> 70 , 1267 (1966).		
Water; H ₂ O; [7732-18-5]			² J. Polak and B. C. Y. Lu, <i>Can. J. Chem.</i> 51 , 4018 (1973).		
Reference liquid–liquid equilibrium data					
Water rich phase			Hydrocarbon rich phase		
<i>T</i> (K)	<i>x</i> _{1,exp}	<i>x</i> _{1,calc}	<i>T</i> (K)	<i>x</i> _{2,exp}	<i>x</i> _{2,calc}
298.2	3.85 × 10 ⁻⁶ (Ref. 1)	4.1 × 10 ⁻⁶	273.2	1.53 × 10 ⁻⁴ (Ref. 2)	2.0 × 10 ⁻⁴

Other references:³L. C. Price, *Am. Assoc. Pet. Geol. Bull.* **60**, 213 (1976).

Table 3.10. 2,3-Dimethylbutane-water

Components			References		
2,3-Dimethylbutane; C ₆ H ₁₄ ; [79-29-8]			¹ B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, <i>Khim. Tekhnol. Topl. Masel</i> 10 , 42 (1965).		
Water; H ₂ O; [7732-18-5]			² J. Polak and B. C. Y. Lu, <i>Can. J. Chem.</i> 51 , 4018 (1973).		
			³ L. C. Price, <i>Am. Assoc. Pet. Geol. Bull.</i> 60 , 213 (1976).		
Reference liquid-liquid equilibrium data					
Water rich phase			Hydrocarbon rich phase		
<i>T</i> (K)	<i>x</i> _{1,exp}	<i>x</i> _{1,calc}	<i>T</i> (K)	<i>x</i> _{2,exp}	<i>x</i> _{2,calc}
298.2	3.99 × 10 ⁻⁶ (Ref. 3)	3.9 × 10 ⁻⁶	273.2	1.43 × 10 ⁻⁴ (Ref. 2)	1.9 × 10 ⁻⁴
313.3	4.01 × 10 ⁻⁶ (Ref. 3)	3.8 × 10 ⁻⁶	283.2	2.80 × 10 ⁻⁴ (Ref. 1)	3.1 × 10 ⁻⁴
328.3	4.95 × 10 ⁻⁶ (Ref. 3)	4.2 × 10 ⁻⁶	293.2	5.26 × 10 ⁻⁴ (Ref. 1)	5.0 × 10 ⁻⁴
372.3	8.38 × 10 ⁻⁶ (Ref. 3)	8.3 × 10 ⁻⁶	303.2	9.18 × 10 ⁻⁴ (Ref. 1)	7.8 × 10 ⁻⁴
394.5	1.19 × 10 ⁻⁵ (Ref. 3)	1.4 × 10 ⁻⁵	313.2	1.54 × 10 ⁻³ (Ref. 1)	1.2 × 10 ⁻³
410.5	2.05 × 10 ⁻⁵ (Ref. 3)	2.1 × 10 ⁻⁵			
422.7	3.37 × 10 ⁻⁵ (Ref. 3)	2.9 × 10 ⁻⁵			

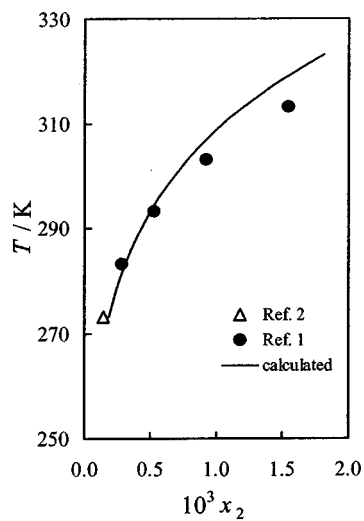
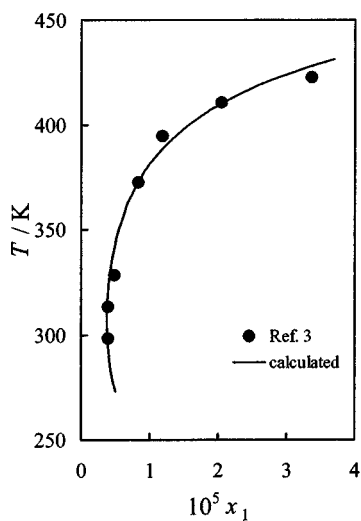


Table 3.11. 2-Methylpentane–water

Components			References		
2-Methylpentane; C ₆ H ₁₄ ; [107-83-5]			¹ C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).		
Water; H ₂ O; [7732-18-5]			² J. Polak and B. C. Y. Lu, Can. J. Chem. 51 , 4018 (1973).		
			³ L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).		
Reference liquid–liquid equilibrium data					
Water rich phase			Hydrocarbon rich phase		
T (K)	$x_{1,exp}$	$x_{1,calc}$	T (K)	$x_{2,exp}$	$x_{2,calc}$
273.2	4.06×10^{-6} (Ref. 2)	3.8×10^{-6}	273.2	1.39×10^{-4} (Ref. 2)	1.9×10^{-4}
298.2	2.88×10^{-6} (Ref. 1)	2.9×10^{-6}			
313.3	2.88×10^{-6} (Ref. 3)	2.9×10^{-6}			
328.9	3.28×10^{-6} (Ref. 3)	3.2×10^{-6}			
372.3	5.67×10^{-6} (Ref. 3)	6.4×10^{-6}			
391.2	9.39×10^{-6} (Ref. 3)	9.8×10^{-6}			
410.5	1.81×10^{-5} (Ref. 3)	1.6×10^{-5}			
422.7	2.36×10^{-5} (Ref. 3)	2.3×10^{-5}			

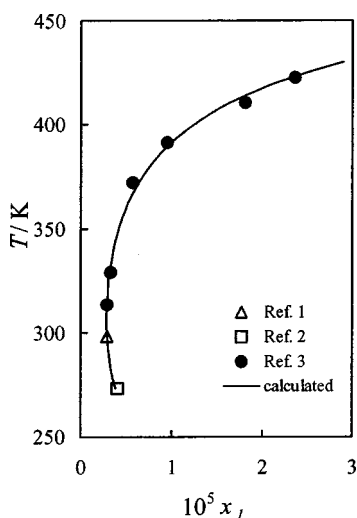
Other references:⁴J. F. Connolly, J. Chem. Eng. Data **11**, 13 (1966).⁵P. J. Leinonen and D. Mackay, Can. J. Chem. Eng. **51**, 230 (1973).

Table 3.12. 3-Methylpentane–water

Components			References		
3-Methylpentane; C ₆ H ₁₄ ; [96-14-0]			¹ J. Polak and B. C. Y. Lu, Can. J. Chem. 51 , 4018 (1973).		
Water; H ₂ O; [7732-18-5]					
Reference liquid–liquid equilibrium data					
Water rich phase			Hydrocarbon rich phase		
T (K)	$x_{1,exp}$	$x_{1,calc}$	T (K)	$x_{2,exp}$	$x_{2,calc}$
273.2	4.49×10^{-6} (Ref. 1)	4.6×10^{-6}	298.2	4.5×10^{-4} (Ref. 1)	6.1×10^{-4}
298.2	3.74×10^{-6} (Ref. 1)	3.5×10^{-6}			

Other references:²C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).³L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).⁴E. S. Rudakov and A. I. Lutsyk, Zh. Fiz. Khim. **53**, 1298 (1979).

Table 3.13. 2,2-Dimethylpentane-water

Components		References	
2,2-Dimethylpentane; C ₇ H ₁₆ ; [590-35-2] Water; H ₂ O; [7732-18-5]		¹ L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).	
Reference liquid-liquid equilibrium data			
Water rich phase			Hydrocarbon rich phase
T (K)	x _{1,exp}	x _{1,calc}	x _{2,calc}
298.2	7.9 × 10 ⁻⁷ (Ref. 1)	8.8 × 10 ⁻⁷	6.6 × 10 ⁻⁴

Table 3.14. 2,3-Dimethylpentane-water

Components		References	
2,3-Dimethylpentane; C ₇ H ₁₆ ; [565-59-3] Water; H ₂ O; [7732-18-5]		¹ L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).	
Reference liquid-liquid equilibrium data			
Water rich phase			Hydrocarbon rich phase
T (K)	x _{1,exp}	x _{1,calc}	x _{2,calc}
298.2	9.43 × 10 ⁻⁷ (Ref. 1)	1.1 × 10 ⁻⁶	5.9 × 10 ⁻⁴

Table 3.15. 2,4-Dimethylpentane-water

Components		References			
2,4-Dimethylpentane; C ₇ H ₁₆ ; [108-08-7] Water; H ₂ O; [7732-18-5]		¹ J. Polak and B. C. Y. Lu, Can. J. Chem. 51 , 4018 (1973). ² L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).			
Reference liquid-liquid equilibrium data					
Water rich phase			Hydrocarbon rich phase		
T (K)	x _{1,exp}	x _{1,calc}	T (K)	x _{2,exp}	x _{2,calc}
273.2	1.17 × 10 ⁻⁶ (Ref. 1)	1.1 × 10 ⁻⁶	273.2	1.73 × 10 ⁻⁴ (Ref. 1)	2.0 × 10 ⁻⁴
298.2	7.92 × 10 ⁻⁶ (Ref. 2)	8.0 × 10 ⁻⁶			

Other references:³C. McAuliffe, Nature (London) **200**, 1092 (1963).⁴C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

Table 3.16. 3,3-Dimethylpentane–water

Components		References	
3,3-Dimethylpentane; C ₇ H ₁₆ ; [562-49-2] Water; H ₂ O; [7732-18-5]		¹ L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).	
Reference liquid–liquid equilibrium data			
T (K)	Water rich phase		Hydrocarbon rich phase
	$x_{1,\text{exp}}$	$x_{1,\text{calc}}$	$x_{2,\text{calc}}$
298.2	1.06×10^{-6} (Ref. 1)	1.2×10^{-6}	6.0×10^{-4}
313.2	1.22×10^{-6} (Ref. 1)	1.2×10^{-6}	1.1×10^{-3}
329.2	1.47×10^{-6} (Ref. 1)	1.4×10^{-6}	2.1×10^{-3}
343.2	1.85×10^{-6} (Ref. 1)	1.6×10^{-6}	3.5×10^{-3}
372.2	2.84×10^{-6} (Ref. 1)	2.9×10^{-6}	9.2×10^{-3}
391.2	4.91×10^{-6} (Ref. 1)	4.7×10^{-6}	1.6×10^{-2}
423.2	1.55×10^{-5} (Ref. 1)	1.2×10^{-5}	3.9×10^{-2}

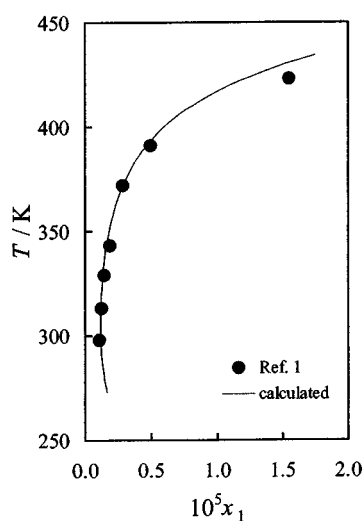


Table 3.17. 2-Methylhexane–water

Components		References		
2-Methylhexane; C ₇ H ₁₆ ; [591-76-4] Water; H ₂ O; [7732-18-5]		¹ B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel 10 , 42 (1965). ² L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).		
Reference liquid–liquid equilibrium data				
T (K)	Water rich phase		Hydrocarbon rich phase	
	$x_{1,\text{exp}}$	$x_{1,\text{calc}}$	T (K)	$x_{2,\text{calc}}$
298.3	4.57×10^{-7} (Ref. 2)	6.3×10^{-7}	283.2	3.12×10^{-4} (Ref. 1)
			293.2	5.73×10^{-4} (Ref. 1)
			303.2	1.012×10^{-3} (Ref. 1)
				3.2×10^{-4}
				5.0×10^{-4}
				7.8×10^{-4}

Table 3.18. 3-Methylhexane-water

Components			References		
3-Methylhexane; C ₇ H ₁₆ ; [589-34-4]			¹ J. Polak and B. C. Y. Lu, Can. J. Chem. 51 , 4018 (1973).		
Water; H ₂ O; [7732-18-5]					
Reference liquid-liquid equilibrium data					
Water rich phase			Hydrocarbon rich phase		
<i>T</i> (K)	<i>x</i> _{1,exp}	<i>x</i> _{1,calc}	<i>T</i> (K)	<i>x</i> _{2,exp}	<i>x</i> _{2,calc}
273.2	9.41 × 10 ⁻⁷ (Ref. 1)	1.1 × 10 ⁻⁶	273.2	1.39 × 10 ⁻⁴ (Ref. 1)	1.9 × 10 ⁻⁴
298.2	8.89 × 10 ⁻⁷ (Ref. 1)	7.7 × 10 ⁻⁷			

Other references:²L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).

Table 3.19. 3-Methylheptane-water

Components			References		
3-Methylheptane; C ₈ H ₁₈ ; [589-81-1]			¹ L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).		
Water; H ₂ O; [7732-18-5]					
Reference liquid-liquid equilibrium data					
Water rich phase			Hydrocarbon rich phase		
<i>T</i> (K)	<i>x</i> _{1,exp}	<i>x</i> _{1,calc}	<i>x</i> _{2,calc}		
298.2	1.25 × 10 ⁻⁷ (Ref. 1)	1.6 × 10 ⁻⁷	6.1 × 10 ⁻⁴		

Table 3.20. 2,2,4-Trimethylpentane-water

Components			References		
2,2,4-Trimethylpentane; C ₈ H ₁₈ ; [540-84-1]			¹ L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. 50 , 1344 (1976).		
Water; H ₂ O; [7732-18-5]			² B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel 10 , 42 (1965).		
			³ J. Polak and B. C. Y. Lu, Can. J. Chem. 51 , 4018 (1973).		
Reference liquid-liquid equilibrium data					
Water rich phase			Hydrocarbon rich phase		
<i>T</i> (K)	<i>x</i> _{1,exp}	<i>x</i> _{1,calc}	<i>T</i> (K)	<i>x</i> _{2,exp}	<i>x</i> _{2,calc}
273.2	3.88 × 10 ⁻⁷ (Ref. 3)	3.6 × 10 ⁻⁷	273.2	1.97 × 10 ⁻⁴ (Ref. 2)	2.1 × 10 ⁻⁴
293.2	3.00 × 10 ⁻⁷ (Ref. 1)	2.6 × 10 ⁻⁷	283.2	3.74 × 10 ⁻⁴ (Ref. 2)	3.4 × 10 ⁻⁴
298.2	3.23 × 10 ⁻⁷ (Ref. 3)	2.6 × 10 ⁻⁷	293.2	4.40 × 10 ⁻⁴ (Ref. 1)	5.4 × 10 ⁻⁴
			298.2	5.07 × 10 ⁻⁴ (Ref. 3)	6.7 × 10 ⁻⁴

Other references:⁴E. G. Baker, Geochim. Cosmochim. Acta **19**, 309 (1960).⁵T. I. Berkengeim, Zavod. Lab. **10**, 592 (1941).⁶M. B. Gramajo de Doz, C. M. Bonatti, N., Solimo, and H. N. Barnes, J. Chem. Thermodyn. **33**, 1663 (2001).⁷C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).⁸D. J. Miller and S. B. Hawthorne, J. Chem. Eng. Data **45**, 78 (2000).⁹N. Peschke and S. I. Sandler, J. Chem. Eng. Data **40**, 315 (1995).¹⁰L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).

Table 3.21. 2,3,4-Trimethylpentane–water

Components		References	
2,3,4-Trimethylpentane; C ₈ H ₁₈ ; [565-75-3] Water; H ₂ O; [7732-18-5]		¹ J. Polak and B. C. Y. Lu, Can. J. Chem. 51 , 4018 (1973).	
Reference liquid–liquid equilibrium data			
T (K)	Water rich phase		Hydrocarbon rich phase
	$x_{1,\text{exp}}$	$x_{1,\text{calc}}$	$x_{2,\text{calc}}$
273.2	3.69×10^{-7} (Ref. 1)	4.5×10^{-7}	1.9×10^{-4}
298.2	3.62×10^{-7} (Ref. 1)	3.2×10^{-7}	5.9×10^{-4}
Other references:			
² L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).			

Table 3.22. 2,2,5-Trimethylhexane–water

Components		References		
2,2,5-Trimethylhexane; C ₉ H ₂₀ ; [3522-94-9] Water; H ₂ O; [7732-18-5]		¹ J. Polak and B. C. Y. Lu, Can. J. Chem. 51 , 4018 (1973).		
Reference liquid–liquid equilibrium data				
T (K)	Water rich phase		Hydrocarbon rich phase	
	$x_{1,\text{exp}}$	$x_{1,\text{calc}}$	T (K)	$x_{2,\text{calc}}$
273.2	1.11×10^{-7} (Ref. 1)	8.6×10^{-8}	273.2	1.78×10^{-4} (Ref. 1)
			298.2	5.34×10^{-4} (Ref. 1)
Other references:				
² C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).				

Table 3.23. Cyclopentane-water

Components		References	
Cyclopentane; C ₅ H ₁₀ ; [287-92-3]		¹ F. R. Groves, J. Chem. Eng. Data 33 , 136 (1988).	
Water; H ₂ O; [7732-18-5]		² L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).	
Reference liquid-liquid equilibrium data			
T (K)	Water rich phase		Hydrocarbon rich phase
	$x_{1,exp}$	$x_{1,calc}$	$x_{2,calc}$
298.2	4.22×10^{-5} (Ref.1)	4.3×10^{-5}	3.9×10^{-4}
313.3	4.19×10^{-5} (Ref.2)	4.5×10^{-5}	7.5×10^{-4}
328.9	4.62×10^{-5} (Ref.2)	5.0×10^{-5}	1.4×10^{-3}
372.3	7.61×10^{-5} (Ref.2)	8.8×10^{-5}	6.5×10^{-3}
391.2	9.56×10^{-5} (Ref.2)	1.2×10^{-4}	1.2×10^{-2}
410.5	1.57×10^{-4} (Ref.2)	1.8×10^{-4}	2.1×10^{-2}
426.3	2.04×10^{-4} (Ref.2)	2.5×10^{-4}	3.3×10^{-2}

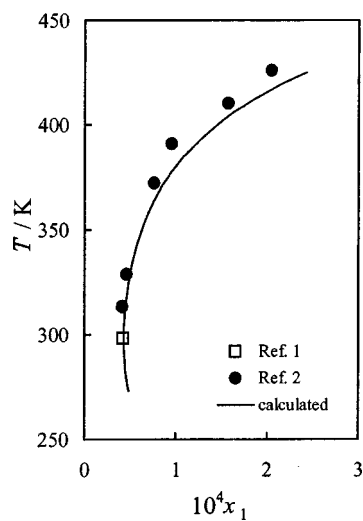
Other references:³B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel. **10**, 42 (1965).⁴A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **19**, 77 (1964).⁵C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).⁶R. A. Pierotti and A. A. Liabastre, U.S. NITS, PB Rep., No 21163, 113 pp, 1972.

Table 3.24. Cyclohexane–water

Components			References		
Cyclohexane; C ₆ H ₁₂ ; [110-82-7]			¹ L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, <i>Zh. Fiz. Khim.</i> 50 , 1344 (1976).		
Water; H ₂ O; [7732-18-5]			² R. Durand, <i>C. R. Acad. Sci.</i> 226 , 409 (1948).		
			³ P. K. Glasoe and S. D. Schultz, <i>J. Chem. Eng. Data</i> 17 , 66 (1972).		
			⁴ S. Goldman, <i>Can. J. Chem.</i> 52 , 1668 (1974).		
			⁵ F. R. Groves, <i>J. Chem. Eng. Data</i> 33 , 136 (1988).		
			⁶ R. A. Pierotti and A. A. Liabastre, U.S. NITS, PB Rep., No 21163, 113 pp, 1972.		
			⁷ J. W. Roddy and C. F. Coleman, <i>Talanta</i> 15 , 1281 (1968).		
			⁸ F. P. Schwarz, <i>Anal. Chem.</i> 52 , 10 (1980).		
			⁹ D. N. Tarassenkow and E. N. Poloshinzewa, <i>Ber. Dtsch. Chem. Ges.</i> 65 , 184 (1932).		
			¹⁰ C. Tsonopoulos and G. M. Wilson, <i>AIChE J.</i> 29 , 990 (1983).		
Reference liquid–liquid equilibrium data					
Water rich phase			Hydrocarbon rich phase		
T (K)	x _{1,exp}	x _{1,calc}	T (K)	x _{2,exp}	x _{2,calc}
278.3	1.84 × 10 ⁻⁵ (Ref. 6)	1.5 × 10 ⁻⁵	283.15	1.60 × 10 ⁻⁴ (Ref. 4)	2.0 × 10 ⁻⁴
289.2	1.30 × 10 ⁻⁵ (Ref. 2)	1.4 × 10 ⁻⁵	287.15	2.30 × 10 ⁻⁴ (Ref. 9)	2.4 × 10 ⁻⁴
293.2	1.50 × 10 ⁻⁵ (Ref. 1)	1.3 × 10 ⁻⁵	288.15	2.80 × 10 ⁻⁴ (Ref. 3)	2.6 × 10 ⁻⁴
296.7	1.10 × 10 ⁻⁵ (Ref. 8)	1.3 × 10 ⁻⁵	293.15	2.80 × 10 ⁻⁴ (Ref. 4)	3.3 × 10 ⁻⁴
298.2	1.25 × 10 ⁻⁵ (Ref. 5)	1.3 × 10 ⁻⁵	298.15	3.75 × 10 ⁻⁴ (Ref. 7)	4.0 × 10 ⁻⁴
313.2	1.56 × 10 ⁻⁵ (Ref. 10)	1.4 × 10 ⁻⁵	303.15	4.50 × 10 ⁻⁴ (Ref. 4)	5.0 × 10 ⁻⁴
373.2	3.79 × 10 ⁻⁵ (Ref. 10)	3.2 × 10 ⁻⁵	308.15	5.30 × 10 ⁻⁴ (Ref. 4)	6.2 × 10 ⁻⁴
422.0	1.03 × 10 ⁻⁴ (Ref. 10)	1.0 × 10 ⁻⁴	313.15	8.87 × 10 ⁻⁴ (Ref. 10)	7.6 × 10 ⁻⁴
473.2	3.92 × 10 ⁻⁴ (Ref. 10)	4.0 × 10 ⁻⁴	373.15	5.12 × 10 ⁻³ (Ref. 10)	6.3 × 10 ⁻³
482.2	4.93 × 10 ⁻⁴ (Ref. 10)	5.1 × 10 ⁻⁴	423.15	2.40 × 10 ⁻² (Ref. 10)	2.6 × 10 ⁻²
			473.15	7.93 × 10 ⁻² (Ref. 10)	8.6 × 10 ⁻²

Other references:

- ¹¹T. I. Berkengeim, *Zavod. Lab.* **10**, 592 (1941).
¹²P. Backx and S. Goldman, *J. Phys. Chem.* **85**, 2975 (1981).
¹³C. Black, G. G. Joris, and H. S. Taylor, *J. Chem. Phys.* **16**, 537 (1948).
¹⁴K. Brollos, K. Peter, and G. M. Schneider, *Ber. Bunsen-Ges. Phys. Chem.* **74**, 682 (1970).
¹⁵S. D. Burd, Jr. and W. G. Braun, *Proc. Am. Pet. Inst., Div. Refin.* **48**, 464 (1968).
¹⁶B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, *Khim. Tekhnol. Topl. Masel* **10**, 42 (1965).
¹⁷M. D. Gregory, S. D. Christian, and H. E. Affsprung, *J. Phys. Chem.* **71**, 2283 (1967).
¹⁸A. N. Guseva and E. I. Parnov, *Radiokhimiya* **5**, 507 (1963).
¹⁹A. N. Guseva and E. I. Parnov, *Zh. Fiz. Khim.* **37**, 2763 (1963).
²⁰J. R. Johnson, S. D. Christian, and H. E. Affsprung, *J. Chem. Soc. A*, 77 (1966).
²¹J. Kirchnerova and G. C. B. Cave, *Can. J. Chem.* **54**, 3909 (1976).
²²I. M. Korenman and R. P. Arefeva, Patent USSR, 553 524, 1977.04.05.
²³I. M. Korenman and R. P. Arefeva, *Zh. Prikl. Khim. (Leningrad)* **51**, 957 (1978).
²⁴A. P. Kudchadker and J. J. McKetta, *AIChE J.* **7**, 707 (1961).
²⁵P. J. Leinonen and D. Mackay, *Can. J. Chem. Eng.* **51**, 230 (1973).
²⁶D. Mackay and W. Y. Shiu, *Can. J. Chem. Eng.* **53**, 239 (1975).
²⁷D. Mackay, W. J. Shiu, and A. W. Wolkoff, *ASTM Spec. Tech. Pub.* **573**, 251 (1975).
²⁸C. McAuliffe, *J. Phys. Chem.* **70**, 1267 (1966).
²⁹J. W. McBain and K. J. Lissant, *J. Phys. Colloid Chem.* **55**, 665 (1951).
³⁰R. M. Plenkina, R. O. Pryanikova, and G. D. Efremova, *Zh. Fiz. Khim.* **45**, 2389 (1971).
³¹L. C. Price, *Am. Assoc. Pet. Geol. Bull.* **60**, 213 (1976).
³²C. J. Rebert and K. E. Hayworth, *AIChE J.* **13**, 118 (1967).
³³E. S. Rudakov and A. I. Lutsyk, *Zh. Fiz. Khim.* **53**, 1298 (1979).
³⁴I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, *Bull. Chem. Soc. Jpn.* **60**, 517 (1987).
³⁵V. G. Skripka, Tr., *Vses. Neftgazov. Nauch.-Issled. Inst.* **61**, 139 (1976).
³⁶R. M. Stephenson, *J. Chem. Eng. Data* **37**, 80 (1992).
³⁷Ya. D. Zel'venskii, A. A. Efremov, and G. M. Larin, *Khim. Tekhnol. Topl. Masel* **10**, 3 (1965).

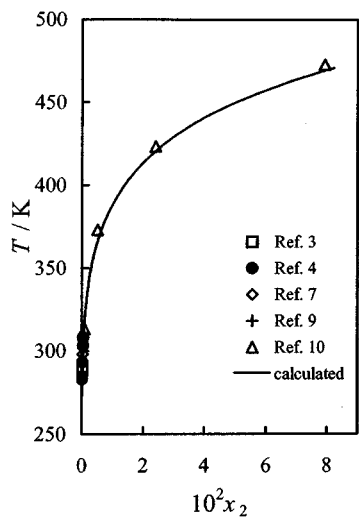
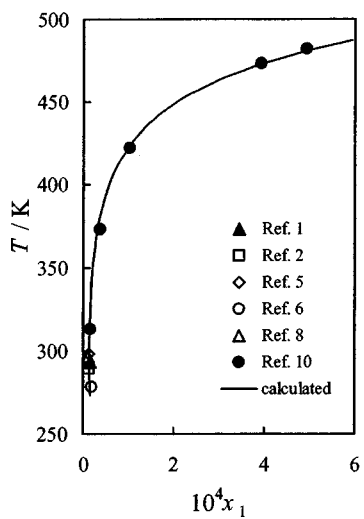


Table 3.25. Methylcyclopentane–water

Components		References	
Methylcyclopentane; C ₆ H ₁₂ ; [96-37-7] Water; H ₂ O; [7732-18-5]		¹ E. S. Rudakov and A. I. Lutsyk, Zh. Fiz. Khim. 53 , 1298 (1979).	
Reference liquid–liquid equilibrium data			
T (K)	Water rich phase		Hydrocarbon rich phase
	$x_{1,\text{exp}}$	$x_{1,\text{calc}}$	$x_{2,\text{calc}}$
298.2	9.6×10^{-6} (Ref. 1)	1.0×10^{-5}	4.6×10^{-4}

Other references:²B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).³A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **19**, 77 (1964).⁴C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).⁵L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).

Table 3.26. Cycloheptane–water

Components		References	
Cycloheptane; C ₇ H ₁₄ ; [291-64-5] Water; H ₂ O; [7732-18-5]		¹ F. R. Groves, J. Chem. Eng. Data 33 , 136 (1988). ² C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).	
Reference liquid–liquid equilibrium data			
T (K)	Water rich phase		Hydrocarbon rich phase
	$x_{1,\text{exp}}$	$x_{1,\text{calc}}$	$x_{2,\text{calc}}$
298.2	5.50×10^{-6} (Ref. 2)	4.3×10^{-6}	3.9×10^{-4}
303.2	4.99×10^{-6} (Ref. 1)	4.3×10^{-6}	4.9×10^{-4}

Table 3.27. Methylcyclohexane-water

Components		References	
Methylcyclohexane; C ₇ H ₁₄ ; [108-87-2] Water; H ₂ O; [7732-18-5]		¹ L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).	
Reference liquid-liquid equilibrium data			
T (K)	Water rich phase		Hydrocarbon rich phase
	$x_{1,\text{exp}}$	$x_{1,\text{calc}}$	$x_{2,\text{calc}}$
298.2	2.90×10^{-6} (Ref. 1)	2.9×10^{-6}	4.7×10^{-4}
313.3	3.30×10^{-6} (Ref. 1)	3.1×10^{-6}	8.9×10^{-4}
328.9	3.50×10^{-6} (Ref. 1)	3.6×10^{-6}	1.6×10^{-3}
372.3	6.20×10^{-6} (Ref. 1)	8.1×10^{-6}	6.9×10^{-3}
393.2	1.46×10^{-5} (Ref. 1)	1.4×10^{-5}	1.3×10^{-2}
410.5	2.55×10^{-5} (Ref. 1)	2.3×10^{-5}	2.0×10^{-2}

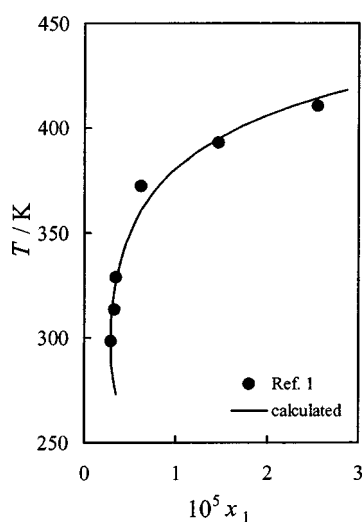
Other references:²B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).³F. R. Groves, J. Chem. Eng. Data **33**, 136 (1988).⁴A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **19**, 77 (1964).⁵S. Hellinger and S. I. Sandler, J. Chem. Eng. Data **40**, 321 (1995).⁶C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).⁷E. S. Rudakov and A. I. Lutsyk, Zh. Fiz. Khim. **53**, 1298 (1979).

Table 3.28. Cyclooctane-water

Components		References	
Cyclooctane; C ₈ H ₁₆ ; [292-64-8] Water; H ₂ O; [7732-18-5]		¹ C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).	
Reference liquid-liquid equilibrium data			
T (K)	Water rich phase		Hydrocarbon rich phase
	$x_{1,\text{exp}}$	$x_{1,\text{calc}}$	$x_{2,\text{calc}}$
298.2	1.27×10^{-6} (Ref. 1)	1.2×10^{-6}	4.1×10^{-4}

Table 3.29. *cis*-1,2-Dimethylcyclohexane–water

Components		References	
<i>cis</i> -1,2-Dimethylcyclohexane; C ₈ H ₁₆ ; [2207-01-4] Water; H ₂ O; [7732-18-5]		¹ C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).	
Reference liquid–liquid equilibrium data			
T (K)	Water rich phase		Hydrocarbon rich phase
	$x_{1,\text{exp}}$	$x_{1,\text{calc}}$	$x_{2,\text{calc}}$
298.2	9.6×10^{-7} (Ref. 1)	7.9×10^{-7}	4.8×10^{-4}

Table 3.30. Ethylcyclohexane–water

Components				References			
Ethylcyclohexane, C ₈ H ₁₆ [1678-91-7] Water; H ₂ O; [7732-18-5]				¹ J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M., AIChE J. 31 , 376 (1985).			
Reference liquid–liquid equilibrium data							
Water rich phase				Hydrocarbon rich phase			
T (K)	P (kPa)	$x_{1,\text{exp}}$	$x_{1,\text{calc}}$	T (K)	P (kPa)	$x_{2,\text{exp}}$	$x_{2,\text{calc}}$
367.6	117	2.40×10^{-6} (Ref. 1)	2.2×10^{-6}	310.9	9.9	8.10×10^{-4} (Ref. 1)	7.9×10^{-4}
479.5	2360	1.2×10^{-4} (Ref. 1)	1.2×10^{-4}	367.6	117	6.50×10^{-3} (Ref. 1)	5.6×10^{-3}
536.1	6690	1.18×10^{-3} (Ref. 1)	1.2×10^{-3}	423.4	647	3.00×10^{-2} (Ref. 1)	2.6×10^{-2}
552.8	8830	2.37×10^{-3} (Ref. 1)	2.5×10^{-3}	479.5	2360	1.07×10^{-1} (Ref. 1)	9.5×10^{-2}
				536.1	6690	2.90×10^{-1} (Ref. 1)	3.3×10^{-1}
				552.8	8830	4.14×10^{-1} (Ref. 1)	5.1×10^{-1}
				561.4 ^a	9930	6.03×10^{-1} (Ref. 1)	7.3×10^{-1}

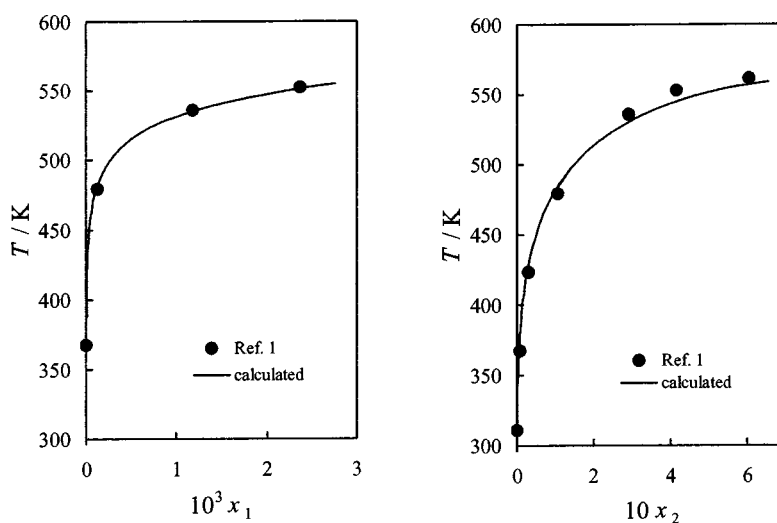
^aUCST**Other reference:**²A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2, Khim. **19**, 77 (1964).

Table 3.31. 1-Butylcyclohexane-water

Components				References			
1-Butylcyclohexane; C ₁₀ H ₂₀ ; [1678-93-9]				¹ I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. 43 , 535 (1997).			
Water; H ₂ O; [7732-18-5]							
Reference liquid-liquid equilibrium data							
Water rich phase				Hydrocarbon rich phase			
<i>T</i> (K)	<i>P</i> (kPa)	<i>x</i> _{1,exp}	<i>x</i> _{1,calc}	<i>T</i> (K)	<i>P</i> (kPa)	<i>x</i> _{2,exp}	<i>x</i> _{2,calc}
477.6	1902.3	1.60 × 10 ⁻⁵ (Ref. 1)	1.5 × 10 ⁻⁵	366.48		6.13 × 10 ⁻³ (Ref. 1)	6.0 × 10 ⁻³
				422.04	506.8	2.87 × 10 ⁻² (Ref. 1)	2.6 × 10 ⁻²
				477.59	1902.3	1.01 × 10 ⁻¹ (Ref. 1)	9.1 × 10 ⁻²
				533.15	5422.0	2.66 × 10 ⁻¹ (Ref. 1)	2.7 × 10 ⁻¹
				549.82	7107.8	3.47 × 10 ⁻¹ (Ref. 1)	3.8 × 10 ⁻¹

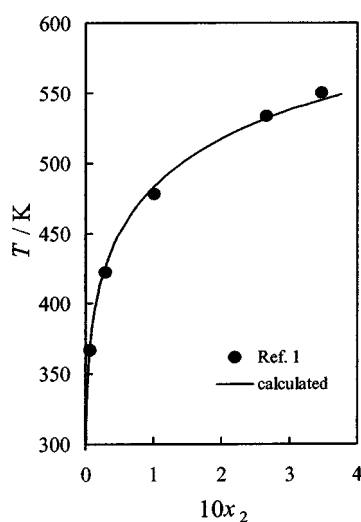


Table 3.32. Pentylcyclopentane-water

Components		References	
Pentylcyclopentane; C ₁₀ H ₂₀ ; [3741-00-2]		¹ L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).	
Water; H ₂ O; [7732-18-5]			
Reference liquid-liquid equilibrium data			
<i>T</i> (K)	Water rich phase		Hydrocarbon rich phase
	<i>x</i> _{1,exp}	<i>x</i> _{1,calc}	<i>x</i> _{2,calc}
298.2	1.5 × 10 ⁻⁸ (Ref. 1)	1.7 × 10 ⁻⁸	5.4 × 10 ⁻⁴