

Recommended Liquid–Liquid Equilibrium Data. Part 2. Unsaturated Hydrocarbon–Water Systems

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The recommended liquid–liquid equilibrium (LLE) data for 24 binary unsaturated hydrocarbon–water systems have been obtained after critical evaluation of all data (80 data sets) reported in the open literature up to the middle of 2003. A new equation was developed for prediction of the unsaturated hydrocarbon solubility. Using the predicted hydrocarbon solubilities the concentration of water in the second liquid phase was calculated. The LLE calculations were performed with the equation of state appended with a chemical term (EoS_C). The recommended data were presented in the form of individual pages containing tables, all the references, and optionally figures. © 2004 American Institute of Physics. [DOI: 10.1063/1.1647146]

Key words: binary systems; liquid–liquid equilibria; recommended data; reference data; unsaturated hydrocarbon; 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 binary unsaturated hydrocarbon–water systems, taken from the open literature up to the middle of 2003 and completed with the reference data. Solubility data for hydrocarbon–water systems were the object of IUPAC Commission on Solubility Data and presented as the Volumes 37 and 38 of the IUPAC Solubility Data Series, edited by Shaw.^{2,3} This work takes into account new data, which were published since that time

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TABLE 1. Data for calculation of solubilities of unsaturated hydrocarbons in water by means of Eq. (1)

	CAS	Formula, Name	T_c (K)	P_c (kPa)	b (cm ³)	$\ln x_{\min}$	T_{\min}
1	542-92-7	C ₅ H ₆ , 1,3-cyclopentadiene	499	4239	84.8	-8.80	298
2	142-29-0	C ₅ H ₈ , cyclopentene	509	4789	76.6	-8.57	298
3	78-79-5	C ₅ H ₈ , 2-methyl-1,3-butadiene	479	4010	86.1	-8.90	306
4	627-19-0	C ₅ H ₈ , 1-pentyne	481	4170	83.1	-7.95	306
5	513-35-9	C ₅ H ₁₀ , 2-methyl-2-butene	481	3860	89.8	-9.54	306
6	109-67-1	C ₅ H ₁₀ , 1-pentene	465	3513	95.3	-9.94	306
7	628-41-1	C ₆ H ₈ , 1,4-cyclohexadiene	574	4609	89.7	-8.43	298
8	110-83-8	C ₆ H ₁₀ , cyclohexene	554	4249	93.9	-9.83	298
9	592-42-7	C ₆ H ₁₀ , 1,5-hexadiene	500	3378	106.6	-9.66	306
10	693-02-7	C ₆ H ₁₀ , 1-hexyne	516	3620	102.7	-9.38	306
11	563-78-0	C ₆ H ₁₂ , 2,3-dimethyl-1-butene	496	3500	102.1	-10.43	306
12	592-41-6	C ₆ H ₁₂ , 1-hexene	504	3143	115.5	-11.41	306
13	763-29-1	C ₆ H ₁₂ , 2-methyl-1-pentene	504	3400	106.8	-10.78	306
14	544-25-2	C ₇ H ₈ , 1,3,5-cycloheptatriene	594	4330	98.8	-9.09	298
15	628-71-7	C ₇ H ₁₂ , 1-heptyne	547	3210	122.8	-10.84	306
16	591-49-1	C ₇ H ₁₂ , 1-methylcyclohexene	594	3754	114.0	-11.30	298
17	592-76-7	C ₇ H ₁₄ , 1-heptene	537	2836	136.5	-12.94	306
18	592-77-8	C ₇ H ₁₄ , 2-heptene,	533	2930	131.0	-12.54	306
19	3710-30-3	C ₈ H ₁₄ , 1,7-octadiene	564	2724	149.1	-12.76	306
20	629-05-0	C ₈ H ₁₄ , 1-octyne	574	2880	143.6	-12.36	306
21	111-66-0	C ₈ H ₁₆ , 1-octene	567	2568	159.0	-14.59	306
22	3452-09-3	C ₉ H ₁₆ , 1-nonyne	598	2610	165.0	-13.93	306
23	5989-27-5	C ₁₀ H ₁₆ , 4-isopropenyl-1-methylcyclohexane	648	2788	167.5	-14.11	298
24	872-05-9	C ₁₀ H ₂₀ , 1-decene	617	2130	208.6	-18.21	306

as well as new methods of the LLE correlation. In this work we investigated 80 data sets for 36 unsaturated hydrocarbon–water systems obtained from 21 references. At least the reference data for 24 systems have been obtained.

Solubilities in hydrocarbon–water systems are very low so even small errors of the measurements lead to big relative error of the measured concentrations, which in some cases can achieve 100% or more. If one system is evaluated only then the estimation of data quality is always problematic, especially if only few experimental points are available. In this work the critical evaluation procedures were based on the same approach as those presented in the previous papers by Mączyński *et al.*^{4,5} The investigation of data included two steps:

- (1) Simultaneous regression of the hydrocarbon solubilities in all investigated systems using newly developed equation. The hydrocarbon solubilities calculated from the smoothing equation are more accurate than experimental data due to compensation of negative and positive errors during the regression.
- (2) LLE calculations, which yield water solubility in the hydrocarbons. The input data for these calculations were the hydrocarbon solubilities predicted from the smoothing equation in the previous step. The LLE calculations were done with the equation of state appended with a chemical term (EoS_C) proposed by Góral.¹

The hydrocarbon solubilities calculated from the smoothing equation and the water solubilities calculated with EoS_C were used as the reference data in the evaluation. The mentioned two steps are described in Secs. 2 and 3.

2. Solubility of Unsaturated Hydrocarbons in Water

The mole fraction of a hydrocarbon in water (x_1) at temperature (T) along the three phase equilibrium line can be approximated with Eq. (1) derived in the previous paper of this series,⁵

$$\ln x_1 = \ln x_{1,\min} + (\Delta_{\text{sln}}C_p/R)[T_{\min}/T + \ln(T/T_{\min}) - 1], \quad (1)$$

where $\Delta_{\text{sln}}C_p$ is heat capacity corresponding to transfer of one mole of hydrocarbon to infinite solution. This equation describes solubility curve exhibiting a minimum solubility ($x_{1,\min}$) at $T = T_{\min}$. The solubility of various hydrocarbons at the minimum can differ by several orders of magnitude. The bigger molecules exhibit lower solubility, because 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–Kwong⁶ 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

$$b = 0.08664RT_c/P_c. \quad (2)$$

It was shown in Refs. 4 and 5 that $\ln x_{1,\min}$ in alkane–water systems depends linearly on b . The unsaturated hydrocarbons investigated in this paper are more soluble than the alkanes

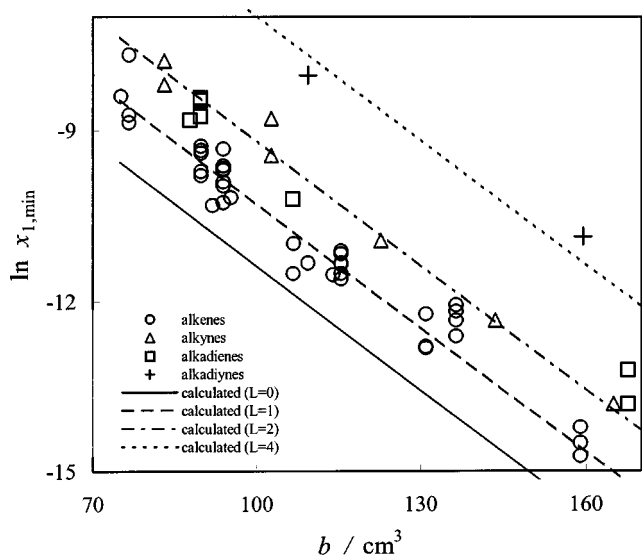


Fig. 1. Minimum solubilities ($x_{1,\min}$) of hydrocarbons vs excluded volume (b).

due to coassociation. To account for this phenomenon the expression for $\ln x_{1,\min}$ used previously for alkanes was generalized by appending an additional term

$$\ln x_{1,\min} = c_1 + c_2 b + c_\pi L, \quad (3)$$

where L is number of π bonds in the molecule of the hydrocarbon, e.g., $L=0$ for alkanes, $L=1$ for alkenes, $L=2$ for alkadienes and alkynes, and $L=4$ for alkadiynes. Validity of Eq. (3) is shown in Fig. 1.

Figure 1 shows solubilities reported for the temperature interval 280–314 K. These temperatures correspond to vicinity of the minimum of the solubility curve. Around the minimum the solubility practically does not depend on temperature hence values of $\ln x_1$ measured at these temperatures were treated as experimental approximations of $\ln x_{1,\min}$. The full line was determined in the previous paper (Ref. 5), using 169 points for 29 alkanes including n -alkanes, isoalkanes, and cycloalkanes. The other lines in Fig. 1 have the same slope but are shifted due to the additional term in Eq. (3). The coefficient c_π in this term was adjusted to experimental points shown in Fig. 1 using the fixed values of c_1 and c_2 . The resulting standard error of the experimental points was 0.369. When also c_2 was adjusted then the corresponding error was 0.362. This improvement is insignificant so c_1 and c_2 used previously for alkane–water mixtures were adopted. Thus the following coefficients were used in Eq. (3):

$$c_1 = -4.08, \quad c_2 = -0.073 \text{ mol} \cdot \text{cm}^{-3}, \quad c_\pi = 1.10. \quad (4)$$

For the conjugated π bonds $c_\pi = 0.79$. For $L=0$ Eq. (3) reduces to the approximating formula used in Ref. 5. Standard error of Eq. (3) can be estimated with the equation:

$$s(\ln x_{1,\min}) = (D_{11} + 2D_{12}b + D_{22}b^2 + D_{33}L^2)^{0.5}, \quad (5)$$

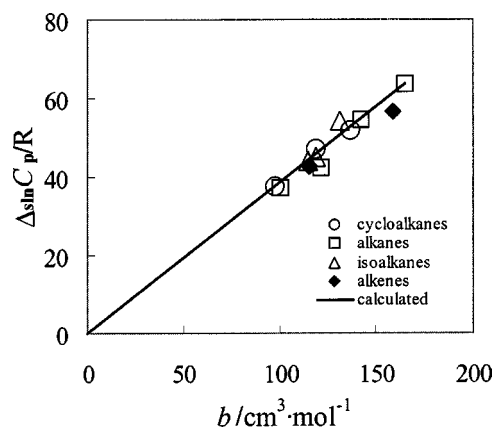


Fig. 2. Heat capacities of solution of the hydrocarbons divided by gas constant ($\Delta_{\text{sln}} C_p / R$) vs excluded volume of hydrocarbon (b).

where $D_{33} = 0.0011$ results from regression of the points in Fig. 1 with the fixed values of c_1 and c_2 . Other coefficients were reported in an earlier publication.⁵ Their values are as follows:

$$D_{11} = 9.9 \times 10^{-3};$$

$$D_{12} = -6.9 \times 10^{-5} \text{ mol} \cdot \text{cm}^{-3}; \quad (6)$$

$$D_{22} = 5.2 \times 10^{-7} (\text{mol} \cdot \text{cm}^{-3})^2.$$

Equation (3) is based on all investigated data so it is much more accurate than individual experimental points. This equation 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 $\ln x_{1,\min}$ predicted with Eq. (3). Thus Eq. (3) is a point of departure for the next stages of the evaluation.

The coefficient $\Delta_{\text{sln}} C_p / R$ in Eq. (1) was approximated by Eq. (7)

$$\Delta_{\text{sln}} C_p / R = c_3 b. \quad (7)$$

The value of c_3 was obtained by regression of the solubility data for alkanes with Eq. (1) where $\ln x_{1,\min}$ was fixed by Eq. (3) and $T_{\min} = 298$ K for cyclic hydrocarbons, $T_{\min} = 306$ K for other mixtures. These values of T_{\min} were found from analysis of experimental solubility curves. The following values of c_3 and its standard error, $s(c_3)$ were obtained:

$$c_3 = 0.376 \text{ cm}^{-3} \cdot \text{mol}, \quad s(c_3) = 2.6 \times 10^{-3} \text{ mol} \cdot \text{cm}^{-3}. \quad (8)$$

The same equations were also applied to three alkene–water systems, which were measured in wide temperature range by Economou *et al.*⁷ The experimental solubility curve for 1-hexene is well described. The experimental points for solubility of 1-octene in water are approximated fairly well but systematic deviations are observed. For 1-decene the experimental solubility curve does not go through $\ln x_{1,\min}$ predicted with Eq. (3).

The validity of Eq. (7) is illustrated in Fig. 2. This plot

was demonstrated in the previous paper, Ref. 5, but now the points corresponding to 1-hexene and 1-octene systems are supplemented.

Figure 2 suggest that Eqs. (7) and (8) are valid also for systems investigated in this paper but in order to draw definite conclusion more high temperature data are necessary. Nevertheless at temperatures not too distant from T_{\min} the second term in Eq. (1) is so small that the mentioned uncertainty is insignificant. Thus we conclude that Eq. (1) [with Eqs. (3), (4), (7), and (8)] can be applied to the investigated systems at the vicinity of minimum as well as at moderate temperatures up to say 330 K.

3. Solubility of Water in Unsaturated Hydrocarbons

In this work the solubilities predicted with Eq. (1) were used for the calculation of water concentration in the second liquid phase. To perform the LLE calculations a method of correlation of phase equilibrium developed by Góral¹ was used. This method (EoS_C) was successfully used in previous papers, Refs. 4 and 5, for correlation and prediction of LLE in alkane–water systems. EoS_C is based on RK EoS appended with a term, which accounts for hydrogen bonding. It was assumed that association of water could be approximated with the continuous association model in which 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 temperature dependent association constant $K_{\text{H-O}}$. The details of the calculations were given by Maczyński *et al.*^{4,5}

Water is more soluble in unsaturated hydrocarbons than in alkanes. This shift of the water solubility depends on number of π bonds in the hydrocarbon molecule. To account for this phenomenon it was assumed that each π bond can coassociate with free hydrogen atom of water. Each hydrogen bond of this kind was described with the same equilibrium constant $K_{\pi\text{-H}}$. The conjugated π bonds were described with another equilibrium constant ($K'_{\pi\text{-H}}$) fulfilling

$$K'_{\pi\text{-H}} = (2/3)K_{\pi\text{-H}}, \quad (9)$$

$K_{\pi\text{-H}}$ was approximated with the following equation:

$$K_{\pi\text{-H}} = (CK_{\text{H-O}})^{0.5}, \quad (10)$$

where $K_{\text{H-O}}$ is constant of self-association of water, which was calculated with formula given in the previous paper (Ref. 5). The constant C was optimized in order to obtain good agreement between the calculated and experimental solubility of water in the unsaturated hydrocarbons. This optimization gave $C = 2.2 \times 10^{-5} \text{ MPa}^{-1}$, which was used for calculation of the water solubility in all investigated systems.

The input information for the described LLE calculations is solubility of unsaturated hydrocarbons in water, calculated with Eq. (1). The output is the predicted concentration of water in the second liquid phase.

For the water solubility only 44 experimental points were available in the literature. For 29 points deviations between the experimental and the calculated value were lower than 30%. In view of accuracy of the data the agreement between the calculated and experimental water solubilities is very satisfactory. One can compare this result with verification of unsaturated hydrocarbon solubility data where Fig. 1 and Eq. (3) discarded 50 out of 110 points using the same 30% limit.

Most of the experimental points are measured at 298 K or in the vicinity of this temperature. Only for three systems was solubility of water measured in a wide temperature range. These are data for solubility of water in 1-hexene, 1-octene, and 1-decene reported by Economou *et al.*⁷ These data at room temperature are a little lower than the values predicted by EoS_C and the data of other authors. In higher temperatures the experimental points for the three systems overlap except for the last point for 1-decene, which seems to be too low. This overlapping seem to be in contradiction with behavior of the corresponding systems of *n*-alkanes where some common curve at medium temperatures differentiates at high temperatures. The same behavior exhibit the solubilities calculated with EoS_C. As a result the solubilities of water in the alkenes calculated with EoS_C agree well with the experimental points at temperatures up to about 60 K below three phase critical temperature (T_{3c}) but they are too high in the vicinity of T_{3c} .

For convenience of the reader the solubility curves predicted with EoS_C were approximated with Eq. (9) proposed by Economou *et al.*⁷

$$\ln x_2 = d_1 + d_2 \cdot (1/T_r - 1) + d_3 \cdot (1 - T_r)^{1/3} + d_4 \cdot (1 - T_r). \quad (11)$$

Originally $T_r = T/T_{3c}$, where T_{3c} is three phase critical temperature. In most cases T_{3c} is not known and instead of T_{3c} some adjustable temperature T^0 is used in Eq. (9). For unsaturated hydrocarbons investigated in this work the parameters of Eq. (9) are given in Table 2. Equation (9) should be used in the range of experimental data, which were used for testing the EoS_C calculations.

4. Conclusions

Solubility of unsaturated hydrocarbons in water can be calculated with good accuracy with Eq. (1) at the vicinity of minimum, e.g., at room and moderate temperatures. Due to lack of reliable data it is difficult to estimate accuracy of Eq. (1) at high temperatures. Solubility of water in unsaturated hydrocarbons can be calculated with EoS_C in conjunction with Eq. (1). To apply the presented equations no experimental solubility data are necessary. This method of prediction was tested using all available solubility data for the unsaturated hydrocarbon–water systems. Unfortunately most of the solubility data were measured at room temperatures. The

TABLE 2. Data for calculation of solubilities of water in unsaturated hydrocarbons by means of Eq. (11)

	CAS	Formula, Name	d_1	d_2	d_3	d_4	T^0
1	542-92-7	C ₅ H ₆ , 1,3-cyclopentadiene	-1.221	-2.646	0.656	-9.580	492.9
2	142-29-0	C ₅ H ₈ , cyclopentene	-1.296	-2.727	0.428	-9.356	501.2
3	78-79-5	C ₅ H ₈ , 2-methyl-1,3-butadiene	-1.358	-2.481	0.394	-9.823	476.1
4	627-19-0	C ₅ H ₈ , 1-pentyne	-1.396	-0.697	1.235	-12.629	477.9
5	513-35-9	C ₅ H ₁₀ , 2-methyl-2-butene	-1.408	-2.941	0.381	-9.576	477.9
6	109-67-1	C ₅ H ₁₀ , 1-pentene	-1.499	-3.363	0.364	-9.332	462.9
7	628-41-1	C ₆ H ₈ , 1,4-cyclohexadiene	-0.249	-1.027	0.384	-10.706	546.2
8	110-83-8	C ₆ H ₁₀ , cyclohexene	-0.307	-3.095	-1.147	-6.791	533.6
9	592-42-7	C ₆ H ₁₀ , 1,5-hexadiene	-0.989	-1.624	0.876	-10.836	493.8
10	693-02-7	C ₆ H ₁₀ , 1-hexyne	-0.924	-1.118	0.958	-11.461	506.6
11	563-78-0	C ₆ H ₁₂ , 2,3-dimethyl-1-butene	-1.235	-2.943	0.495	-9.510	490.5
12	592-41-6	C ₆ H ₁₂ , 1-hexene	-1.118	-3.190	0.602	-9.144	497.1
13	763-29-1	C ₆ H ₁₂ , 2-methyl-1-pentene	-1.163	-2.959	0.537	-9.395	497.0
14	544-25-2	C ₇ H ₈ , 1,3,5-cycloheptatriene	0.489	-1.227	-1.196	-8.963	558.3
15	628-71-7	C ₇ H ₁₂ , 1-heptyne	-0.646	-0.919	1.062	-11.884	529.0
16	591-49-1	C ₇ H ₁₂ , 1-methylcyclohexene	-0.138	-2.877	-0.624	-7.412	558.4
17	592-76-7	C ₇ H ₁₄ , 1-heptene	-1.090	-2.642	1.406	-10.413	522.1
18	592-77-8	C ₇ H ₁₄ , 2-heptene,	-0.564	-3.132	-0.218	-8.104	518.8
19	3710-30-3	C ₈ H ₁₄ , 1,7-octadiene	-0.246	-1.498	0.411	-10.326	540.0
20	629-05-0	C ₈ H ₁₄ , 1-octyne	-0.030	-1.406	-0.148	-9.793	546.5
21	111-66-0	C ₈ H ₁₆ , 1-octene	-0.256	-3.091	0.082	-8.020	550.8
22	3452-09-3	C ₉ H ₁₆ , 1-nonyne	0.058	-2.198	0.084	-8.477	560.7
23	5989-27-5	C ₁₀ H ₁₆ , 4-isopropenyl-1-methylcyclohexane	-0.478	2.058	2.523	-18.610	587.2
24	872-05-9	C ₁₀ H ₂₀ , 1-decene	0.160	-3.339	-0.639	-6.273	577.2

presented tests and good agreement between the calculated solubilities and the recommended data lead us to believe in good accuracy of the calculations as well as internal consistency and good quality of the recommended data.

5. Description of Tables Containing the Recommended Data

Each system is presented in a separate table, which includes 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% in respect to mole fraction of the solute. This criterion discarded 66 out of a total number of 154 experimental points investigated in this work. If more data at the same temperature fulfills this criterion then only one selected experimental point was chosen and placed in the table. The selection was done taking into account agreement with the recommended data at other temperatures and the agreement with the calculated solubility. The tables contain experimental mole fractions of the solute and the corresponding calculated values. The symbol x_1 denotes mole fraction of unsaturated hydrocarbon in the water—rich phase and x_2 denotes mole fraction of water in the unsaturated hydrocarbon—rich phase. Values denoted by $x_{1,calc}$ were calculated with Eq. (1). Coefficients of this equation are given

in Table 1. Values of $x_{2,calc}$ were calculated with Eq. (9). Coefficients of this equation are given in Table 2. These coefficients were found in the following way: at first LLE calculations were performed with EOSC using solubility of unsaturated hydrocarbon predicted with Eq. (1). Next the calculated solubilities of water were approximated with Eq. (9).

Additionally, for mixtures investigated in a sufficiently large temperature interval two types of figures are given. The figures where T is plotted versus x_1 show solubility of unsaturated hydrocarbons in water. The figures where T is plotted versus x_2 show solubility of water in the corresponding unsaturated hydrocarbon.

6. References

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3. Recommended LLE data for unsaturated hydrocarbon–water systems

Table 3.1. 1,3-Cyclopentadiene–water

Components		References	
(1) 1,3-Cyclopentadiene; C ₅ H ₆ ; [542-92-7]		¹ A. Streitweiser and L. L. Nebenzahl, <i>J. Am. Chem. Soc.</i> 98 , 2188 (1976).	
(2) Water; H ₂ O; [7732-18-5]			
Reference liquid–liquid equilibrium data			
T (K)	Water rich phase		Hydrocarbon rich phase
	$x_{1,\text{exp}}$	$x_{1,\text{calc}}$	$x_{2,\text{calc}}$
298.0	1.8×10^{-4} (Ref. 1)	1.5×10^{-4}	1.9×10^{-3}

Table 3.2. Cyclopentene–water

Components		References	
(1) Cyclopentene; C ₅ H ₈ ; [142-29-0]		¹ G. S. Natarajan and K. A. Venkatachalam, <i>J. Chem. Eng. Data</i> 17 , 328 (1972).	
(2) Water; H ₂ O; [7732-18-5]			
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	1.62×10^{-4} (Ref. 1)	1.9×10^{-4}	1.3×10^{-3}

Other references:²C. McAuliffe, *J. Phys. Chem.* **70**, 1267 (1966).³R. A. Pierotti and A. A. Liabastre, U.S. NITS, PB Rep., No 21163, 113 pp (1972).

Table 3.3. 2-Methyl-1,3-butadiene–water

Components		References			
(1) 2-Methyl-1,3-butadiene; C ₅ H ₈ ; [78-79-5]		¹ C. McAuliffe, <i>J. Phys. Chem.</i> 70 , 1267 (1966).			
(2) Water; H ₂ O; [7732-18-5]		² S. P. Pavlova, S. Yu. Pavlov, L. A. Serafimov, and L. S. Kofman, <i>Prom-st Sint. Kauch.</i> 3 , 18 (1966).			
Reference liquid–liquid equilibrium data					
T (K)	Water rich phase		Hydrocarbon rich phase		
	$x_{1,\text{exp}}$	$x_{1,\text{calc}}$	T (K)	$x_{2,\text{exp}}$	$x_{2,\text{calc}}$
293.2	1.44×10^{-4} (Ref. 2)	1.4×10^{-4}	313.2	3.58×10^{-3} (Ref.2)	3.2×10^{-3}
298.2	1.70×10^{-4} (Ref. 1)	1.4×10^{-4}	333.2	5.53×10^{-3} (Ref.2)	6.1×10^{-3}
313.2	1.76×10^{-4} (Ref. 2)	1.4×10^{-4}			

Table 3.4. 1-Pentyne–water

Components		References	
(1) 1-Pentyne; C ₅ H ₈ ; [627-19-0]		¹ C. McAuliffe, <i>J. Phys. Chem.</i> 70 , 1267 (1966).	
(2) Water; H ₂ O; [7732-18-5]			
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	4.15×10^{-4} (Ref. 1)	3.6×10^{-4}	3.4×10^{-3}

Other references:²Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, *J. Chem. Eng. Data* **27**, 451 (1982).

Table 3.5. 2-Methyl-2-butene-water

Components			References		
(1) 2-Methyl-2-butene; C ₅ H ₁₀ ; [513-35-9]			¹ G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng. Data 17 , 328 (1972).		
(2) Water; H ₂ O; [7732-18-5]			² S. P. Pavlova, S. Yu. Pavlov, L. A. Serafimov, and L. S. Kofman, Prom-st Sint. Kauch. 3 , 18 (1966).		
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	9.30 × 10 ⁻⁵ (Ref. 1)	7.7 × 10 ⁻⁵	293.2	1.51 × 10 ⁻³ (Ref. 2)	1.3 × 10 ⁻³
293.2	8.80 × 10 ⁻⁵ (Ref. 1)	7.5 × 10 ⁻⁵	313.2	2.29 × 10 ⁻³ (Ref. 2)	2.5 × 10 ⁻³
298.2	8.30 × 10 ⁻⁵ (Ref. 1)	7.3 × 10 ⁻⁵	333.2	3.52 × 10 ⁻³ (Ref. 2)	4.8 × 10 ⁻³
313.2	6.06 × 10 ⁻⁵ (Ref. 2)	7.3 × 10 ⁻⁵			
323.2	6.42 × 10 ⁻⁵ (Ref. 2)	7.6 × 10 ⁻⁵			
333.2	6.87 × 10 ⁻⁵ (Ref. 2)	8.1 × 10 ⁻⁵			

Other references:³B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Table 3.6. 1-Pentene-water

Components			References
(1) 1-Pentene; C ₅ H ₁₀ ; [109-67-1]			¹ C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).
(2) 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}	x _{2,calc}
298.2	3.8 × 10 ⁻⁵ (Ref. 1)	4.9 × 10 ⁻⁵	1.6 × 10 ⁻³

Table 3.7. 1,4-Cyclohexadiene-water

Components			References
(1) 1,4-Cyclohexadiene; C ₆ H ₈ ; [628-41-1]			¹ C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).
(2) Water; H ₂ O; [7732-18-5]			² R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No. 21163, 1972, 113 pp.
Reference liquid-liquid equilibrium data			
Water rich phase			Hydrocarbon rich phase
T (K)	x _{1,exp}	x _{1,calc}	x _{2,calc}
278.3	1.91 × 10 ⁻⁴ (Ref. 2)	2.4 × 10 ⁻⁴	2.1 × 10 ⁻³
288.4	2.15 × 10 ⁻⁴ (Ref. 2)	2.2 × 10 ⁻⁴	2.7 × 10 ⁻³
298.2	1.57 × 10 ⁻⁴ (Ref. 1)	2.2 × 10 ⁻⁴	3.4 × 10 ⁻³
298.3	2.10 × 10 ⁻⁴ (Ref. 2)	2.2 × 10 ⁻⁴	3.5 × 10 ⁻³
308.4	2.17 × 10 ⁻⁴ (Ref. 2)	2.2 × 10 ⁻⁴	4.5 × 10 ⁻³
318.4	2.27 × 10 ⁻⁴ (Ref. 2)	2.4 × 10 ⁻⁴	5.7 × 10 ⁻³

Table 3.8. Cyclohexene–water

Components			References		
(1) Cyclohexene; C ₆ H ₁₀ ; [110-83-8]			¹ L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, <i>Zh. Fiz. Khim.</i> 50 , 1344 (1976).		
(2) 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 C. McAuliffe, <i>J. Phys. Chem.</i> 70 , 1267 (1966).		
			⁴ R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No 21163, 1972, 113 pp.		
			⁵ F. P. Schwarz, <i>Anal. Chem.</i> 52 , 10 (1980).		
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}
278.3	6.14 × 10 ⁻⁵ (Ref. 4)	5.8 × 10 ⁻⁵	293.2	1.44 × 10 ⁻³ (Ref. 2)	1.1 × 10 ⁻³
288.4	6.55 × 10 ⁻⁵ (Ref. 4)	5.5 × 10 ⁻⁵	303.2	1.93 × 10 ⁻³ (Ref. 2)	1.6 × 10 ⁻³
293.2	5.00 × 10 ⁻⁵ (Ref. 1)	5.4 × 10 ⁻⁵	313.2	2.56 × 10 ⁻³ (Ref. 2)	2.1 × 10 ⁻³
296.7	6.16 × 10 ⁻⁵ (Ref. 5)	5.4 × 10 ⁻⁵			
298.2	4.67 × 10 ⁻⁵ (Ref. 3)	5.4 × 10 ⁻⁵			
298.3	6.56 × 10 ⁻⁵ (Ref. 4)	5.4 × 10 ⁻⁵			
308.4	6.63 × 10 ⁻⁵ (Ref. 4)	5.5 × 10 ⁻⁵			
318.4	6.81 × 10 ⁻⁵ (Ref. 4)	5.8 × 10 ⁻⁵			
Other references:					
⁶ E. Duque-Estrada, A. H. Bayne, and D. A. Manalan, <i>Instr. Lab. Rept.</i> , Dept. Chem. Eng., MIT, April 22, 1964.					
⁷ E. J. Farkas, <i>Anal. Chem.</i> 37 , 1173 (1965).					
⁸ J. W. McBain and K. J. Lissant, <i>J. Phys. Colloid Chem.</i> 55 , 665 (1951).					
⁹ G. S. Natarajan and K. A. Venkatachalam, <i>J. Chem. Eng. Data</i> 17 , 328 (1972).					

Table 3.9. 1,5-Hexadiene–water

Components		References	
(1) 1,5-Hexadiene; C ₆ H ₁₀ ; [592-42-7]		¹ C. Black, G. G. Joris, and H. S. Taylor, <i>J. Chem. Phys.</i> 16 , 537 (1948).	
(2) 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,calc}	<i>T</i> (K)	<i>x</i> _{2,exp}
286.2	7.0 × 10 ⁻⁵	286.2	2.8 × 10 ⁻³ (Ref. 1)
			<i>x</i> _{2,calc}
			2.3 × 10 ⁻³
Other references:			
² C. McAuliffe, <i>J. Phys. Chem.</i> 70 , 1267 (1966).			

Table 3.10. 1-Hexyne–water

Components		References	
(1) 1-Hexyne; C ₆ H ₁₀ ; [693-02-7]		¹ C. McAuliffe, <i>J. Phys. Chem.</i> 70 , 1267 (1966).	
(2) 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	7.89 × 10 ⁻⁵ (Ref. 1)	8.6 × 10 ⁻⁵	3.3 × 10 ⁻³
Other references:			
² Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, <i>J. Chem. Eng. Data</i> 27 , 451 (1982).			

Table 3.11. 2,3-Dimethyl-1-butene-water

Components		References		
(1) 2,3-Dimethyl-1-butene; C ₆ H ₁₂ ; [563-78-0]		¹ B. A. Englin, A. F. Plate, V. M. Tugolukov, and		
(2) Water; H ₂ O; [7732-18-5]		M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel 10 , 42 (1965).		
Reference liquid-liquid equilibrium data				
Water rich phase		Hydrocarbon rich phase		
<i>T</i> (K)	<i>x</i> _{1,calc}	<i>T</i> (K)	<i>x</i> _{2,exp}	<i>x</i> _{2,calc}
303.2	3.0 × 10 ⁻⁵	303.2	2.14 × 10 ⁻³ (Ref. 1)	1.8 × 10 ⁻³

Table 3.12. 1-Hexene-water

Components		References				
(1) 1-Hexene; C ₆ H ₁₂ ; [592-41-6]		¹ L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. 50 , 1344 (1976).				
(2) 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 B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel 10 , 42 (1965).				
		⁴ P. J. Leinonen and D. Mackay, Can. J. Chem. Eng. 51 , 230 (1973).				
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>x</i> _{2,exp}	<i>x</i> _{2,calc}
293.2		1.00 × 10 ⁻⁵ (Ref. 1)	1.2 × 10 ⁻⁵	293.2	1.60 × 10 ⁻³ (Ref. 1)	1.3 × 10 ⁻³
298.2		1.18 × 10 ⁻⁵ (Ref. 4)	1.1 × 10 ⁻⁵	303.2	2.23 × 10 ⁻³ (Ref. 3)	1.9 × 10 ⁻³
310.9	206.8	1.20 × 10 ⁻⁵ (Ref. 2)	1.1 × 10 ⁻⁵	366.7	318.4	1.015 × 10 ⁻² (Ref. 2)
366.5		2.40 × 10 ⁻⁵ (Ref. 2)	2.2 × 10 ⁻⁵	420.4	1247.3	4.329 × 10 ⁻² (Ref. 2)
422.0		8.50 × 10 ⁻⁵ (Ref. 2)	8.4 × 10 ⁻⁵			6.2 × 10 ⁻²
477.6		4.40 × 10 ⁻⁴ (Ref. 2)	4.6 × 10 ⁻⁴			
494.3		7.30 × 10 ⁻⁴ (Ref. 2)	8.0 × 10 ⁻⁴			

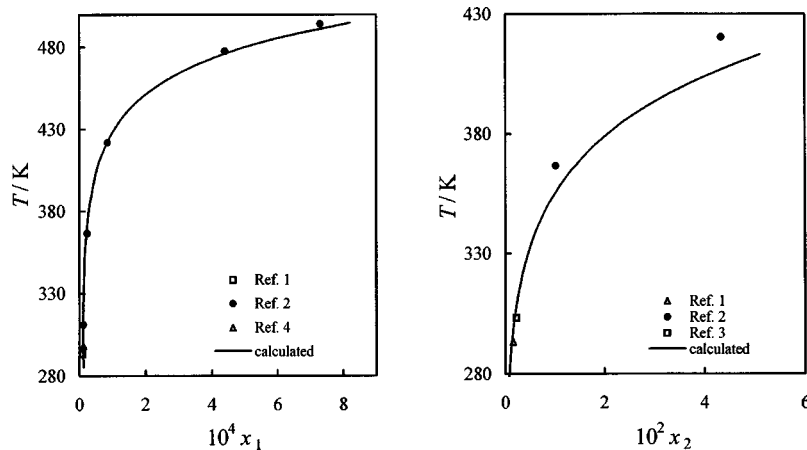
Other references:⁵C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).⁶G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng. Data **17**, 328 (1972).⁷Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Table 3.13. 2-Methyl-1-pentene–water

Components		References	
(1) 2-Methyl-1-pentene; C ₆ H ₁₂ ; [763-29-1]		¹ C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).	
(2) Water; H ₂ O; [7732-18-5]			
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	1.7×10^{-5} (Ref. 1)	2.1×10^{-5}	1.5×10^{-3}

Table 3.14. 1,3,5-Cycloheptatriene–water

Components		References			
(1) 1,3,5-Cycloheptatriene; C ₇ H ₈ ; [544-25-2]		¹ B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel 10 , 42 (1965).			
(2) Water; H ₂ O; [7732-18-5]		² C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).			
		³ R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No 21163, 1972, 113 pp.			
Reference liquid–liquid equilibrium data					
T (K)	Water rich phase		T (K)	Hydrocarbon rich phase	
	$x_{1,\text{exp}}$	$x_{1,\text{calc}}$		$x_{2,\text{exp}}$	$x_{2,\text{calc}}$
278.3	1.14×10^{-4} (Ref. 3)	1.2×10^{-4}	303.2	3.21×10^{-3} (Ref. 1)	3.8×10^{-3}
288.4	1.30×10^{-4} (Ref. 3)	1.2×10^{-4}	313.2	3.94×10^{-3} (Ref. 1)	4.9×10^{-3}
298.2	1.21×10^{-4} (Ref. 2)	1.1×10^{-4}	323.2	5.06×10^{-3} (Ref. 1)	6.2×10^{-3}
298.3	1.31×10^{-4} (Ref. 3)	1.1×10^{-4}			
308.4	1.45×10^{-4} (Ref. 3)	1.2×10^{-4}			
318.4	1.50×10^{-4} (Ref. 3)	1.2×10^{-4}			

Table 3.15. 1-Heptyne–water

Components		References	
(1) 1-Heptyne; C ₇ H ₁₂ ; [628-71-7]		¹ C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).	
(2) Water; H ₂ O; [7732-18-5]			
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	1.76×10^{-5} (Ref. 1)	2.0×10^{-5}	3.2×10^{-3}

Table 3.16. 1-Methylcyclohexene–water

Components		References	
(1) 1-Methylcyclohexene; C ₇ H ₁₂ ; [591-49-1]		¹ C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).	
(2) Water; H ₂ O; [7732-18-5]			
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	9.7×10^{-6} (Ref. 1)	1.2×10^{-5}	1.4×10^{-3}

Table 3.17. 1-Heptene-water

Components		References		
(1) 1-Heptene; C ₇ H ₁₄ ; [592-76-7]		¹ B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, <i>Khim. Tekhnol. Topl. Masel</i> 10 , 42 (1965).		
(2) 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,calc}	<i>T</i> (K)	<i>x</i> _{2,exp}	<i>x</i> _{2,calc}
283.2	2.8 × 10 ⁻⁶	283.2	1.01 × 10 ⁻³ (Ref. 1)	9.1 × 10 ⁻⁴
293.2	2.5 × 10 ⁻⁶	293.2	1.36 × 10 ⁻³ (Ref. 1)	1.3 × 10 ⁻³
303.2	2.4 × 10 ⁻⁶	303.2	2.04 × 10 ⁻³ (Ref. 1)	1.8 × 10 ⁻³

Other references:²C. Black, G. G. Joris, and H. S. Taylor, *J. Chem. Phys.* **16**, 537 (1948).³G. S. Natarajan and K. A. Venkatachalam, *J. Chem. Eng. Data* **17**, 328 (1972).⁴Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, *J. Chem. Eng. Data* **27**, 451 (1982).

Table 3.18. 2-Heptene-water

Components		References	
(1) 2-Heptene; C ₇ H ₁₄ ; [592-77-8]		¹ C. McAuliffe, <i>J. Phys. Chem.</i> 70 , 1267 (1966).	
(2) Water; H ₂ O; [7732-18-5]		² F. P. Schwarz, <i>Anal. Chem.</i> 52 , 10 (1980).	
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}
296.7	2.75 × 10 ⁻⁶ (Ref. 2)	3.7 × 10 ⁻⁶	1.4 × 10 ⁻³
298.2	2.70 × 10 ⁻⁶ (Ref. 1)	3.6 × 10 ⁻⁶	1.5 × 10 ⁻³

Other references:³G. S. Natarajan and K. A. Venkatachalam, *J. Chem. Eng. Data* **17**, 328 (1972).

Table 3.19. 1,7-Octadiene-water

Components		References		
(1) 1,7-Octadiene; C ₈ H ₁₄ ; [3710-30-3]		¹ A. O. Emelyanov, L. V. Melnik, and B. N. Bobylev, <i>Zh. Prikl. Khim. (Leningrad)</i> 64 , 1700 (1991).		
(2) 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,calc}	<i>T</i> (K)	<i>x</i> _{2,exp}	<i>x</i> _{2,calc}
360.2	5.8 × 10 ⁻⁶	360.2	1.49 × 10 ⁻² (Ref. 1)	1.6 × 10 ⁻²

Table 3.20. 1-Octyne-water

Components		References	
(1) 1-Octyne; C ₈ H ₁₄ ; [629-05-0]		¹ C. McAuliffe, <i>J. Phys. Chem.</i> 70 , 1267 (1966).	
(2) 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	4.4 × 10 ⁻⁶ (Ref. 1)	4.4 × 10 ⁻⁶	3.1 × 10 ⁻³

Table 3.21. 1-Octene–water

Components				References			
(1) 1-Octene; C ₈ H ₁₆ ; [111-66-0]				¹ I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. 43 , 535 (1997).			
(2) Water; H ₂ O; [7732-18-5]				² C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).			
Reference liquid–liquid equilibrium data							
Water rich phase				Hydrocarbon rich phase			
T (K)	P (kPa)	x _{1,exp}	x _{1,calc}	T (K)	P (kPa)	x _{2,exp}	x _{2,calc}
298.15		4.0 × 10 ⁻⁷ (Ref. 2)	4.7 × 10 ⁻⁷	310.93		1.68 × 10 ⁻³ (Ref. 1)	2.3 × 10 ⁻³
310.93		5.0 × 10 ⁻⁷ (Ref. 1)	4.7 × 10 ⁻⁷	366.48	124	8.70 × 10 ⁻³ (Ref. 1)	1.2 × 10 ⁻²
477.59	2423	9.1 × 10 ⁻⁵ (Ref. 1)	7.9 × 10 ⁻⁵	422.04	662	4.51 × 10 ⁻² (Ref. 1)	4.9 × 10 ⁻²
				477.59	2423	1.56 × 10 ⁻¹ (Ref. 1)	1.7 × 10 ⁻¹
				533.15	6840	4.19 × 10 ⁻¹ (Ref. 1)	5.5 × 10 ⁻¹
				549.82	9260	5.38 × 10 ⁻¹ (Ref. 1)	7.7 × 10 ⁻¹

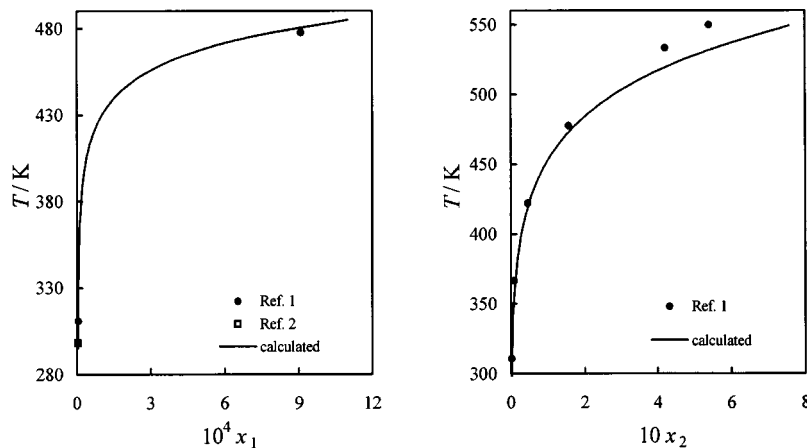
Other references:³G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng. Data **17**, 328 (1972).⁴Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Table 3.22. 1-Nonyne–water

Components		References	
(1) 1-Nonyne; C ₉ H ₁₆ ; [3452-09-3]		¹ C. McAuliffe, J. Phys. Chem. 70 , 1267 (1966).	
(2) 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}	x _{2,calc}
298.2	1.0 × 10 ⁻⁶ (Ref. 1)	9.2 × 10 ⁻⁷	3.1 × 10 ⁻³

Table 3.23. 4-Isopropenyl-1-methylcyclohexane-water

Components		References	
(1) 4-Isopropenyl-1-methylcyclohexane; C ₁₀ H ₁₆ ; [5989-27-5]		¹ D. J. Miller and S. B. Hawthorne, J. Chem. Eng. Data 45 , 315 (2000).	
(2) Water; H ₂ O; [7732-18-5]			
Reference liquid-liquid equilibrium data			
T (K)	Water rich phase		Hydrocarbon rich phase
	$x_{1,exp}$	$x_{1,calc}$	$x_{2,calc}$
423.0	2.1×10^{-5} (Ref. 1)	2.4×10^{-5}	3.9×10^{-2}

Other references:²H. A. Massaldi and C. J. King, J. Chem. Eng. Data **18**, 393 (1973).

Table 3.24. 1-Decene-water

Components		References			
(1) 1-Decene; C ₁₀ H ₂₀ ; [872-05-9]		¹ I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. 43 , 535 (1997).			
(2) Water; H ₂ O; [7732-18-5]					
Reference liquid-liquid equilibrium data					
Water rich phase		Hydrocarbon rich phase			
T (K)	$x_{1,calc}$	T (K)	P (kPa)	$x_{2,exp}$	$x_{2,calc}$
374.2	5.5×10^{-8}	374.2	121	1.33×10^{-2} (Ref.1)	1.3×10^{-2}
424.7	5.5×10^{-7}	424.2	552	4.22×10^{-2} (Ref.1)	4.5×10^{-2}
475.2	9.0×10^{-6}	475.2	1840	1.28×10^{-1} (Ref.1)	1.3×10^{-1}

Other references:²G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng. Data **17**, 328 (1972).