# Recommended Liquid–Liquid Equilibrium Data. Part 3. Alkylbenzene–Water Systems

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The recommended liquid–liquid equilibrium (LLE) data for 21 binary alkylbenzene–water systems have been obtained after critical evaluation of all data (392 data sets) reported in the open literature up to the middle of 2003. An equation for prediction of the alkylbenzene solubilities was developed. The predicted alkylbenzene solubilities were used for calculation of water solubility in the second liquid phase. The LLE calculations were done with the equation of state appended with a chemical term proposed by Góral. The recommended data were presented in the form of individual pages containing tables, all the references, and optionally figures. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1797038]

Key words: benzene and alkylbenzenes; 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 binary alkylbenzene–water systems, taken from the open literature up to the middle of 2003 and completed with predicted data. In this work we investigated 392 data sets obtained from 169 references.[1]

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.[2,3] This work takes into account new data, which were published since that time. The critical evaluation procedures were based on the same approach as

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those presented in the previous papers by Mączyński *et al.*[4] and Góral *et al.*[5] The investigation of data includes two steps described in the next two sections.

## 2. Solubility of Alkylbenzenes in Water

In the previous papers by Mączyński *et al.*[4] and Góral *et al.*,[5] the solubility of hydrocarbons in water was approximated with equation:

$$\ln x_1 = \ln x_{1,\min} + C[T_{\min}/T + \ln(T/T_{\min}) - 1]. \quad (1)$$

It was found, however, that Eq. (1) applied to the solubility data of alkylbenzenes produces small but systematic deviations. Therefore, the derivation of Eq. (1) is examined below and a modified equation is proposed.

The starting point of the derivation is condition of the phase equilibrium:

$$\mu_1 = \mu_1^* + RT \ln(x_1 f_1), \quad (2)$$

where $\mu_1$ denotes chemical potential of the hydrocarbon in the hydrocarbon rich phase and the expression in the right side of Eq. (2) gives chemical potential of the hydrocarbon solute in water, where $x_1$ is mole fraction of the hydrocarbon in water, $f_1$ is activity coefficient standardized to infinite solution, and $\mu_1^*$ is the chemical potential of the hydrocarbon in the corresponding standard state. The solubility of the hydrocarbons is so small that in the whole temperature range $f_1 = 1$ can be used. Differentiation of both sides of Eq. (2) gives, after simple rearrangement:

$$\partial \ln(x_1)/\partial(1/T) = -(h_1^* - h_1)/R, \quad (3)$$

where $h_1^*$ and $h_1$ are partial molar enthalpies corresponding to the chemical potentials $\mu_1^*$ and $\mu_1$, respectively. Equation (3) can be further rearranged to form:

$$\partial \ln(x_1)/\partial(1/T) = -[(h_1^* - h_1^\circ) - (h_1 - h_1^\circ)]/R, \quad (4)$$

where $h_1^\circ$ is molar enthalpy of the pure hydrocarbon. At low temperatures the hydrocarbon rich phase contains almost pure hydrocarbon hence $(h_1 - h_1^\circ) \approx 0$. Therefore, one can assume that the right side of Eq. (4) depends mainly on $(h_1^* - h_1^\circ)$, which is equal to heat of transfer of one mole of the pure hydrocarbon to the infinite water solution. Calorimetric measurements suggest that $(h_1^* - h_1^\circ)$ increases linearly with temperature passing through zero at room temperature ($T_{\min}$). In this case, Eq. (4) can be expressed as follows:

$$\partial \ln(x_1)/\partial(1/T) = C(T - T_{\min}), \quad (5)$$

where $C$ is some constant. Integration of Eq. (5) leads to Eq. (1).

In a more rigorous approach, both terms in Eq. (4) must be taken into account. When the temperature increases, the concentration of the hydrocarbon rich phase shifts towards the concentration of the water rich phase. This is accompanied by a nonlinear increase of the corresponding partial heat of mixing $(h_1 - h_1^\circ)$, which slows down the linear increasing of the first term in Eq. (4). Therefore, we approximate the right side of Eq. (4) with a logarithmic function, which increases with temperature more slowly than the linear function used in Eq. (5)

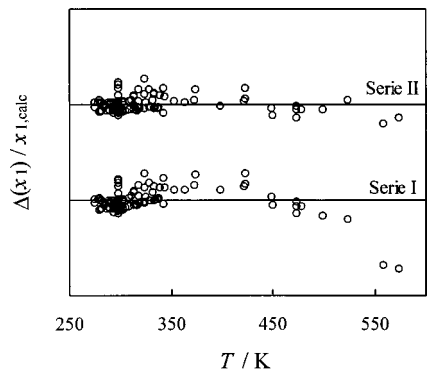


FIG. 1. Relative deviations of experimental mole fractions of benzene in water, $\Delta(x_1)/x_{1,\mathrm{calc}}$ resulting from Eq. (1) (I series) or Eq. (7) (II series). The relative deviations for given series are indicated by the deviations of the points from the corresponding horizontal line, where the distance between neighboring lines corresponds to 50% deviation.

$$\partial \ln(x_1)/\partial(1/T) = C' \ln(T/T_{\min}), \quad (6)$$

Equation (6), upon integration, gives Eq. (7).

$$\ln x_1 = \ln x_{1,\min} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)], \quad (7)$$

where $D$ is an adjustable constant, $x_{1,\min}$ is mole fraction of the hydrocarbon at minimum of the solubility and $T_{\min}$ is the corresponding temperature.

Figure 1 shows the deviations resulting from Eqs. (1) and (7) fitted to the solubility data of benzene. (Figure 1 also contains points measured at temperatures higher than three phase critical temperature. At these temperatures the hydrocarbon rich phase disappears, but the vapor–liquid equilibrium still exists.) The deviations corresponding to Eq. (1) show a characteristic pattern also observed in other mixtures, provided they are measured in sufficiently large temperature interval. Comparison of both equations for such mixtures is given in Table 1.

Figure 1 and Table 1 show that Eq. (7) approximates the experimental data more accurately. Therefore, Eq. (7) was used for the approximate value of the alkylbenzene solubility investigated in this paper.

At the first stage of this investigation Eq. (7) was applied to experimental data in order to establish value of $T_{\min}$. The minimum is rather flat so the adjusted value of $T_{\min}$ is sensitive to errors of the data but in some mixtures there are huge amounts of experimental points measured at room temperatures, which allows establishing $T_{\min}$ relatively accurately. The fitted values of $T_{\min}$ were as follows: benzene (290 K), methylbenzene (290 K), ethylbenzene (293 K), 1,3-dimethylbenzene (288 K), and 1,4-dimethylbenzene (288 K). In other mixtures experimental points measured at the room temperatures were too scarce or too scattered hence we adopted $T_{\min} = 290$ K for all the investigated mixtures of alkylbenzenes.

TABLE 1. Standard errors ($s_1$,$s_2$) of ln($x_1$) resulting from Eqs. (1) and (7), respectively ($M$ number of experimental points; $T_{min}$..$T_{max}$ temperature range of the experimental data).

| Name | $s_1$ | $s_2$ | $M$ | ($T_{min}$..$T_{max}$) |
|---|---|---|---|---|
| benzene | 0.046 | 0.034 | 111 | (274..523) |
| methylbenzene | 0.070 | 0.059 | 96 | (273..548) |
| ethylbenzene | 0.097 | 0.092 | 85 | (273..507) |
| 1,3-dimethylbenzene | 0.146 | 0.110 | 36 | (273..544) |
| 1,4-dimethylbenzene | 0.083 | 0.059 | 20 | (273..553) |
| 1,3-diethylbenzene | 0.050 | 0.121 | 6 | (311..550) |
| 1-methyl-4-(1-methylethyl)benzene | 0.045 | 0.019 | 6 | (298..473) |
| 1,4-bis(1-methylethyl)benzene | 0.124 | 0.048 | 6 | (311..550) |

Next the data for each mixture were approximated with Eq. (7), where the parameters ln($x_{1,min}$) and $D$ were fitted to the experimental points using $T_{min}$=290 K. The obtained values of $\ln x_{1,min}$ and $D$ are plotted in Figs. 2 and 3 versus the excluded volume ($b$) used in Redlich–Kwong[6] Equation of State (RK EoS), where $b$ is calculated from critical temperature, $T_c$, and critical pressure, $P_c$, given in the Table 2

$$b=0.08664\cdot RT_c/P_c. \tag{8}$$

The linear relations shown in Figs. 2 and 3 are analogical to the linear relations presented in the previous papers[4,5] for $n$-alkanes and unsaturated hydrocarbons. Figures 2 and 3 suggest that Eq. (7) can be rewritten in form

$$\ln x_1=(c_1+c_2b)+(c_3+c_4b)[(T_{min}/T)\ln(T_{min}/T)+1-(T_{min}/T)]. \tag{9}$$

The coefficients ($c_1$, $c_2$, $c_3$, and $c_4$) were found by a simultaneous regression of the alkylbenzene solubility data. Before the regression process, the plots of the solubility data were inspected in order to remove the most outlying experimental points. The initial verification rejected 210 points. The remaining 556 points were used in the regression. The following values of the coefficients in Eq. (9) were obtained:

$$c_1=-2.605;\quad c_2=-0.06296\ \text{mol}\cdot\text{cm}^{-3};$$
$$c_3=7.979;\quad c_4=0.2668\ \text{mol}\cdot\text{cm}^{-3}. \tag{10}$$

The standard error of the experimental value of $\ln x_{1,min}$, estimated from deviations of the 556 points, was 0.18. Standard error of $\ln x_{1,min}$, resulting from Eq. (9), was determined with the help of the variance–covariance matrix obtained with a least squares method. This error depends on $T$ and $b$. For the limiting values of $T$ and $b$, standard errors ($s$) of $\ln x_1$ resulting from Eq. (9) are as follows:

$$s(T=290,b=80)=0.01;$$
$$s(t=290,b=220)=0.02;$$
$$s(T=550,b=80)=0.06;$$
$$s(T=550,b=220)=0.10;$$

where $T$ is given in Kelvin and $b$ in cm$^3$ mol$^{-1}$.

## 3. Solubility of Water in Alkylbenzenes

In this work, the solubility predicted with Eq. (9) was used for the calculation of the water concentration in the second liquid phase. To perform the LLE calculations, a method of correlation of phase equilibrium developed by Góral[1] was used. This method (EoSC) was successfully used in previous papers[4,5] for the correlation and prediction of LLE in alkane–water and unsaturated hydrocarbons–water systems. EoSC is based on RK EoS appended with a term, which accounts for hydrogen bonding. It assumes that the association of water can 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 tem-

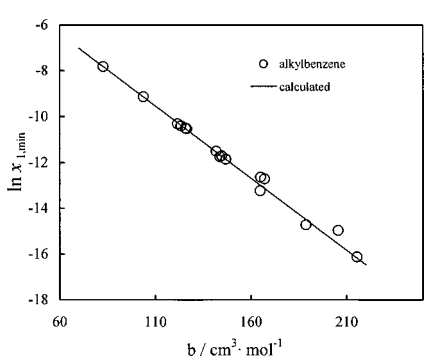


FIG. 2. Minimum solubility ($x_{1,min}$) of alkylbenzenes vs excluded volume ($b$).

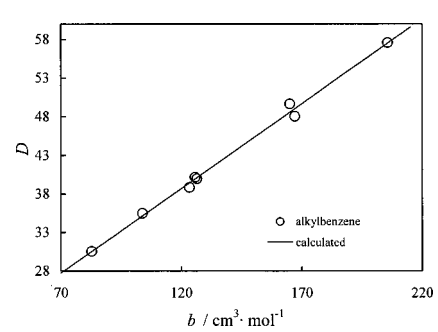


FIG. 3. Coefficient $D$ in Eq. (7) vs excluded volume of alkylbenzenes ($b$).

TABLE 2. Data for calculation of the alkylbenzene solubility by means of Eq. (9), where $T_{min}=290$ K

| | CAS | Name | $T_c$ (K) | $P_c$ (kPa) | $b$ (cm$^3$ mol$^{-1}$) | $\ln x_{1,min}$ |
|---|---|---|---|---|---|---|
| 1 | 71-43-2 | benzene | 562 | 4898 | 82.7 | −7.81 |
| 2 | 108-88-3 | methylbenzene | 592 | 4106 | 103.8 | −9.14 |
| 3 | 100-41-4 | ethylbenzene | 617 | 3606 | 123.3 | −10.37 |
| 4 | 103-65-1 | propylbenzene | 638 | 3200 | 143.7 | −11.65 |
| 5 | 104-51-8 | butylbenzene | 661 | 2887 | 164.8 | −12.98 |
| 6 | 538-68-1 | pentylbenzene | 679 | 2590 | 188.8 | −14.49 |
| 7 | 1077-16-3 | hexylbenzene | 696 | 2330 | 215.3 | −16.16 |
| 8 | 98-82-8 | (1-methylethyl)benzene | 631 | 3209 | 141.7 | −11.53 |
| 9 | 135-98-8 | *sec*-butylbenzene | 649 | 2890 | 161.8 | −12.79 |
| 10 | 98-06-6 | *tert*-butylbenzene | 645 | 2800 | 165.9 | −13.05 |
| 11 | 95-47-6 | 1,2-dimethylbenzene | 630 | 3734 | 121.6 | −10.26 |
| 12 | 108-38-3 | 1,3-dimethylbenzene | 617 | 3536 | 125.7 | −10.52 |
| 13 | 106-42-3 | 1,4-dimethylbenzene | 616 | 3511 | 126.4 | −10.56 |
| 14 | 141-93-5 | 1,3-diethylbenzene | 655 | 2860 | 165.0 | −12.99 |
| 15 | 611-14-3 | 1-ethyl-2-methylbenzene | 647 | 3290 | 141.7 | −11.53 |
| 16 | 99-87-6 | 1-methyl-4-(1-methylethyl) benzene | 652 | 2810 | 167.1 | −13.13 |
| 17 | 100-18-5 | 1,4bis(1-methylethyl)benzene | 671 | 2351 | 205.6 | −15.55 |
| 18 | 526-73-8 | 1,2,3-trimethylbenzene | 664 | 3454 | 138.6 | −11.33 |
| 19 | 95-63-6 | 1,2,4-trimethylbenzene | 649 | 3232 | 144.7 | −11.72 |
| 20 | 108-67-8 | 1,3,5-trimethylbenzene | 637 | 3127 | 146.8 | −11.85 |
| 21 | 100-42-5 | ethenylbenzene | 635 | 3841 | 119.2 | −13.05 |

perature dependent association constant $K_{H-O}$. The details of the LLE calculations and the parameters of the water self-association model are given in previous papers.[4,5]

Water is more soluble in alkylbenzenes than in alkanes. To account for this phenomenon it was assumed that each aromatic ring can co-associate with the free hydrogen atom of water. The hydrogen bond of this kind was described by the temperature dependent equilibrium constant ($K_{\pi-H}$)

$$K_{\pi-H}=K_0 \exp[(-\Delta H_{\pi-H}/R)(1/T-1/T_0)], \quad (11)$$

where $T_0=273$ K is the reference temperature. $K_0$ and $(-\Delta H_{\pi-H}/R)$ were optimized in order to obtain good agreement between the calculated and experimental solubility of water in the alkylbenzenes. This optimization gave

$$K_0=0.0103 \ \ \mathrm{MPa}^{-1}, \quad (12)$$

which was used for calculation of the water solubility in all investigated systems.

It is known that the enthalpy of the coassociation of various alkylbenzenes with the same electrone acceptor increases with number of the alkyl groups attached to the benzene ring. See, for example, the data of Thompson and Maine.[7] The same behavior was observed in the investigated systems. It was found that good results of the LLE calculations were obtained with the following empirical formula:

$$(-\Delta H_{\pi-H}/R)=h_1+h_2T_c, \quad (13)$$

where $T_c$ is critical temperature of the alkylbenzene (in Kelvin) and $h_1$ and $h_2$ are empirical constants:

$$h_1=-2670 \ \ \mathrm{K}; \quad h_2=6.0 \quad (14)$$

This formula gives increasing values of $(-\Delta H_{\pi-H})$ from 5.82 kJ mol$^{-1}$ for benzene up to 12.52 kJ mol$^{-1}$ for hexylbenzene.

The results of the LLE calculations are the predicted values (as temperature function) of water solubility in the investigated alkylbenzenes. The input information is solubility of alkylbenzene in water, calculated with Eq. (9). The solubility of water in the alkylbenzenes was used only at the beginning of this investigation to fix the three parameters used in the model of the co-association ($K_0$, $h_1$, $h_2$). These parameters were constant for all the investigated mixtures. The parameters of the model of self-association of water were unchanged in respect to the previous papers.[4,5]

For the solubility of water in alkylbenzenes 405 experimental points for 15 systems were available in literature. The most outlying 36 points were rejected from further investigations. The remained 369 points were compared with the calculated values. This comparison gives average standard error of the experimental data equal to 11% of the measured water mole fraction. In view of accuracy of the data the agreement between the calculated and experimental water solubilities is very satisfactory. It was estimated that the LLE calculations at low temperatures permit a determination of the mole fraction of water with 1% accuracy. This accuracy is lower at high temperatures.

The relative deviations between the experimental and calculated water mole fractions in various alkylbenzenes are shown in Fig. 4.

For convenience of the reader the solubility curves predicted with EoSC were approximated with Eq. (15) proposed by Economou *et al.*[8]

$$\ln x_2=d_1+d_2(1/T_r-1)+d_3(1-T_r)^{1/3}+d_4(1-T_r). \quad (15)$$

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 $T_0 \geqslant T_{3c}$ is used in Eq. (15). For

TABLE 3. Data for calculation of water solubility in alkylbenzenes by means of Eq. (15)

| | CAS | Name | $d_1$ | $d_2$ | $d_3$ | $d_4$ | $T^0$ |
|---|---|---|---|---|---|---|---|
| 1 | 71-43-2 | benzene | −0.509 | −4.316 | −0.203 | −3.637 | 541.7 |
| 2 | 108-88-3 | methylbenzene | −0.495 | −3.700 | −0.102 | −4.641 | 553.0 |
| 3 | 100-41-4 | ethylbenzene | −0.383 | −3.167 | −0.009 | −5.655 | 566.9 |
| 4 | 103-65-1 | propylbenzene | −0.304 | −2.764 | 0.166 | −6.621 | 577.5 |
| 5 | 104-51-8 | butylbenzene | −0.232 | −2.326 | 0.400 | −7.774 | 588.0 |
| 6 | 538-68-1 | pentylbenzene | −0.180 | −2.021 | 0.666 | −8.750 | 596.1 |
| 7 | 1077-16-3 | hexylbenzene | −0.135 | −1.779 | 0.971 | −9.671 | 603.5 |
| 8 | 98-82-8 | (1-methylethyl)benzene | −0.329 | −2.962 | 0.152 | −6.247 | 574.0 |
| 9 | 135-98-8 | *sec*-butylbenzene | −0.268 | −2.638 | 0.322 | −7.077 | 582.7 |
| 10 | 98-06-6 | *tert*-butylbenzene | −0.281 | −2.831 | 0.360 | −6.777 | 580.8 |
| 11 | 95-47-6 | 1,2-dimethylbenzene | −0.332 | −2.775 | −0.027 | −6.308 | 573.6 |
| 12 | 108-38-3 | 1,3-dimethylbenzene | −0.383 | −3.168 | −0.019 | −5.636 | 566.8 |
| 13 | 106-42-3 | 1,4-dimethylbenzene | −0.386 | −3.206 | −0.003 | −5.597 | 566.4 |
| 14 | 141-93-5 | 1,3-diethylbenzene | −0.248 | −2.450 | 0.336 | −7.447 | 585.6 |
| 15 | 611-14-3 | 1-ethyl-2-methylbenzene | −0.274 | −2.480 | 0.179 | −7.156 | 581.8 |
| 16 | 99-87-6 | 1-methyl-4-(1-methylethyl) benzene | −0.259 | −2.611 | 0.366 | −7.192 | 584.0 |
| 17 | 100-18-5 | 1,4bis(1-methylethyl)benzene | −0.202 | −1.908 | 0.300 | −8.422 | 592.7 |
| 18 | 526-73-8 | 1,2,3-trimethylbenzene | −0.220 | −1.939 | 0.288 | −8.329 | 589.8 |
| 19 | 95-63-6 | 1,2,4-trimethylbenzene | −0.267 | −2.429 | 0.187 | −7.262 | 582.8 |
| 20 | 108-67-8 | 1,3,5-trimethylbenzene | −0.307 | −2.743 | 0.101 | −6.560 | 577.1 |
| 21 | 100-42-5 | ethenylbenzene | −0.314 | −0.910 | 2.643 | −13.598 | 576.1 |

the alkylbenzenes investigated in this work, the parameters of Eq. (15) are given in Table 3. Equation (15) should be used in range of experimental data, which were used for testing the EoSC calculations.

## 4. Conclusions

The solubility of alkylbenzenes in water can be calculated with Eq. (9) up to three-phase critical temperature or even higher (as was shown by data for benzene–water system). The solubility of water in alkylbenzenes can be calculated with EoSC in conjunction with Eq. (9). To apply the presented equations no experimental solubility data are necessary. This method of prediction was tested using all available solubility data for the alkylbenzene–water systems. The presented tests and good agreement between the calculated solubilities and the recommended data suggest that there is good accuracy in the calculations as well as internal consistency and good quality of the recommended data.

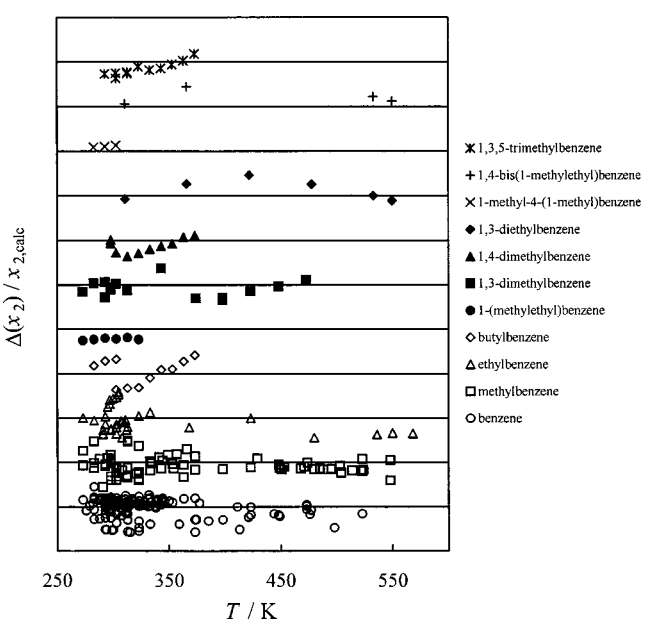


FIG. 4. Relative deviations of experimental mole fractions of water in the investigated alkylbenzenes, $\Delta(x_2)/x_{2,\mathrm{calc}}$, calculated in respect to the values given by Eq. (15). The relative deviations for given mixture are indicated by the deviations of the points from the corresponding horizontal line, where the distance between neighboring lines corresponds to 50% deviation.

## 5. Description of Tables Containing the Recommended Data

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

The tables contain data which deviate from the calculated solubilities by less than 30%. If more data at the same temperature fulfills the assumed limit, then only one selected experimental point was chosen and placed in the table. The selection was done taking into account agreement with the recommended data at other temperatures and the agreement with the calculated (reference) solubility. The tables contain experimental mole fractions of the solute and the corresponding calculated values. The symbol $x_1$ denotes the mole fraction of alkylbenzene in the water-rich phase, and $x_2$ denotes the mole fraction of water in the alkylbenzene-rich phase. Values denoted by $x_{1,\mathrm{calc}}$ were calculated with Eq. (9). The data necessary for using Eq. (9) are given in Table 2. Values of $x_{2,\mathrm{calc}}$ were calculated with Eq. (15). Coefficients of this equation are given in Table 3. These coefficients were found in the following way: at first LLE calculations were

performed with EoSC using solubility of alkylbenzenes predicted with Eq. (9). Next the calculated solubilities of water were approximated with Eq. (15).

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

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# 4. Recommended LLE data for alkylbenzenes–water systems

Table 4.1. Benzene–water

**Components**:
(1) Benzene; $C_6H_6$; [71-43-2]
(2) Water; $H_2O$; [7732-18-5]

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Reference liquid–liquid equilibrium data

| Water rich phase | | | | Hydrocarbon rich phase | | | |
|---|---|---|---|---|---|---|---|
| $T$ (K) | $P$ (kPa) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $T$ (K) | $P$ (kPa) | $x_{2,\mathrm{exp}}$ | $x_{2,\mathrm{calc}}$ |
| 273.2 | | $3.87\times10^{-4}$ (Ref. 32) | $4.3\times10^{-4}$ | 273.2 | | $1.31\times10^{-3}$ (Ref. 32) | $1.2\times10^{-3}$ |
| 273.4 | | $4.232\times10^{-4}$ (Ref. 27) | $4.3\times10^{-4}$ | 276.2 | | $1.30\times10^{-3}$ (Ref. 20) | $1.4\times10^{-3}$ |
| 274.0 | | $4.25\times10^{-4}$ (Ref. 1) | $4.3\times10^{-4}$ | 278.6 | | $1.50\times10^{-3}$ (Ref. 33) | $1.5\times10^{-3}$ |
| 275.2 | | $4.31\times10^{-4}$ (Ref. 24) | $4.2\times10^{-4}$ | 282.4 | | $1.783\times10^{-3}$ (Ref. 30) | $1.7\times10^{-3}$ |
| 277.7 | | $4.25\times10^{-4}$ (Ref. 8) | $4.2\times10^{-4}$ | 282.6 | | $1.92\times10^{-3}$ (Ref. 29) | $1.7\times10^{-3}$ |
| 278.2 | | $3.73\times10^{-4}$ (Ref. 34) | $4.2\times10^{-4}$ | 282.7 | | $1.50\times10^{-3}$ (Ref. 39) | $1.7\times10^{-3}$ |
| 278.8 | | $4.02\times10^{-4}$ (Ref. 3) | $4.2\times10^{-4}$ | 283.2 | | $1.93\times10^{-3}$ (Ref. 15) | $1.8\times10^{-3}$ |
| 279.4 | | $4.159\times10^{-4}$ (Ref. 27) | $4.1\times10^{-4}$ | 287.7 | | $1.80\times10^{-3}$ (Ref. 39) | $2.1\times10^{-3}$ |
| 279.5 | | $4.27\times10^{-4}$ (Ref. 8) | $4.1\times10^{-4}$ | 288.1 | | $2.31\times10^{-3}$ (Ref. 23) | $2.1\times10^{-3}$ |
| 279.9 | | $4.02\times10^{-4}$ (Ref. 3) | $4.1\times10^{-4}$ | 288.2 | | $2.26\times10^{-3}$ (Ref. 17) | $2.1\times10^{-3}$ |
| 280.3 | | $4.18\times10^{-4}$ (Ref. 8) | $4.1\times10^{-4}$ | 291.1 | | $2.56\times10^{-3}$ (Ref. 23) | $2.3\times10^{-3}$ |
| 282.2 | | $4.18\times10^{-4}$ (Ref. 8) | $4.1\times10^{-4}$ | 293.2 | | $2.52\times10^{-3}$ (Ref. 15) | $2.5\times10^{-3}$ |
| 282.6 | | $4.13\times10^{-4}$ (Ref. 1) | $4.1\times10^{-4}$ | 293.3 | | $2.77\times10^{-3}$ (Ref. 29) | $2.5\times10^{-3}$ |
| 283.2 | | $4.04\times10^{-4}$ (Ref. 43) | $4.1\times10^{-4}$ | 294.2 | | $2.00\times10^{-3}$ (Ref. 13) | $2.6\times10^{-3}$ |
| 284.4 | | $4.147\times10^{-4}$ (Ref. 27) | $4.1\times10^{-4}$ | 295.2 | | $2.90\times10^{-3}$ (Ref. 43) | $2.7\times10^{-3}$ |
| 285.0 | | $4.09\times10^{-4}$ (Ref. 8) | $4.1\times10^{-4}$ | 295.7 | | $2.60\times10^{-3}$ (Ref. 39) | $2.7\times10^{-3}$ |
| 285.3 | | $4.09\times10^{-4}$ (Ref. 8) | $4.1\times10^{-4}$ | 295.9 | | $2.606\times10^{-3}$ (Ref. 38) | $2.7\times10^{-3}$ |
| 285.7 | | $3.97\times10^{-4}$ (Ref. 3) | $4.1\times10^{-4}$ | 296.1 | | $2.98\times10^{-3}$ (Ref. 23) | $2.8\times10^{-3}$ |
| 287.2 | | $4.08\times10^{-4}$ (Ref. 27) | $4.1\times10^{-4}$ | 296.2 | | $2.60\times10^{-3}$ (Ref. 20) | $2.8\times10^{-3}$ |
| 288.1 | | $4.792\times10^{-4}$ (Ref. 31) | $4.1\times10^{-4}$ | 297.7 | | $3.14\times10^{-3}$ (Ref. 29) | $2.9\times10^{-3}$ |
| 288.2 | | $3.99\times10^{-4}$ (Ref. 3) | $4.1\times10^{-4}$ | 297.9 | | $2.96\times10^{-3}$ (Ref. 37) | $2.9\times10^{-3}$ |
| 288.3 | | $4.14\times10^{-4}$ (Ref. 8) | $4.1\times10^{-4}$ | 298.1 | | $3.14\times10^{-3}$ (Ref. 23) | $2.9\times10^{-3}$ |
| 289.2 | | $3.35\times10^{-4}$ (Ref. 14) | $4.1\times10^{-4}$ | 298.2 | | $3.09\times10^{-3}$ (Ref. 26) | $3.0\times10^{-3}$ |
| 290.0 | | $4.09\times10^{-4}$ (Ref. 1) | $4.1\times10^{-4}$ | 299.2 | | $2.34\times10^{-3}$ (Ref. 6) | $3.1\times10^{-3}$ |
| 290.1 | | $4.062\times10^{-4}$ (Ref. 27) | $4.1\times10^{-4}$ | 299.8 | | $2.40\times10^{-3}$ (Ref. 13) | $3.1\times10^{-3}$ |
| 290.2 | | $3.95\times10^{-4}$ (Ref. 16) | $4.1\times10^{-4}$ | 301.1 | | $3.47\times10^{-3}$ (Ref. 23) | $3.3\times10^{-3}$ |
| 291.1 | | $4.14\times10^{-4}$ (Ref. 8) | $4.1\times10^{-4}$ | 302.7 | | $3.67\times10^{-3}$ (Ref. 29) | $3.4\times10^{-3}$ |
| 291.8 | | $4.073\times10^{-4}$ (Ref. 27) | $4.1\times10^{-4}$ | 303.1 | | $3.70\times10^{-3}$ (Ref. 23) | $3.5\times10^{-3}$ |
| 293.1 | | $4.809\times10^{-4}$ (Ref. 31) | $4.1\times10^{-4}$ | 303.2 | | $3.50\times10^{-3}$ (Ref. 36) | $3.5\times10^{-3}$ |
| 293.2 | | $4.133\times10^{-4}$ (Ref. 5) | $4.1\times10^{-4}$ | 303.3 | | $3.597\times10^{-3}$ (Ref. 30) | $3.5\times10^{-3}$ |
| 293.3 | | $4.07\times10^{-4}$ (Ref. 8) | $4.1\times10^{-4}$ | 303.7 | | $3.674\times10^{-3}$ (Ref. 38) | $3.5\times10^{-3}$ |
| 293.8 | | $3.97\times10^{-4}$ (Ref. 3) | $4.1\times10^{-4}$ | 305.1 | | $3.97\times10^{-3}$ (Ref. 23) | $3.7\times10^{-3}$ |
| 294.0 | | $4.01\times10^{-4}$ (Ref. 12) | $4.1\times10^{-4}$ | 305.2 | | $3.50\times10^{-3}$ (Ref. 39) | $3.7\times10^{-3}$ |
| 295.2 | | $4.306\times10^{-4}$ (Ref. 43) | $4.1\times10^{-4}$ | 306.2 | | $3.784\times10^{-3}$ (Ref. 38) | $3.8\times10^{-3}$ |
| 296.7 | | $4.20\times10^{-4}$ (Ref. 35) | $4.1\times10^{-4}$ | 308.0 | | $4.40\times10^{-3}$ (Ref. 29) | $4.1\times10^{-3}$ |
| 297.2 | | $4.16\times10^{-4}$ (Ref. 1) | $4.1\times10^{-4}$ | 308.2 | | $4.19\times10^{-3}$ (Ref. 18) | $4.1\times10^{-3}$ |
| 298.0 | 100 | $4.00\times10^{-4}$ (Ref. 28) | $4.1\times10^{-4}$ | 310.7 | | $5.00\times10^{-3}$ (Ref. 22) | $4.4\times10^{-3}$ |
| 298.1 | | $4.02\times10^{-4}$ (Ref. 3) | $4.1\times10^{-4}$ | 310.9 | 7000 | $4.18\times10^{-3}$ (Ref. 40) | $4.4\times10^{-3}$ |
| 298.2 | | $4.11\times10^{-4}$ (Ref. 25) | $4.1\times10^{-4}$ | 311.0 | 7000 | $4.66\times10^{-3}$ (Ref. 40) | $4.5\times10^{-3}$ |
| 299.0 | | $4.193\times10^{-4}$ (Ref. 27) | $4.1\times10^{-4}$ | 311.1 | 7000 | $4.87\times10^{-3}$ (Ref. 40) | $4.5\times10^{-3}$ |
| 299.2 | | $3.99\times10^{-4}$ (Ref. 16) | $4.1\times10^{-4}$ | 311.5 | 7000 | $4.21\times10^{-3}$ (Ref. 40) | $4.5\times10^{-3}$ |
| 300.5 | | $4.02\times10^{-4}$ (Ref. 3) | $4.1\times10^{-4}$ | 311.8 | 7000 | $4.33\times10^{-3}$ (Ref. 40) | $4.6\times10^{-3}$ |
| 302.2 | | $4.02\times10^{-4}$ (Ref. 16) | $4.2\times10^{-4}$ | 313.2 | | $4.76\times10^{-3}$ (Ref. 17) | $4.8\times10^{-3}$ |
| 303.2 | 100 | $4.24\times10^{-4}$ (Ref. 11) | $4.2\times10^{-4}$ | 313.3 | | $4.845\times10^{-3}$ (Ref. 30) | $4.8\times10^{-3}$ |
| 304.2 | | $4.23\times10^{-4}$ (Ref. 1) | $4.2\times10^{-4}$ | 313.8 | | $5.041\times10^{-3}$ (Ref. 38) | $4.9\times10^{-3}$ |
| 305.2 | | $4.12\times10^{-4}$ (Ref. 16) | $4.2\times10^{-4}$ | 314.6 | | $5.23\times10^{-3}$ (Ref. 37) | $5.0\times10^{-3}$ |
| 308.2 | | $4.20\times10^{-4}$ (Ref. 16) | $4.3\times10^{-4}$ | 315.1 | | $5.153\times10^{-3}$ (Ref. 38) | $5.1\times10^{-3}$ |
| 308.3 | | $4.848\times10^{-4}$ (Ref. 31) | $4.3\times10^{-4}$ | 315.2 | | $3.80\times10^{-3}$ (Ref. 13) | $5.1\times10^{-3}$ |
| 311.2 | | $4.50\times10^{-4}$ (Ref. 1) | $4.3\times10^{-4}$ | 316.9 | | $5.76\times10^{-3}$ (Ref. 29) | $5.3\times10^{-3}$ |
| 313.1 | | $4.34\times10^{-4}$ (Ref. 3) | $4.4\times10^{-4}$ | 317.2 | | $5.88\times10^{-3}$ (Ref. 37) | $5.4\times10^{-3}$ |
| 313.2 | 30.54 | $4.435\times10^{-4}$ (Ref. 41) | $4.4\times10^{-4}$ | 319.1 | | $6.064\times10^{-3}$ (Ref. 38) | $5.7\times10^{-3}$ |
| 313.7 | | $4.39\times10^{-4}$ (Ref. 16) | $4.4\times10^{-4}$ | 322.6 | | $6.78\times10^{-3}$ (Ref. 29) | $6.3\times10^{-3}$ |
| 315.2 | | $4.40\times10^{-4}$ (Ref. 16) | $4.5\times10^{-4}$ | 323.1 | | $6.567\times10^{-3}$ (Ref. 30) | $6.4\times10^{-3}$ |
| 317.2 | | $4.45\times10^{-4}$ (Ref. 16) | $4.5\times10^{-4}$ | 323.2 | | $6.50\times10^{-3}$ (Ref. 19) | $6.4\times10^{-3}$ |
| 317.9 | | $4.69\times10^{-4}$ (Ref. 1) | $4.6\times10^{-4}$ | 323.6 | | $6.97\times10^{-3}$ (Ref. 37) | $6.5\times10^{-3}$ |
| 318.2 | | $4.55\times10^{-4}$ (Ref. 3) | $4.6\times10^{-4}$ | 325.1 | | $6.902\times10^{-3}$ (Ref. 38) | $6.8\times10^{-3}$ |
| 318.9 | | $5.304\times10^{-4}$ (Ref. 31) | $4.6\times10^{-4}$ | 325.4 | | $7.078\times10^{-3}$ (Ref. 38) | $6.9\times10^{-3}$ |
| 319.2 | | $4.57\times10^{-4}$ (Ref. 16) | $4.6\times10^{-4}$ | 326.4 | | $7.211\times10^{-3}$ (Ref. 38) | $7.1\times10^{-3}$ |
| 323.0 | | $4.71\times10^{-4}$ (Ref. 3) | $4.8\times10^{-4}$ | 327.9 | | $7.521\times10^{-3}$ (Ref. 38) | $7.4\times10^{-3}$ |
| 323.2 | 100 | $5.10\times10^{-4}$ (Ref. 11) | $4.8\times10^{-4}$ | 328.2 | | $7.90\times10^{-3}$ (Ref. 20) | $7.4\times10^{-3}$ |
| 324.2 | | $4.78\times10^{-4}$ (Ref. 16) | $4.8\times10^{-4}$ | 329.2 | | $7.80\times10^{-3}$ (Ref. 39) | $7.7\times10^{-3}$ |
| 324.7 | | $4.94\times10^{-4}$ (Ref. 1) | $4.8\times10^{-4}$ | 330.7 | | $8.00\times10^{-3}$ (Ref. 22) | $8.0\times10^{-3}$ |
| 327.7 | | $4.97\times10^{-4}$ (Ref. 3) | $5.0\times10^{-4}$ | 331.4 | | $8.91\times10^{-3}$ (Ref. 37) | $8.2\times10^{-3}$ |
| 328.2 | 100 | $5.49\times10^{-4}$ (Ref. 7) | $5.0\times10^{-4}$ | 331.7 | | $9.41\times10^{-3}$ (Ref. 37) | $8.2\times10^{-3}$ |
| 329.2 | | $5.03\times10^{-4}$ (Ref. 16) | $5.1\times10^{-4}$ | 333.1 | | $8.657\times10^{-3}$ (Ref. 30) | $8.5\times10^{-3}$ |
| 332.0 | | $5.40\times10^{-4}$ (Ref. 1) | $5.2\times10^{-4}$ | 333.2 | 150 | $9.50\times10^{-3}$ (Ref. 11) | $8.6\times10^{-3}$ |
| 333.0 | | $5.22\times10^{-4}$ (Ref. 3) | $5.3\times10^{-4}$ | 334.1 | | $9.294\times10^{-3}$ (Ref. 38) | $8.8\times10^{-3}$ |
| 333.2 | | $5.641\times10^{-4}$ (Ref. 5) | $5.3\times10^{-4}$ | 338.2 | | $9.90\times10^{-3}$ (Ref. 22) | $9.8\times10^{-3}$ |

| | | | |
|---|---|---|---|
| 334.2 | | $5.31\times10^{-4}$ (Ref. 16) | $5.3\times10^{-4}$ |
| 336.2 | | $5.42\times10^{-4}$ (Ref. 16) | $5.5\times10^{-4}$ |
| 338.0 | | $5.57\times10^{-4}$ (Ref. 3) | $5.6\times10^{-4}$ |
| 338.6 | | $5.94\times10^{-4}$ (Ref. 1) | $5.6\times10^{-4}$ |
| 342.2 | | $5.67\times10^{-4}$ (Ref. 3) | $5.9\times10^{-4}$ |
| 342.4 | | $6.49\times10^{-4}$ (Ref. 4) | $5.9\times10^{-4}$ |
| 343.2 | 250 | $6.25\times10^{-4}$ (Ref. 11) | $5.9\times10^{-4}$ |
| 352.7 | | $8.62\times10^{-4}$ (Ref. 42) | $6.7\times10^{-4}$ |
| 353.2 | 250 | $6.99\times10^{-4}$ (Ref. 11) | $6.8\times10^{-4}$ |
| 363.2 | 350 | $8.00\times10^{-4}$ (Ref. 11) | $7.8\times10^{-4}$ |
| 373.0 | 6500 | $8.90\times10^{-4}$ (Ref. 28) | $9.1\times10^{-4}$ |
| 373.2 | 275.8 | $9.49\times10^{-4}$ (Ref. 41) | $9.1\times10^{-4}$ |
| 374.2 | 287 | $1.02\times10^{-3}$ (Ref. 2) | $9.2\times10^{-4}$ |
| 398.0 | 577 | $1.40\times10^{-3}$ (Ref. 2) | $1.4\times10^{-3}$ |
| 420.9 | 1053 | $2.17\times10^{-3}$ (Ref. 2) | $2.1\times10^{-3}$ |
| 423.0 | 6500 | $2.20\times10^{-3}$ (Ref. 28) | $2.2\times10^{-3}$ |
| 423.2 | 1054.9 | $2.42\times10^{-3}$ (Ref. 41) | $2.2\times10^{-3}$ |
| 448.0 | 1901 | $3.49\times10^{-3}$ (Ref. 2) | $3.4\times10^{-3}$ |
| 448.6 | 1859 | $3.40\times10^{-3}$ (Ref. 2) | $3.5\times10^{-3}$ |
| 473.0 | 6500 | $5.00\times10^{-3}$ (Ref. 28) | $5.5\times10^{-3}$ |
| 473.2 | 3020 | $5.40\times10^{-3}$ (Ref. 41) | $5.5\times10^{-3}$ |
| 473.4 | 3045 | $5.64\times10^{-3}$ (Ref. 2) | $5.6\times10^{-3}$ |
| 477.0 | 3218 | $6.07\times10^{-3}$ (Ref. 2) | $6.0\times10^{-3}$ |
| 477.2 | | $6.844\times10^{-3}$ (Ref. 21) | $6.0\times10^{-3}$ |
| 498.2 | | $9.00\times10^{-3}$ (Ref. 21) | $8.9\times10^{-3}$ |
| 514.2 | | $1.067\times10^{-2}$ (Ref. 21) | $1.2\times10^{-2}$ |
| 523.2 | 6600 | $1.54\times10^{-2}$ (Ref. 10) | $1.4\times10^{-2}$ |
| 527.2 | | $1.217\times10^{-2}$ (Ref. 21) | $1.5\times10^{-2}$ |

| | | | |
|---|---|---|---|
| 338.5 | | $1.05\times10^{-2}$ (Ref. 38) | $9.9\times10^{-3}$ |
| 339.2 | | $1.10\times10^{-2}$ (Ref. 20) | $1.0\times10^{-2}$ |
| 340.4 | | $1.121\times10^{-2}$ (Ref. 38) | $1.0\times10^{-2}$ |
| 340.7 | | $1.08\times10^{-2}$ (Ref. 39) | $1.1\times10^{-2}$ |
| 342.7 | | $1.14\times10^{-2}$ (Ref. 22) | $1.1\times10^{-2}$ |
| 343.2 | 250 | $1.22\times10^{-2}$ (Ref. 11) | $1.1\times10^{-2}$ |
| 344.2 | | $1.274\times10^{-2}$ (Ref. 37) | $1.2\times10^{-2}$ |
| 344.4 | 7000 | $1.24\times10^{-2}$ (Ref. 40) | $1.2\times10^{-2}$ |
| 346.2 | | $1.29\times10^{-2}$ (Ref. 39) | $1.2\times10^{-2}$ |
| 346.4 | | $1.302\times10^{-2}$ (Ref. 38) | $1.2\times10^{-2}$ |
| 350.2 | | $1.45\times10^{-2}$ (Ref. 20) | $1.4\times10^{-2}$ |
| 353.2 | 250 | $1.54\times10^{-2}$ (Ref. 11) | $1.5\times10^{-2}$ |
| 359.0 | 170 | $1.40\times10^{-2}$ (Ref. 9) | $1.7\times10^{-2}$ |
| 363.2 | 350 | $2.07\times10^{-2}$ (Ref. 11) | $1.9\times10^{-2}$ |
| 373.2 | 350 | $2.65\times10^{-2}$ (Ref. 11) | $2.4\times10^{-2}$ |
| 374.2 | 287 | $2.135\times10^{-2}$ (Ref. 2) | $2.5\times10^{-2}$ |
| 377.0 | 7000 | $2.74\times10^{-2}$ (Ref. 40) | $2.6\times10^{-2}$ |
| 385.0 | 340 | $2.70\times10^{-2}$ (Ref. 9) | $3.2\times10^{-2}$ |
| 398.0 | 577 | $3.658\times10^{-2}$ (Ref. 2) | $4.2\times10^{-2}$ |
| 411.0 | 7000 | $5.580\times10^{-2}$ (Ref. 40) | $5.6\times10^{-2}$ |
| 413.0 | 690 | $4.50\times10^{-2}$ (Ref. 9) | $5.8\times10^{-2}$ |
| 420.9 | 1053 | $6.081\times10^{-2}$ (Ref. 2) | $6.8\times10^{-2}$ |
| 423.0 | 1073 | $6.513\times10^{-2}$ (Ref. 2) | $7.1\times10^{-2}$ |
| 423.2 | 1054.9 | $7.13\times10^{-2}$ (Ref. 41) | $7.2\times10^{-2}$ |
| 434.0 | 1030 | $6.40\times10^{-2}$ (Ref. 9) | $8.9\times10^{-2}$ |
| 444.3 | 7000 | $1.00\times10^{-1}$ (Ref. 40) | $1.1\times10^{-1}$ |
| 448.0 | 1901 | $1.058\times10^{-1}$ (Ref. 2) | $1.2\times10^{-1}$ |
| 448.6 | 1859 | $1.053\times10^{-1}$ (Ref. 2) | $1.2\times10^{-1}$ |
| 473.2 | 3020 | $1.85\times10^{-1}$ (Ref. 41) | $1.8\times10^{-1}$ |
| 473.4 | 3045 | $1.792\times10^{-1}$ (Ref. 2) | $1.8\times10^{-1}$ |
| 476.1 | 7000 | $1.77\times10^{-1}$ (Ref. 40) | $1.9\times10^{-1}$ |
| 477.0 | 3218 | $1.886\times10^{-1}$ (Ref. 2) | $2.0\times10^{-1}$ |
| 498.2 | 4100 | $2.23\times10^{-1}$ (Ref. 10) | $2.8\times10^{-1}$ |
| 523.2 | 6600 | $3.94\times10^{-1}$ (Ref. 10) | $4.3\times10^{-1}$ |

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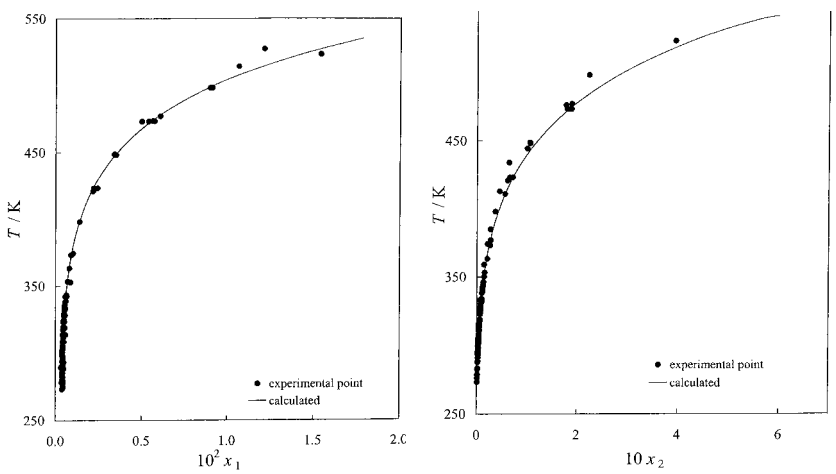

Table 4.2. Methylbenzene–water

**Components**
(1) Methylbenzene; $C_7H_8$; [108-88-3]
(2) Water; $H_2O$; [7732-18-5]

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Reference liquid–liquid equilibrium data

| Water rich phase | | | | Hydrocarbon rich phase | | | |
|---|---|---|---|---|---|---|---|
| $T$ (K) | $P$ (kPa) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $T$ (K) | $P$ (kPa) | $x_{2,\mathrm{exp}}$ | $x_{2,\mathrm{calc}}$ |
| 273.2 | | $1.14\times10^{-4}$ (Ref. 22) | $1.2\times10^{-4}$ | 273.2 | | $1.17\times10^{-3}$ (Ref. 18) | $1.2\times10^{-3}$ |
| 273.7 | | $1.10\times10^{-4}$ (Ref. 7) | $1.1\times10^{-4}$ | 283.2 | | $1.71\times10^{-3}$ (Ref. 19) | $1.7\times10^{-3}$ |
| 277.7 | | $1.20\times10^{-4}$ (Ref. 3) | $1.1\times10^{-4}$ | 288.2 | | $2.11\times10^{-3}$ (Ref. 10) | $2.0\times10^{-3}$ |
| 278.2 | | $1.111\times10^{-4}$ (Ref. 22) | $1.1\times10^{-4}$ | 291.2 | | $1.70\times10^{-3}$ (Ref. 25) | $2.2\times10^{-3}$ |
| 279.5 | | $1.18\times10^{-4}$ (Ref. 3) | $1.1\times10^{-4}$ | 293.2 | | $2.35\times10^{-3}$ (Ref. 8) | $2.4\times10^{-3}$ |
| 280.3 | | $1.15\times10^{-4}$ (Ref. 3) | $1.1\times10^{-4}$ | 295.2 | | $2.68\times10^{-3}$ (Ref. 26) | $2.6\times10^{-3}$ |
| 282.2 | | $1.15\times10^{-4}$ (Ref. 3) | $1.1\times10^{-4}$ | 298.2 | | $2.80\times10^{-3}$ (Ref. 12) | $2.8\times10^{-3}$ |
| 283.1 | | $1.236\times10^{-4}$ (Ref. 17) | $1.1\times10^{-4}$ | 303.2 | 100 | $3.14\times10^{-3}$ (Ref. 8) | $3.3\times10^{-3}$ |
| 283.2 | | $1.09\times10^{-4}$ (Ref. 22) | $1.1\times10^{-4}$ | 308.2 | | $3.50\times10^{-3}$ (Ref. 13) | $3.8\times10^{-3}$ |
| 285.0 | | $1.12\times10^{-4}$ (Ref. 3) | $1.1\times10^{-4}$ | 311.7 | | $3.60\times10^{-3}$ (Ref. 25) | $4.2\times10^{-3}$ |
| 285.3 | | $1.13\times10^{-4}$ (Ref. 3) | $1.1\times10^{-4}$ | 312.8 | | $5.60\times10^{-3}$ (Ref. 24) | $4.4\times10^{-3}$ |
| 288.2 | | $1.08\times10^{-4}$ (Ref. 22) | $1.1\times10^{-4}$ | 313.2 | 100 | $4.16\times10^{-3}$ (Ref. 4) | $4.4\times10^{-3}$ |
| 288.3 | | $1.11\times10^{-4}$ (Ref. 3) | $1.1\times10^{-4}$ | 321.2 | | $4.90\times10^{-3}$ (Ref. 25) | $5.6\times10^{-3}$ |
| 289.2 | | $9.20\times10^{-5}$ (Ref. 9) | $1.1\times10^{-4}$ | 323.2 | 100 | $5.30\times10^{-3}$ (Ref. 4) | $5.9\times10^{-3}$ |
| 291.1 | | $1.13\times10^{-4}$ (Ref. 3) | $1.1\times10^{-4}$ | 333.2 | 150 | $7.11\times10^{-3}$ (Ref. 4) | $7.8\times10^{-3}$ |
| 293.1 | | $1.292\times10^{-4}$ (Ref. 17) | $1.1\times10^{-4}$ | 333.3 | | $7.88\times10^{-3}$ (Ref. 24) | $7.8\times10^{-3}$ |
| 293.2 | | $1.11\times10^{-4}$ (Ref. 14) | $1.1\times10^{-4}$ | 333.7 | | $7.80\times10^{-3}$ (Ref. 25) | $7.9\times10^{-3}$ |
| 293.3 | | $1.11\times10^{-4}$ (Ref. 3) | $1.1\times10^{-4}$ | 341.2 | | $1.02\times10^{-2}$ (Ref. 25) | $9.6\times10^{-3}$ |
| 294.0 | | $9.36\times10^{-5}$ (Ref. 5) | $1.1\times10^{-4}$ | 343.2 | 250 | $9.46\times10^{-3}$ (Ref. 4) | $1.0\times10^{-2}$ |
| 295.2 | | $9.62\times10^{-5}$ (Ref. 26) | $1.1\times10^{-4}$ | 343.6 | | $1.045\times10^{-2}$ (Ref. 24) | $1.0\times10^{-2}$ |
| 296.7 | | $1.29\times10^{-4}$ (Ref. 23) | $1.1\times10^{-4}$ | 349.2 | | $1.29\times10^{-2}$ (Ref. 25) | $1.2\times10^{-2}$ |
| 298.0 | 5000 | $1.07\times10^{-4}$ (Ref. 16) | $1.1\times10^{-4}$ | 353.2 | 250 | $1.28\times10^{-2}$ (Ref. 4) | $1.3\times10^{-2}$ |
| 298.1 | | $1.021\times10^{-4}$ (Ref. 21) | $1.1\times10^{-4}$ | 354.2 | | $1.251\times10^{-2}$ (Ref. 24) | $1.3\times10^{-2}$ |
| 298.2 | | $1.12\times10^{-4}$ (Ref. 18) | $1.1\times10^{-4}$ | 357.2 | | $1.58\times10^{-2}$ (Ref. 25) | $1.4\times10^{-2}$ |
| 303.2 | | $1.12\times10^{-4}$ (Ref. 11) | $1.1\times10^{-4}$ | 363.2 | 350 | $1.62\times10^{-2}$ (Ref. 4) | $1.7\times10^{-2}$ |
| 308.2 | | $1.09\times10^{-4}$ (Ref. 15) | $1.1\times10^{-4}$ | 363.4 | | $1.421\times10^{-2}$ (Ref. 24) | $1.7\times10^{-2}$ |
| 308.3 | | $1.314\times10^{-4}$ (Ref. 17) | $1.1\times10^{-4}$ | 366.2 | | $2.08\times10^{-2}$ (Ref. 25) | $1.8\times10^{-2}$ |
| 313.2 | | $1.20\times10^{-4}$ (Ref. 24) | $1.2\times10^{-4}$ | 372.6 | 153 | $1.923\times10^{-2}$ (Ref. 1) | $2.1\times10^{-2}$ |
| 318.2 | | $1.25\times10^{-4}$ (Ref. 20) | $1.2\times10^{-4}$ | 373.2 | 350 | $2.26\times10^{-2}$ (Ref. 4) | $2.1\times10^{-2}$ |
| 318.5 | | $1.313\times10^{-4}$ (Ref. 17) | $1.2\times10^{-4}$ | 398.0 | 384 | $3.411\times10^{-2}$ (Ref. 1) | $3.7\times10^{-2}$ |
| 323.0 | 5000 | $1.25\times10^{-4}$ (Ref. 16) | $1.3\times10^{-4}$ | 422.6 | 753 | $5.789\times10^{-2}$ (Ref. 1) | $6.1\times10^{-2}$ |

| | | | |
|---|---|---|---|
| 323.2 | 100 | $1.27\times10^{-4}$ (Ref. 4) | $1.3\times10^{-4}$ |
| 328.2 | | $1.40\times10^{-4}$ (Ref. 7) | $1.4\times10^{-4}$ |
| 333.2 | 150 | $1.44\times10^{-4}$ (Ref. 4) | $1.5\times10^{-4}$ |
| 340.6 | 6800 | $1.83\times10^{-4}$ (Ref. 2) | $1.6\times10^{-4}$ |
| 343.2 | 250 | $1.71\times10^{-4}$ (Ref. 4) | $1.7\times10^{-4}$ |
| 343.6 | | $1.80\times10^{-4}$ (Ref. 24) | $1.7\times10^{-4}$ |
| 353.2 | 250 | $1.98\times10^{-4}$ (Ref. 4) | $2.0\times10^{-4}$ |
| 354.2 | | $2.50\times10^{-4}$ (Ref. 24) | $2.0\times10^{-4}$ |
| 363.2 | 350 | $2.32\times10^{-4}$ (Ref. 4) | $2.3\times10^{-4}$ |
| 363.4 | | $2.30\times10^{-4}$ (Ref. 24) | $2.3\times10^{-4}$ |
| 372.6 | 153 | $2.86\times10^{-4}$ (Ref. 1) | $2.8\times10^{-4}$ |
| 373.0 | 5000 | $2.70\times10^{-4}$ (Ref. 16) | $2.8\times10^{-4}$ |
| 373.2 | 350 | $1.68\times10^{-4}$ (Ref. 4) | $2.8\times10^{-4}$ |
| 384.1 | 6800 | $3.60\times10^{-4}$ (Ref. 2) | $3.5\times10^{-4}$ |
| 398.0 | 384 | $4.63\times10^{-4}$ (Ref. 1) | $4.6\times10^{-4}$ |
| 403.2 | 6800 | $5.27\times10^{-4}$ (Ref. 2) | $5.1\times10^{-4}$ |
| 417.2 | 6800 | $6.93\times10^{-4}$ (Ref. 2) | $6.9\times10^{-4}$ |
| 422.6 | 753 | $7.94\times10^{-4}$ (Ref. 1) | $7.7\times10^{-4}$ |
| 423.0 | 5000 | $6.60\times10^{-4}$ (Ref. 16) | $7.8\times10^{-4}$ |
| 445.0 | 6800 | $1.18\times10^{-3}$ (Ref. 2) | $1.3\times10^{-3}$ |
| 448.4 | 1425 | $1.30\times10^{-3}$ (Ref. 1) | $1.4\times10^{-3}$ |
| 448.5 | 1404 | $1.23\times10^{-3}$ (Ref. 1) | $1.4\times10^{-3}$ |
| 473.0 | 5000 | $1.90\times10^{-3}$ (Ref. 16) | $2.4\times10^{-3}$ |
| 473.2 | 2500 | $2.38\times10^{-3}$ (Ref. 6) | $2.4\times10^{-3}$ |
| 473.6 | 2363 | $2.59\times10^{-3}$ (Ref. 1) | $2.4\times10^{-3}$ |
| 485.2 | 6800 | $2.68\times10^{-3}$ (Ref. 2) | $3.1\times10^{-3}$ |
| 518.0 | 6800 | $5.47\times10^{-3}$ (Ref. 2) | $6.6\times10^{-3}$ |
| 523.2 | 5800 | $7.03\times10^{-3}$ (Ref. 6) | $7.4\times10^{-3}$ |
| 548.2 | 8600 | $1.29\times10^{-2}$ (Ref. 6) | $1.3\times10^{-3}$ |
| 422.8 | 6800 | $5.80\times10^{-2}$ (Ref. 2) | $6.1\times10^{-2}$ |
| 429.2 | 6800 | $7.30\times10^{-2}$ (Ref. 2) | $7.0\times10^{-2}$ |
| 448.4 | 1425 | $9.826\times10^{-2}$ (Ref. 1) | $1.0\times10^{-1}$ |
| 448.5 | 1404 | $9.525\times10^{-2}$ (Ref. 1) | $1.0\times10^{-1}$ |
| 451.1 | 6800 | $9.80\times10^{-2}$ (Ref. 2) | $1.1\times10^{-1}$ |
| 453.3 | 6800 | $1.05\times10^{-1}$ (Ref. 2) | $1.1\times10^{-1}$ |
| 467.8 | 6800 | $1.34\times10^{-1}$ (Ref. 2) | $1.4\times10^{-1}$ |
| 470.9 | 6800 | $1.45\times10^{-1}$ (Ref. 2) | $1.5\times10^{-1}$ |
| 473.6 | 2363 | $1.592\times10^{-1}$ (Ref. 1) | $1.6\times10^{-1}$ |
| 479.8 | 6800 | $1.65\times10^{-1}$ (Ref. 2) | $1.8\times10^{-1}$ |
| 485.1 | 6800 | $1.82\times10^{-1}$ (Ref. 2) | $2.0\times10^{-1}$ |
| 488.4 | 6800 | $1.91\times10^{-1}$ (Ref. 2) | $2.1\times10^{-1}$ |
| 494.7 | 6800 | $2.14\times10^{-1}$ (Ref. 2) | $2.3\times10^{-1}$ |
| 502.5 | 6800 | $2.53\times10^{-1}$ (Ref. 2) | $2.6\times10^{-1}$ |
| 504.2 | 6800 | $2.41\times10^{-1}$ (Ref. 2) | $2.7\times10^{-1}$ |
| 513.5 | 6800 | $2.88\times10^{-1}$ (Ref. 2) | $3.2\times10^{-1}$ |
| 521.6 | 6800 | $3.29\times10^{-1}$ (Ref. 2) | $3.6\times10^{-1}$ |
| 523.2 | 5800 | $3.84\times10^{-1}$ (Ref. 6) | $3.7\times10^{-1}$ |
| 524.3 | 6800 | $3.47\times10^{-1}$ (Ref. 2) | $3.8\times10^{-1}$ |
| 548.2 | 8600 | $5.69\times10^{-1}$ (Ref. 6) | $5.5\times10^{-1}$ |

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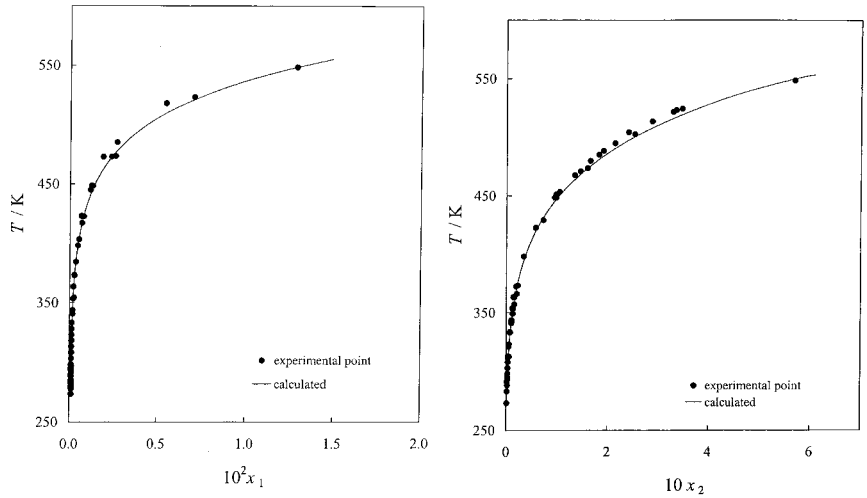


Table 4.3. Ethylbenzene–water

**Components**
(1) Ethylbenzene; $C_8H_{10}$; [100-41-4]
(2) Water; $H_2O$; [7732-18-5]

**References**
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Reference liquid–liquid equilibrium data

| Water rich phase | | | Hydrocarbon rich phase | | | |
|---|---|---|---|---|---|---|
| $T$ (K) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $T$ (K) | $P$ (kPa) | $x_{2,\mathrm{exp}}$ | $x_{2,\mathrm{calc}}$ |
| 273.2 | $3.34\times10^{-5}$ (Ref. 11) | $3.4\times10^{-5}$ | 273.2 | | $1.05\times10^{-3}$ (Ref. 11) | $1.2\times10^{-3}$ |
| 273.7 | $2.86\times10^{-5}$ (Ref. 3) | $3.4\times10^{-5}$ | 283.2 | | $1.62\times10^{-3}$ (Ref. 4) | $1.7\times10^{-3}$ |
| 277.7 | $3.33\times10^{-5}$ (Ref. 1) | $3.3\times10^{-5}$ | 291.4 | | $1.74\times10^{-3}$ (Ref. 5) | $2.2\times10^{-3}$ |
| 278.2 | $3.084\times10^{-5}$ (Ref. 13) | $3.3\times10^{-5}$ | 291.5 | | $1.81\times10^{-3}$ (Ref. 5) | $2.2\times10^{-3}$ |
| 279.5 | $3.26\times10^{-5}$ (Ref. 1) | $3.2\times10^{-5}$ | 292.9 | | $1.92\times10^{-3}$ (Ref. 5) | $2.3\times10^{-3}$ |
| 280.3 | $3.16\times10^{-5}$ (Ref. 1) | $3.2\times10^{-5}$ | 293.2 | | $2.19\times10^{-3}$ (Ref. 4) | $2.3\times10^{-3}$ |
| 282.2 | $3.18\times10^{-5}$ (Ref. 1) | $3.2\times10^{-5}$ | 295.5 | | $2.07\times10^{-3}$ (Ref. 5) | $2.5\times10^{-3}$ |
| 283.2 | $3.05\times10^{-5}$ (Ref. 14) | $3.2\times10^{-5}$ | 296.6 | | $2.12\times10^{-3}$ (Ref. 5) | $2.5\times10^{-3}$ |
| 285.0 | $3.07\times10^{-5}$ (Ref. 1) | $3.2\times10^{-5}$ | 297.4 | | $2.28\times10^{-3}$ (Ref. 5) | $2.6\times10^{-3}$ |
| 285.3 | $3.11\times10^{-5}$ (Ref. 1) | $3.2\times10^{-5}$ | 298.2 | | $2.60\times10^{-3}$ (Ref. 11) | $2.7\times10^{-3}$ |
| 287.2 | $3.27\times10^{-5}$ (Ref. 10) | $3.2\times10^{-5}$ | 300.4 | | $2.91\times10^{-3}$ (Ref. 5) | $2.9\times10^{-3}$ |
| 288.2 | $2.90\times10^{-5}$ (Ref. 9) | $3.1\times10^{-5}$ | 303.0 | | $3.50\times10^{-3}$ (Ref. 5) | $3.1\times10^{-3}$ |
| 288.3 | $3.06\times10^{-5}$ (Ref. 1) | $3.1\times10^{-5}$ | 303.2 | | $2.95\times10^{-3}$ (Ref. 4) | $3.1\times10^{-3}$ |
| 290.2 | $3.20\times10^{-5}$ (Ref. 10) | $3.1\times10^{-5}$ | 304.8 | | $3.81\times10^{-3}$ (Ref. 5) | $3.3\times10^{-3}$ |
| 291.1 | $3.12\times10^{-5}$ (Ref. 1) | $3.1\times10^{-5}$ | 305.3 | | $4.05\times10^{-3}$ (Ref. 5) | $3.3\times10^{-3}$ |
| 291.2 | $3.11\times10^{-5}$ (Ref. 10) | $3.1\times10^{-5}$ | 307.4 | | $4.38\times10^{-3}$ (Ref. 5) | $3.5\times10^{-3}$ |
| 292.2 | $3.02\times10^{-5}$ (Ref. 10) | $3.2\times10^{-5}$ | 308.2 | | $3.60\times10^{-3}$ (Ref. 8) | $3.6\times10^{-3}$ |
| 293.2 | $3.19\times10^{-5}$ (Ref. 10) | $3.2\times10^{-5}$ | 308.3 | | $4.56\times10^{-3}$ (Ref. 5) | $3.6\times10^{-3}$ |
| 293.3 | $3.10\times10^{-5}$ (Ref. 1) | $3.2\times10^{-5}$ | 310.9 | 9.1 | $4.30\times10^{-3}$ (Ref. 7) | $3.9\times10^{-3}$ |
| 294.2 | $3.11\times10^{-5}$ (Ref. 10) | $3.2\times10^{-5}$ | 313.2 | | $3.66\times10^{-3}$ (Ref. 2) | $4.1\times10^{-3}$ |

| | | | | | | |
|---|---|---|---|---|---|---|
| 295.2 | $3.09\times10^{-5}$ (Ref. 10) | $3.2\times10^{-5}$ | 323.2 | | $4.57\times10^{-3}$ (Ref. 2) | $5.5\times10^{-3}$ |
| 296.7 | $3.16\times10^{-5}$ (Ref. 10) | $3.2\times10^{-5}$ | 333.2 | | $5.73\times10^{-3}$ (Ref. 2) | $7.1\times10^{-3}$ |
| 298.0 | $3.44\times10^{-5}$ (Ref. 16) | $3.2\times10^{-5}$ | 343.2 | | $8.30\times10^{-3}$ (Ref. 2) | $9.2\times10^{-3}$ |
| 298.1 | $2.48\times10^{-5}$ (Ref. 12) | $3.2\times10^{-5}$ | 353.2 | | $1.07\times10^{-2}$ (Ref. 2) | $1.2\times10^{-2}$ |
| 298.2 | $3.18\times10^{-5}$ (Ref. 15) | $3.2\times10^{-5}$ | 363.2 | | $1.54\times10^{-2}$ (Ref. 2) | $1.5\times10^{-2}$ |
| 299.0 | $3.17\times10^{-5}$ (Ref. 10) | $3.2\times10^{-5}$ | 367.6 | 111 | $1.86\times10^{-2}$ (Ref. 7) | $1.7\times10^{-2}$ |
| 301.2 | $3.16\times10^{-5}$ (Ref. 10) | $3.2\times10^{-5}$ | 373.2 | | $2.02\times10^{-2}$ (Ref. 2) | $1.9\times10^{-2}$ |
| 303.2 | $3.22\times10^{-5}$ (Ref. 10) | $3.3\times10^{-5}$ | 423.4 | 627 | $5.96\times10^{-2}$ (Ref. 7) | $5.5\times10^{-2}$ |
| 308.2 | $3.29\times10^{-5}$ (Ref. 10) | $3.4\times10^{-5}$ | 479.5 | 2320 | $1.63\times10^{-1}$ (Ref. 7) | $1.6\times10^{-1}$ |
| 313.2 | $3.50\times10^{-5}$ (Ref. 10) | $3.5\times10^{-5}$ | 536.1 | 6500 | $4.08\times10^{-1}$ (Ref. 7) | $4.2\times10^{-1}$ |
| 318.2 | $3.62\times10^{-5}$ (Ref. 10) | $3.7\times10^{-5}$ | 550.4 | 8270 | $4.72\times10^{-1}$ (Ref. 7) | $5.2\times10^{-1}$ |
| 323.2 | $3.525\times10^{-5}$ (Ref. 13) | $3.9\times10^{-5}$ | 568.1 | 10680 | $6.91\times10^{-1}$ (Ref. 7) | $6.8\times10^{-1}$ |
| 328.2 | $3.69\times10^{-5}$ (Ref. 3) | $4.2\times10^{-5}$ | | | | |
| 333.2 | $4.07\times10^{-5}$ (Ref. 2) | $4.5\times10^{-5}$ | | | | |
| 343.2 | $4.93\times10^{-5}$ (Ref. 2) | $5.3\times10^{-5}$ | | | | |
| 353.2 | $5.99\times10^{-5}$ (Ref. 2) | $6.3\times10^{-5}$ | | | | |
| 363.2 | $6.95\times10^{-5}$ (Ref. 2) | $7.7\times10^{-5}$ | | | | |
| 373.2 | $8.54\times10^{-5}$ (Ref. 2) | $9.4\times10^{-5}$ | | | | |
| 413.7 | $2.02\times10^{-4}$ (Ref. 6) | $2.4\times10^{-4}$ | | | | |
| 443.7 | $6.04\times10^{-4}$ (Ref. 6) | $5.2\times10^{-4}$ | | | | |
| 483.2 | $1.13\times10^{-3}$ (Ref. 6) | $1.4\times10^{-3}$ | | | | |
| 506.7 | $1.93\times10^{-3}$ (Ref. 6) | $2.6\times10^{-3}$ | | | | |

**Other references**:
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[29]T. J. Morrison and F. Billett, J. Chem. Soc. 3819 (1952).
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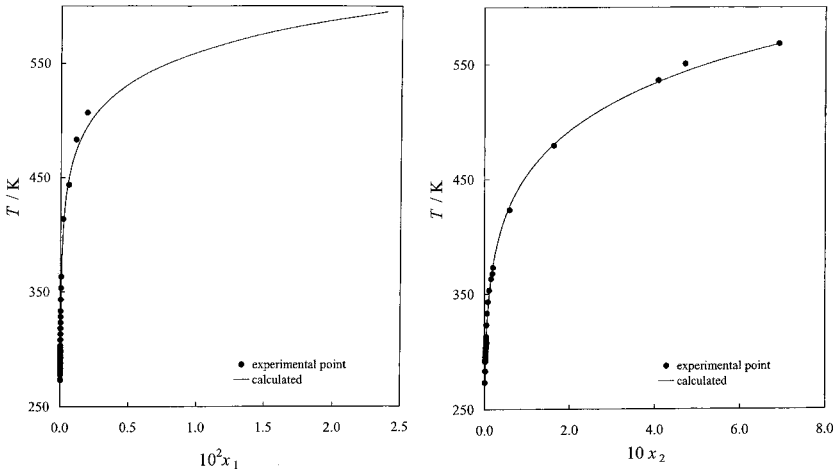

Table 4.4. Propylbenzene–water

| **Components** | **References** |
|---|---|
| (1) Propylbenzene; $C_9H_{12}$; [103-65-1] | [1]P. Dohanyosova, D. Fenclova, P. Vrbka, and V. Dohnal, J. Chem. Eng. Data **46**, 1533 (2001). |
| (2) Water; $H_2O$; [7732-18-5] | [2]H. Fühner, Ber. Dtsch. Chem. Ges. **57**, 510 (1924). |
| | [3]A. N. Guseva and E. I. Parnov, Zh. Fiz. Khim. **38**, 805 (1964). |
| | [4]J. W. Owens, S. P. Wasik, and H. DeVoe, J. Chem. Eng. Data **31**, 47 (1986). |
| | [5]I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, Bull. Chem. Soc. Jpn. **60**, 517 (1987). |
| | [6]S. Sawamura, K. Nagaoka, T. Machikawa, J. Phys. Chem. **105**, 2429 (2001). |

Reference liquid–liquid equilibrium data

| | Water rich phase | | Hydrocarbon rich phase |
|---|---|---|---|
| $T$ (K) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $x_{2,\mathrm{calc}}$ |
| 273.2 | $9.01\times10^{-6}$ (Ref. 6) | $9.5\times10^{-6}$ | $1.2\times10^{-3}$ |
| 273.7 | $6.98\times10^{-6}$ (Ref. 1) | $9.4\times10^{-6}$ | $1.2\times10^{-3}$ |
| 278.2 | $8.65\times10^{-6}$ (Ref. 6) | $9.1\times10^{-6}$ | $1.4\times10^{-3}$ |
| 283.2 | $8.38\times10^{-6}$ (Ref. 6) | $8.8\times10^{-6}$ | $1.6\times10^{-3}$ |
| 288.2 | $9.00\times10^{-6}$ (Ref. 2) | $8.7\times10^{-6}$ | $1.9\times10^{-3}$ |
| 293.2 | $8.16\times10^{-6}$ (Ref. 4) | $8.7\times10^{-6}$ | $2.2\times10^{-3}$ |
| 298.1 | $7.50\times10^{-6}$ (Ref. 5) | $8.9\times10^{-6}$ | $2.6\times10^{-3}$ |
| 298.2 | $8.23\times10^{-6}$ (Ref. 6) | $8.9\times10^{-6}$ | $2.6\times10^{-3}$ |
| 303.2 | $8.41\times10^{-6}$ (Ref. 6) | $9.1\times10^{-6}$ | $3.0\times10^{-3}$ |
| 308.2 | $8.74\times10^{-6}$ (Ref. 6) | $9.4\times10^{-6}$ | $3.4\times10^{-3}$ |
| 313.2 | $9.66\times10^{-6}$ (Ref. 4) | $9.9\times10^{-6}$ | $3.9\times10^{-3}$ |
| 318.2 | $1.01\times10^{-5}$ (Ref. 4) | $1.1\times10^{-5}$ | $4.5\times10^{-3}$ |
| 323.2 | $1.057\times10^{-5}$ (Ref. 6) | $1.1\times10^{-5}$ | $5.2\times10^{-3}$ |
| 328.2 | $1.13\times10^{-5}$ (Ref. 1) | $1.2\times10^{-5}$ | $5.9\times10^{-3}$ |
| 359.0 | $1.98\times10^{-5}$ (Ref. 3) | $2.2\times10^{-5}$ | $1.3\times10^{-2}$ |

**Other references:**

[7]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
[8]H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
[9]R. Ya. Krasnoshchekova and M. Ya. Gubergrits, Vodnye Resursy **2**, 170 (1975).
[10]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).
[11]I. Sanemasa, S. Arakawa, M. Araki, and T. Deguchi, Bull. Chem. Soc. Jpn. **57**, 1539 (1984).
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[15]H. de Voe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (U. S.), **86**, 361 (1981).

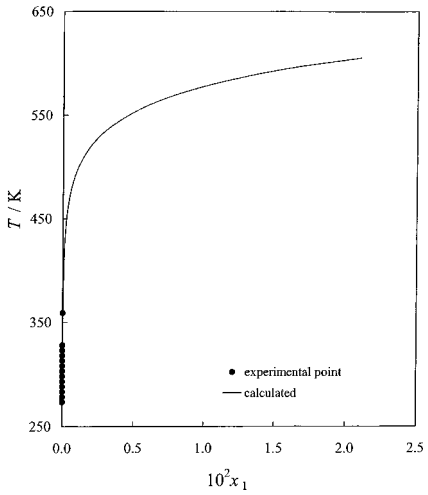


Table 4.5. Butylbenzene–water

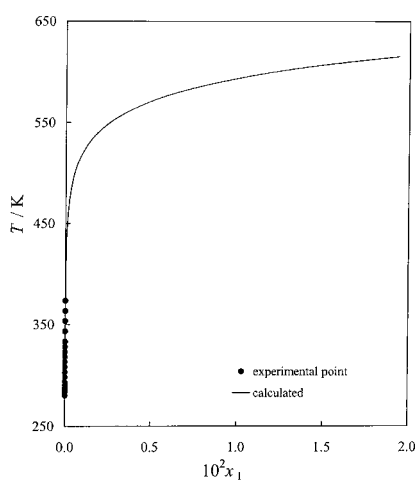
**Components**
(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8]
(2) Water; $H_2O$; [7732-18-5]

**References**
[1]H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 679 (1994).
[2]P. Dohanyosova, D. Fenclova, P. Vrbka, and V. Dohnal, J. Chem. Eng. Data **46**, 1533 (2001).
[3]B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[4]H. A. Massaldi and C. J. King, J. Chem. Eng. Data **18**, 393 (1973).
[5]J. W. Owens, S. P. Wasik, and H. DeVoe, J. Chem. Eng. Data **31**, 47 (1986).

Reference liquid–liquid equilibrium data

| Water rich phase | | | Hydrocarbon rich phase | | |
|---|---|---|---|---|---|
| $T$ (K) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $T$ (K) | $x_{2,\mathrm{exp}}$ | $x_{2,\mathrm{calc}}$ |
| 280.2 | $1.79\times10^{-6}$ (Ref. 5) | $2.4\times10^{-6}$ | 283.2 | $1.74\times10^{-3}$ (Ref. 3) | $1.6\times10^{-3}$ |
| 283.2 | $1.74\times10^{-6}$ (Ref. 5) | $2.3\times10^{-6}$ | 293.2 | $2.46\times10^{-3}$ (Ref. 3) | $2.1\times10^{-3}$ |
| 285.7 | $1.77\times10^{-6}$ (Ref. 5) | $2.3\times10^{-6}$ | 303.2 | $2.36\times10^{-3}$ (Ref. 1) | $2.8\times10^{-3}$ |
| 288.2 | $1.74\times10^{-6}$ (Ref. 5) | $2.3\times10^{-6}$ | 313.2 | $3.15\times10^{-3}$ (Ref. 1) | $3.7\times10^{-3}$ |
| 290.7 | $1.77\times10^{-6}$ (Ref. 5) | $2.3\times10^{-6}$ | 323.2 | $4.13\times10^{-3}$ (Ref. 1) | $4.8\times10^{-3}$ |
| 293.2 | $1.84\times10^{-6}$ (Ref. 5) | $2.3\times10^{-6}$ | 333.2 | $5.95\times10^{-3}$ (Ref. 1) | $6.2\times10^{-3}$ |
| 298.2 | $2.4\times10^{-6}$ (Ref. 4) | $2.4\times10^{-6}$ | 343.2 | $8.37\times10^{-3}$ (Ref. 1) | $8.0\times10^{-3}$ |
| 303.2 | $2.24\times10^{-6}$ (Ref. 1) | $2.4\times10^{-6}$ | 353.2 | $1.07\times10^{-2}$ (Ref. 1) | $1.0\times10^{-2}$ |
| 308.2 | $2.08\times10^{-6}$ (Ref. 5) | $2.5\times10^{-6}$ | 363.2 | $1.48\times10^{-2}$ (Ref. 1) | $1.3\times10^{-2}$ |
| 313.2 | $2.39\times10^{-6}$ (Ref. 1) | $2.7\times10^{-6}$ | 373.2 | $1.99\times10^{-2}$ (Ref. 1) | $1.6\times10^{-2}$ |
| 318.2 | $2.57\times10^{-6}$ (Ref. 5) | $2.8\times10^{-6}$ | | | |
| 323.2 | $2.73\times10^{-6}$ (Ref. 1) | $3.1\times10^{-6}$ | | | |
| 328.2 | $2.86\times10^{-6}$ (Ref. 2) | $3.3\times10^{-6}$ | | | |
| 333.2 | $3.61\times10^{-6}$ (Ref. 1) | $3.6\times10^{-6}$ | | | |
| 343.2 | $4.30\times10^{-6}$ (Ref. 1) | $4.5\times10^{-6}$ | | | |
| 353.2 | $6.40\times10^{-6}$ (Ref. 1) | $5.6\times10^{-6}$ | | | |
| 363.2 | $8.20\times10^{-6}$ (Ref. 1) | $7.2\times10^{-6}$ | | | |
| 373.2 | $1.12\times10^{-5}$ (Ref. 1) | $9.3\times10^{-6}$ | | | |

**Other references:**
[6]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
[7]J. R. Jones and C. B. Monk, J. Chem. Soc. 2633 (1963).
[8]H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
[9]C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
[10]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).



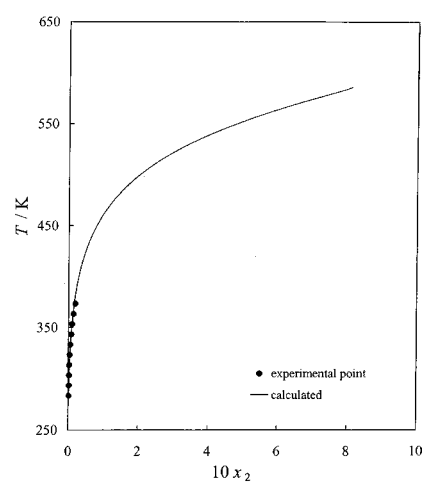



Table 4.6. Pentylbenzene–water

| **Components** | **References** |
|---|---|
| (1) Pentylbenzene; $C_{11}H_{16}$; [538-68-1] | [1]J. W. Owens, S. P. Wasik, and H. DeVoe, J. Chem. Eng. Data **31**, 47 (1986). |
| (2) Water; $H_2O$; [7732-18-5] | [2]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982). |

Reference liquid–liquid equilibrium data

| | Water rich phase | | Hydrocarbon rich phase |
|---|---|---|---|
| $T$ (K) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $x_{2,\mathrm{calc}}$ |
| 280.2 | $4.23\times10^{-7}$ (Ref. 1) | $5.3\times10^{-7}$ | $1.4\times10^{-3}$ |
| 283.2 | $3.86\times10^{-7}$ (Ref. 1) | $5.2\times10^{-7}$ | $1.6\times10^{-3}$ |
| 285.7 | $4.19\times10^{-7}$ (Ref. 1) | $5.1\times10^{-7}$ | $1.7\times10^{-3}$ |
| 288.2 | $3.88\times10^{-7}$ (Ref. 1) | $5.1\times10^{-7}$ | $1.8\times10^{-3}$ |
| 290.7 | $4.17\times10^{-7}$ (Ref. 1) | $5.1\times10^{-7}$ | $1.9\times10^{-3}$ |
| 293.2 | $3.87\times10^{-7}$ (Ref. 1) | $5.1\times10^{-7}$ | $2.1\times10^{-3}$ |
| 298.2 | $4.68\times10^{-7}$ (Ref. 2) | $5.2\times10^{-7}$ | $2.4\times10^{-3}$ |
| 303.2 | $4.40\times10^{-7}$ (Ref. 1) | $5.4\times10^{-7}$ | $2.7\times10^{-3}$ |
| 308.2 | $4.79\times10^{-7}$ (Ref. 1) | $5.6\times10^{-7}$ | $3.1\times10^{-3}$ |
| 313.2 | $5.21\times10^{-7}$ (Ref. 1) | $6.0\times10^{-7}$ | $3.6\times10^{-3}$ |
| 318.2 | $5.75\times10^{-7}$ (Ref. 1) | $6.4\times10^{-7}$ | $4.1\times10^{-3}$ |

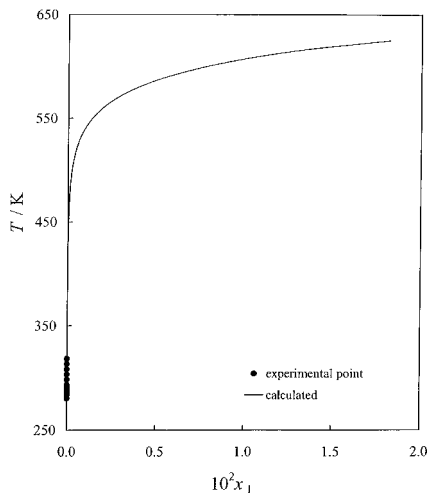


Table 4.7. Hexylbenzene–water

**Components**
(1) Hexylbenzene; $C_{12}H_{18}$; [1077-16-3]
(2) Water; $H_2O$; [7732-18-5]

**References**:
[1]W. E. May, S. P. Wasik, M. M. Miller, Y. B. Tewari, J. M. Brown-Thomas, and R. N. Goldberg, J. Chem. Eng. Data **28**, 197 (1983).
[2]J. W. Owens, S. P. Wasik, and H. DeVoe, J. Chem. Eng. Data **31**, 47 (1986).

Reference liquid–liquid equilibrium data

| | Water rich phase | | Hydrocarbon rich phase |
|---|---|---|---|
| $T$ (K) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $x_{2,\mathrm{calc}}$ |
| 278.2 | $1.02\times10^{-7}$ (Ref. 1) | $1.0\times10^{-7}$ | $1.3\times10^{-3}$ |
| 279.2 | $1.02\times10^{-7}$ (Ref. 1) | $1.0\times10^{-7}$ | $1.3\times10^{-3}$ |
| 280.2 | $9.26\times10^{-8}$ (Ref. 2) | $1.0\times10^{-7}$ | $1.4\times10^{-3}$ |
| 281.2 | $1.02\times10^{-7}$ (Ref. 1) | $9.9\times10^{-8}$ | $1.4\times10^{-3}$ |
| 282.2 | $1.01\times10^{-7}$ (Ref. 1) | $9.8\times10^{-8}$ | $1.5\times10^{-3}$ |
| 283.2 | $1.00\times10^{-7}$ (Ref. 1) | $9.8\times10^{-8}$ | $1.5\times10^{-3}$ |
| 284.2 | $1.03\times10^{-7}$ (Ref. 1) | $9.7\times10^{-8}$ | $1.6\times10^{-3}$ |
| 285.2 | $1.03\times10^{-7}$ (Ref. 1) | $9.7\times10^{-8}$ | $1.6\times10^{-3}$ |
| 286.2 | $1.02\times10^{-7}$ (Ref. 1) | $9.6\times10^{-8}$ | $1.6\times10^{-3}$ |
| 287.2 | $1.03\times10^{-7}$ (Ref. 1) | $9.6\times10^{-8}$ | $1.7\times10^{-3}$ |
| 288.2 | $9.18\times10^{-8}$ (Ref. 2) | $9.6\times10^{-8}$ | $1.7\times10^{-3}$ |
| 289.2 | $1.02\times10^{-7}$ (Ref. 1) | $9.6\times10^{-8}$ | $1.8\times10^{-3}$ |
| 290.2 | $1.01\times10^{-7}$ (Ref. 1) | $9.6\times10^{-8}$ | $1.8\times10^{-3}$ |
| 291.2 | $1.02\times10^{-7}$ (Ref. 1) | $9.6\times10^{-8}$ | $1.9\times10^{-3}$ |
| 292.2 | $1.05\times10^{-7}$ (Ref. 1) | $9.6\times10^{-8}$ | $1.9\times10^{-3}$ |
| 293.2 | $1.06\times10^{-7}$ (Ref. 2) | $9.6\times10^{-8}$ | $2.0\times10^{-3}$ |
| 294.2 | $1.06\times10^{-7}$ (Ref. 1) | $9.7\times10^{-8}$ | $2.1\times10^{-3}$ |
| 295.2 | $1.06\times10^{-7}$ (Ref. 1) | $9.7\times10^{-8}$ | $2.1\times10^{-3}$ |
| 296.2 | $1.09\times10^{-7}$ (Ref. 1) | $9.7\times10^{-8}$ | $2.2\times10^{-3}$ |
| 297.2 | $1.10\times10^{-7}$ (Ref. 1) | $9.8\times10^{-8}$ | $2.2\times10^{-3}$ |
| 298.2 | $1.01\times10^{-7}$ (Ref. 2) | $9.8\times10^{-8}$ | $2.3\times10^{-3}$ |
| 299.2 | $1.11\times10^{-7}$ (Ref. 1) | $9.9\times10^{-8}$ | $2.4\times10^{-3}$ |
| 300.2 | $1.12\times10^{-7}$ (Ref. 1) | $1.0\times10^{-7}$ | $2.4\times10^{-3}$ |
| 302.2 | $1.13\times10^{-7}$ (Ref. 1) | $1.0\times10^{-7}$ | $2.6\times10^{-3}$ |
| 303.2 | $1.11\times10^{-7}$ (Ref. 2) | $1.0\times10^{-7}$ | $2.6\times10^{-3}$ |
| 308.2 | $1.19\times10^{-7}$ (Ref. 2) | $1.1\times10^{-7}$ | $3.0\times10^{-3}$ |
| 313.2 | $1.20\times10^{-7}$ (Ref. 2) | $1.2\times10^{-7}$ | $3.4\times10^{-3}$ |
| 318.2 | $1.45\times10^{-7}$ (Ref. 2) | $1.3\times10^{-7}$ | $3.9\times10^{-3}$ |

**Other references**:
[3]R. Ya. Krasnoshchekova and M. Ya. Gubergrits, Vodnye Resursy **2**, 170 (1975).
[4]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

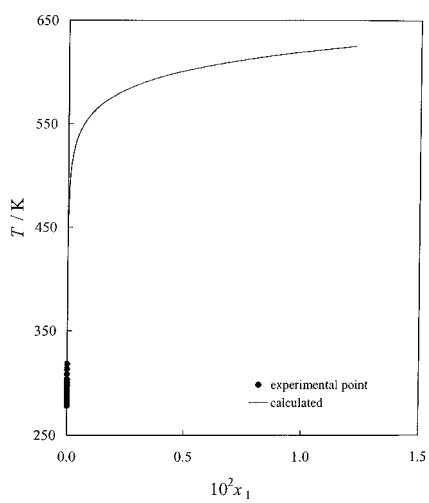


Table 4.8. (1-Methylethyl)benzene–water

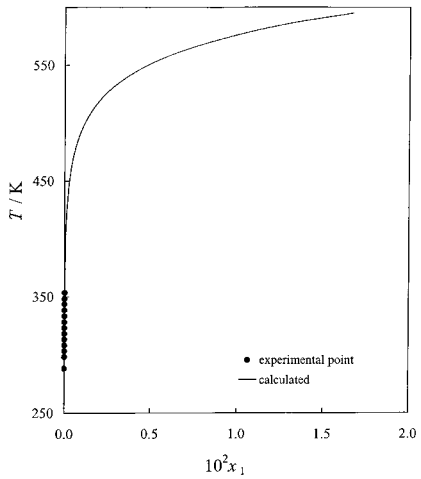
**Components**
(1) (1-Methylethyl)benzene; $C_9H_{12}$; [98-82-8]
(2) Water; $H_2O$; [7732-18-5]

**References**
[1]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
[2]B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[3]D. N. Glew and R. E. Robertson, J. Phys. Chem. **60**, 332 (1956).
[4]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Reference liquid–liquid equilibrium data

| Water rich phase | | | Hydrocarbon rich phase | | |
|---|---|---|---|---|---|
| $T$ (K) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $T$ (K) | $x_{2,\mathrm{exp}}$ | $x_{2,\mathrm{calc}}$ |
| 288.2 | $8.92\times10^{-6}$ (Ref. 4) | $9.9\times10^{-6}$ | 273.2 | $1.04\times10^{-3}$ (Ref. 2) | $1.2\times10^{-3}$ |
| 298.1 | $1.20\times10^{-5}$ (Ref. 3) | $1.0\times10^{-5}$ | 283.2 | $1.46\times10^{-3}$ (Ref. 2) | $1.6\times10^{-3}$ |
| 298.2 | $1.09\times10^{-5}$ (Ref. 1) | $1.0\times10^{-5}$ | 293.2 | $2.02\times10^{-3}$ (Ref. 2) | $2.2\times10^{-3}$ |
| 303.1 | $1.24\times10^{-5}$ (Ref. 3) | $1.0\times10^{-5}$ | 303.2 | $2.71\times10^{-3}$ (Ref. 2) | $3.0\times10^{-3}$ |
| 308.1 | $1.28\times10^{-5}$ (Ref. 3) | $1.1\times10^{-5}$ | 313.2 | $3.66\times10^{-3}$ (Ref. 2) | $4.0\times10^{-3}$ |
| 308.2 | $1.03\times10^{-5}$ (Ref. 4) | $1.1\times10^{-5}$ | 323.2 | $4.72\times10^{-3}$ (Ref. 2) | $5.3\times10^{-3}$ |
| 313.1 | $1.34\times10^{-5}$ (Ref. 3) | $1.1\times10^{-5}$ | | | |
| 318.1 | $1.42\times10^{-5}$ (Ref. 3) | $1.2\times10^{-5}$ | | | |
| 318.2 | $1.16\times10^{-5}$ (Ref. 4) | $1.2\times10^{-5}$ | | | |
| 323.1 | $1.50\times10^{-5}$ (Ref. 3) | $1.3\times10^{-5}$ | | | |
| 328.1 | $1.60\times10^{-5}$ (Ref. 3) | $1.4\times10^{-5}$ | | | |
| 333.1 | $1.72\times10^{-5}$ (Ref. 3) | $1.5\times10^{-5}$ | | | |
| 338.3 | $1.86\times10^{-5}$ (Ref. 3) | $1.6\times10^{-5}$ | | | |
| 343.5 | $2.03\times10^{-5}$ (Ref. 3) | $1.8\times10^{-5}$ | | | |
| 348.3 | $2.21\times10^{-5}$ (Ref. 3) | $2.0\times10^{-5}$ | | | |
| 353.4 | $2.42\times10^{-5}$ (Ref. 3) | $2.2\times10^{-5}$ | | | |

**Other references:**
[5]C. McAuliffe, Nature (London) **200**, 1092 (1963).
[6]C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
[7]L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[8]R. S. Stearns, H. Oppenheimer, E. Simon, and W. D. Harkins, J. Chem. Phys. **15**, 496 (1947).
[9]C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).



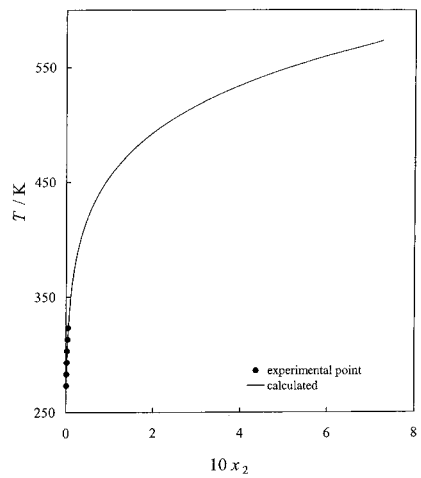



Table 4.9. *sec*-Butylbenzene–water

| Components | References |
|---|---|
| (1) *sec*-Butylbenzene; $C_{10}H_{14}$; [135-98-8]<br>(2) Water; $H_2O$; [7732-18-5] | [1]C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975). |

Reference liquid–liquid equilibrium data

| | Water rich phase | | Hydrocarbon rich phase |
|---|---|---|---|
| $T$ (K) | $x_{1,exp}$ | $x_{1,calc}$ | $x_{2,calc}$ |
| 298.2 | $2.36\times10^{-6}$ (Ref. 1) | $2.8\times10^{-6}$ | $2.5\times10^{-3}$ |

**Other references:**
[2]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
[3]B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[4]L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).

Table 4.10. *tert*-Butylbenzene–water

| Components | References |
|---|---|
| (1) *tert*-Butylbenzene; $C_{10}H_{14}$; [98-06-6]<br>(2) Water; $H_2O$; [7732-18-5] | [1]B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965). |

Reference liquid–liquid equilibrium data

| | Water rich phase | | Hydrocarbon rich phase | |
|---|---|---|---|---|
| $T$ (K) | $x_{1,calc}$ | | $x_{2,exp}$ | $x_{2,calc}$ |
| 283.2 | $2.2\times10^{-6}$ | | $2.03\times10^{-3}$ (Ref. 1) | $1.6\times10^{-3}$ |

**Other references:**
[2]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
[3]C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).

Table 4.11. 1,2-Dimethylbenzene–water

| Components | References |
|---|---|
| (1) 1,2-Dimethylbenzene; $C_8H_{10}$; [95-47-6]<br>(2) Water; $H_2O$; [7732-18-5] | [1]A. Ben-Naim and J. Wilf, J. Chem. Phys. **70**, 771 (1979).<br>[2]E. Högfeldt and B. Bolander, Ark. Kemi **21**, 161 (1964).<br>[3]J. Polak and B. C. Y. Lu, Can. J. Chem. **51**, 4018 (1973).<br>[4]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).<br>[5]I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, Bull. Chem. Soc. Jpn. **60**, 517 (1987). |

Reference liquid–liquid equilibrium data

| Water rich phase | | | Hydrocarbon rich phase | | |
|---|---|---|---|---|---|
| $T$ (K) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $T$/K | $x_{2,\mathrm{exp}}$ | $x_{2,\mathrm{calc}}$ |
| 283.2 | $3.60\times10^{-5}$ (Ref. 1) | $3.5\times10^{-5}$ | 273.2 | $1.09\times10^{-3}$ (Ref. 3) | $1.2\times10^{-3}$ |
| 288.2 | $2.85\times10^{-5}$ (Ref. 4) | $3.5\times10^{-5}$ | 298.2 | $2.60\times10^{-3}$ (Ref. 2) | $2.6\times10^{-3}$ |
| 293.2 | $4.08\times10^{-5}$ (Ref. 1) | $3.5\times10^{-5}$ | | | |
| 298.1 | $3.04\times10^{-5}$ (Ref. 5) | $3.6\times10^{-5}$ | | | |
| 298.2 | $3.61\times10^{-5}$ (Ref. 3) | $3.6\times10^{-5}$ | | | |
| 308.2 | $3.35\times10^{-5}$ (Ref. 4) | $3.8\times10^{-5}$ | | | |
| 318.2 | $3.64\times10^{-5}$ (Ref. 4) | $4.1\times10^{-5}$ | | | |

**Other references:**

[6]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).
[7]A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **18**, 76 (1963).
[8]D. F. Keeley, M. A. Hoffpauir, and J. R. Meriwether, J. Chem. Eng. Data **36**, 456 (1991).
[9]C. McAuliffe, Nature (London) **200**, 1092 (1963).
[10]L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[11]S. Sawamura, K. Suzuki, and Y. J. Taniguchi, J. Solution Chem. **16**, 649 (1987).
[12]C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
[13]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

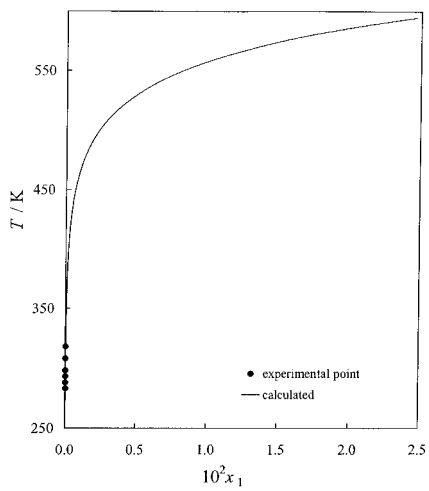



Table 4.12. 1,3-Dimethylbenzene–water

**Components**

(1) 1,3-Dimethylbenzene; $C_8H_{10}$; [108-38-3]
(2) Water; $H_2O$; [7732-18-5]

**References**:

[1]F. E. Anderson and J. M. Prausnitz, Fluid Phase Equilib. **32**, 63 (1986).
[2]F. S. Chernoglazova and Yu. N. Simulin, Zh. Fiz. Khim. **50**, 809 (1976).
[3]B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[4]E. Högfeldt and B. Bolander, Ark. Kemi **21**, 161 (1964).
[5]D. J. Miller and S. B. Hawthorne, J. Chem. Eng. Data **45**, 78 (2000).
[6]J. Polak and B. C. Y. Lu, Can. J. Chem. **51**, 4018 (1973).
[7]W. A. Pryor and R. E. Jentoft, J. Chem. Eng. Data **6**, 36 (1961).
[8]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).
[9]I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, Bull. Chem. Soc. Jpn. **60**, 517 (1987).
[10]S. Sawamura, K. Suzuki, and Y. J. Taniguchi, J. Solution Chem. **16**, 649 (1987).

Reference liquid–liquid equilibrium data

| Water rich phase | | | | Hydrocarbon rich phase | | | |
|---|---|---|---|---|---|---|---|
| $T$ (K) | $P$ (kPa) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $T$ (K) | $P$ (kPa) | $x_{2,\mathrm{exp}}$ | $x_{2,\mathrm{calc}}$ |
| 273.2 | | $3.32\times10^{-5}$ (Ref. 6) | $2.9\times10^{-5}$ | 273.2 | | $1.11\times10^{-3}$ (Ref. 6) | $1.2\times10^{-3}$ |
| 288.2 | | $2.68\times10^{-5}$ (Ref. 8) | $2.7\times10^{-5}$ | 283.2 | | $1.70\times10^{-3}$ (Ref. 3) | $1.7\times10^{-3}$ |
| 293.2 | | $2.70\times10^{-5}$ (Ref. 2) | $2.7\times10^{-5}$ | 293.2 | | $2.37\times10^{-3}$ (Ref. 3) | $2.3\times10^{-3}$ |
| 298.0 | 6000 | $2.90\times10^{-5}$ (Ref. 5) | $2.7\times10^{-5}$ | 298.2 | | $2.60\times10^{-3}$ (Ref. 4) | $2.7\times10^{-3}$ |
| 298.1 | | $2.40\times10^{-5}$ (Ref. 9) | $2.7\times10^{-5}$ | 303.2 | | $3.15\times10^{-3}$ (Ref. 3) | $3.1\times10^{-3}$ |
| 298.2 | | $2.70\times10^{-5}$ (Ref. 10) | $2.7\times10^{-5}$ | 313.2 | | $3.90\times10^{-3}$ (Ref. 2) | $4.1\times10^{-3}$ |
| 308.2 | | $2.85\times10^{-5}$ (Ref. 8) | $2.9\times10^{-5}$ | 343.2 | | $1.11\times10^{-2}$ (Ref. 2) | $9.2\times10^{-3}$ |
| 313.2 | | $3.70\times10^{-5}$ (Ref. 2) | $3.0\times10^{-5}$ | 373.6 | 101 | $1.647\times10^{-2}$ (Ref. 1) | $1.9\times10^{-2}$ |
| 318.2 | | $3.15\times10^{-5}$ (Ref. 8) | $3.2\times10^{-5}$ | 398.2 | 281 | $2.785\times10^{-2}$ (Ref. 1) | $3.3\times10^{-2}$ |
| 323.0 | 6000 | $3.60\times10^{-5}$ (Ref. 5) | $3.4\times10^{-5}$ | 398.3 | 274 | $2.857\times10^{-2}$ (Ref. 1) | $3.3\times10^{-2}$ |
| 373.0 | 6000 | $8.50\times10^{-5}$ (Ref. 5) | $8.2\times10^{-5}$ | 423.2 | 598 | $5.131\times10^{-2}$ (Ref. 1) | $5.5\times10^{-2}$ |
| 378.8 | | $1.13\times10^{-4}$ (Ref. 7) | $9.3\times10^{-5}$ | 448.4 | 1142 | $8.840\times10^{-2}$ (Ref. 1) | $9.0\times10^{-2}$ |
| 397.4 | | $1.75\times10^{-4}$ (Ref. 7) | $1.4\times10^{-4}$ | 473.4 | 2004 | $1.510\times10^{-1}$ (Ref. 1) | $1.4\times10^{-1}$ |
| 423.0 | 6000 | $2.70\times10^{-4}$ (Ref. 5) | $2.7\times10^{-4}$ | | | | |
| 423.2 | 598 | $2.98\times10^{-4}$ (Ref. 1) | $2.7\times10^{-4}$ | | | | |
| 437.4 | | $4.27\times10^{-4}$ (Ref. 7) | $3.9\times10^{-4}$ | | | | |
| 448.4 | 1142 | $5.17\times10^{-4}$ (Ref. 1) | $5.2\times10^{-4}$ | | | | |
| 459.6 | | $7.82\times10^{-4}$ (Ref. 7) | $7.0\times10^{-4}$ | | | | |
| 463.1 | | $7.76\times10^{-4}$ (Ref. 7) | $7.7\times10^{-4}$ | | | | |
| 473.0 | 6000 | $8.80\times10^{-4}$ (Ref. 5) | $1.0\times10^{-3}$ | | | | |
| 473.4 | 2004 | $9.64\times10^{-4}$ (Ref. 1) | $1.0\times10^{-3}$ | | | | |
| 539.8 | | $4.96\times10^{-3}$ (Ref. 7) | $5.7\times10^{-3}$ | | | | |
| 543.8 | | $5.00\times10^{-3}$ (Ref. 7) | $6.3\times10^{-3}$ | | | | |

**Other references:**

[11]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).
[12]R. L. Bohon and W. F. Claussen, J. Am. Chem. Soc. **73**, 1571 (1951).
[13]A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **18**, 76 (1963).
[14]D. F. Keeley, M. A. Hoffpauir, and J. R. Meriwether, J. Chem. Eng. Data **36**, 456 (1991).
[15]L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[16]C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
[17]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
[18]A. Vesala, Acta Chem. Scand., Ser. A **28**, 839 (1974).

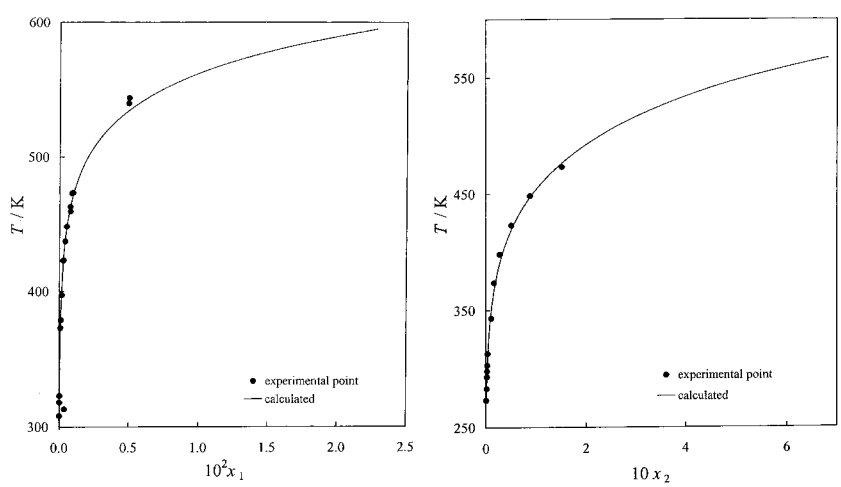


Table 4.13. 1,4-Dimethylbenzene–water

**Components**:
(1) 1,4-Dimethylbenzene; $C_8H_{10}$; [106-42-3]
(2) Water; $H_2O$; [7732-18-5]

**References**
[1]A. Ben-Naim and J. Wilf, J. Chem. Phys. **70**, 771 (1979).
[2]H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 679 (1994).
[3]E. Högfeldt and B. Bolander, Ark. Kemi **21**, 161 (1964).
[4]J. Polak and B. C. Y. Lu, Can. J. Chem. **51**, 4018 (1973).
[5]L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[6]W. A. Pryor and R. E. Jentoft, J. Chem. Eng. Data **6**, 36 (1961).
[7]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).
[8]I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, Bull. Chem. Soc. Jpn. **60**, 517 (1987).

Reference liquid–liquid equilibrium data

| Water rich phase | | | Hydrocarbon rich phase | | |
|---|---|---|---|---|---|
| $T$ (K) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $T$ (K) | $x_{2,\mathrm{exp}}$ | $x_{2,\mathrm{calc}}$ |
| 273.2 | $2.78\times10^{-5}$ (Ref. 4) | $2.8\times10^{-5}$ | 298.2 | $2.70\times10^{-3}$ (Ref. 3) | $2.7\times10^{-3}$ |
| 283.2 | $3.21\times10^{-5}$ (Ref. 1) | $2.6\times10^{-5}$ | 303.2 | $2.71\times10^{-3}$ (Ref. 2) | $3.1\times10^{-3}$ |
| 288.2 | $2.67\times10^{-5}$ (Ref. 7) | $2.6\times10^{-5}$ | 313.2 | $3.48\times10^{-3}$ (Ref. 2) | $4.2\times10^{-3}$ |
| 293.2 | $3.25\times10^{-5}$ (Ref. 1) | $2.6\times10^{-5}$ | 323.2 | $4.75\times10^{-3}$ (Ref. 2) | $5.5\times10^{-3}$ |
| 298.1 | $2.73\times10^{-5}$ (Ref. 8) | $2.6\times10^{-5}$ | 333.2 | $6.51\times10^{-3}$ (Ref. 2) | $7.2\times10^{-3}$ |
| 298.2 | $2.66\times10^{-5}$ (Ref. 5) | $2.6\times10^{-5}$ | 343.2 | $8.70\times10^{-3}$ (Ref. 2) | $9.3\times10^{-3}$ |
| 303.2 | $2.86\times10^{-5}$ (Ref. 2) | $2.7\times10^{-5}$ | 353.2 | $1.15\times10^{-2}$ (Ref. 2) | $1.2\times10^{-2}$ |
| 308.2 | $2.92\times10^{-5}$ (Ref. 7) | $2.8\times10^{-5}$ | 363.2 | $1.57\times10^{-2}$ (Ref. 2) | $1.5\times10^{-2}$ |
| 313.2 | $3.18\times10^{-5}$ (Ref. 2) | $2.9\times10^{-5}$ | 373.2 | $2.02\times10^{-2}$ (Ref. 2) | $1.9\times10^{-2}$ |
| 318.2 | $3.02\times10^{-5}$ (Ref. 7) | $3.1\times10^{-5}$ | | | |
| 323.2 | $3.44\times10^{-5}$ (Ref. 2) | $3.3\times10^{-5}$ | | | |
| 333.2 | $4.04\times10^{-5}$ (Ref. 2) | $3.7\times10^{-5}$ | | | |
| 343.2 | $4.83\times10^{-5}$ (Ref. 2) | $4.4\times10^{-5}$ | | | |
| 353.2 | $5.71\times10^{-5}$ (Ref. 2) | $5.3\times10^{-5}$ | | | |
| 360.4 | $7.79\times10^{-5}$ (Ref. 6) | $6.1\times10^{-5}$ | | | |
| 363.2 | $6.70\times10^{-5}$ (Ref. 2) | $6.4\times10^{-5}$ | | | |
| 373.2 | $8.74\times10^{-5}$ (Ref. 2) | $7.9\times10^{-5}$ | | | |
| 435.7 | $4.264\times10^{-4}$ (Ref. 6) | $3.6\times10^{-4}$ | | | |
| 461.3 | $7.686\times10^{-4}$ (Ref. 6) | $7.1\times10^{-4}$ | | | |
| 516.4 | $2.956\times10^{-3}$ (Ref. 6) | $3.1\times10^{-3}$ | | | |
| 555.7 | $7.624\times10^{-3}$ (Ref. 6) | $8.4\times10^{-3}$ | | | |

**Other references:**
[9]F. E. Anderson and J. M. Prausnitz, Fluid Phase Equilib. **32**, 63 (1986).
[10]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).
[11]R. L. Bohon and W. F. Claussen, J. Am. Chem. Soc. **73**, 1571 (1951).
[12]A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **18**, 76 (1963).
[13]M. Haruki, Y. Iwai, S. Nagao, and Y. Arai, J. Chem. Eng. Data **46**, 950 (2001).
[14]D. F. Keeley, M. A. Hoffpauir, and J. R. Meriwether, J. Chem. Eng. Data **36**, 456 (1991).
[15]J. Kirchnerova and G. C. B. Cave, Can. J. Chem. **54**, 3909 (1976).
[16]J. M. Lo, C. L. Tseng, and J. Y. Yang, Anal. Chem. **58**, 1596 (1986).
[17]S. Sawamura, K. Suzuki, and Y. J. Taniguchi, J. Solution Chem. **16**, 649 (1987).
[18]C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
[19]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

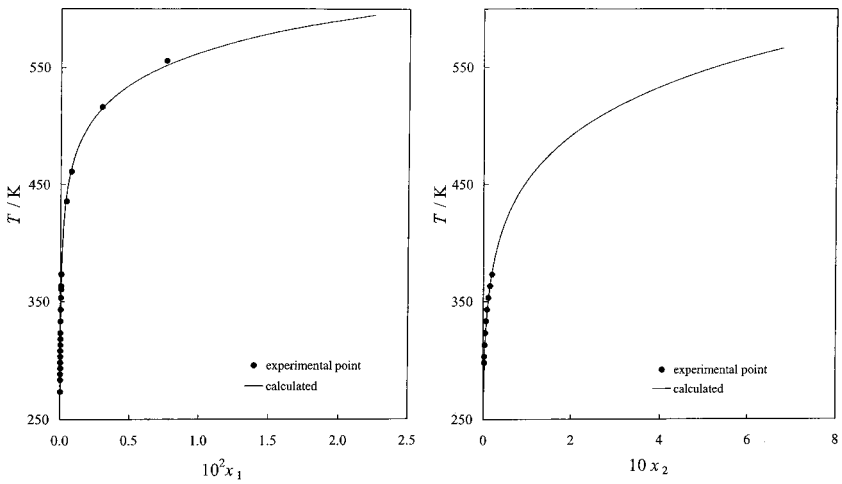



Table 4.14. 1,3-Diethylbenzene–water

**Components**
(1) 1,3-Diethylbenzene; $C_{10}H_{14}$; [141-93-5]
(2) Water; $H_2O$; [7732-18-5]

**References**
[1]I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).

Reference liquid–liquid equilibrium data

| Water rich phase | | | | Hydrocarbon rich phase | | | |
|---|---|---|---|---|---|---|---|
| $T$ (K) | $P$ (kPa) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $T$ (K) | $P$ (kPa) | $x_{2,\mathrm{exp}}$ | $x_{2,\mathrm{calc}}$ |
| 366.5 | | $1.00\times10^{-5}$ (Ref. 1) | $7.7\times10^{-6}$ | 310.9 | | $3.42\times10^{-3}$ (Ref. 1) | $3.5\times10^{-3}$ |
| 422.0 | 508.1 | $4.30\times10^{-5}$ (Ref. 1) | $4.0\times10^{-5}$ | 366.5 | | $1.62\times10^{-2}$ (Ref. 1) | $1.4\times10^{-2}$ |
| 477.6 | 1891.2 | $2.70\times10^{-4}$ (Ref. 1) | $2.4\times10^{-4}$ | 422.0 | 508.1 | $5.93\times10^{-2}$ (Ref. 1) | $4.7\times10^{-2}$ |
| 533.2 | 5405 | $1.57\times10^{-3}$ (Ref. 1) | $1.5\times10^{-3}$ | 477.6 | 1891.2 | $1.57\times10^{-1}$ (Ref. 1) | $1.4\times10^{-1}$ |
| 549.8 | 7074 | $3.07\times10^{-3}$ (Ref. 1) | $2.6\times10^{-3}$ | 533.2 | 5405 | $3.67\times10^{-1}$ (Ref. 1) | $3.7\times10^{-1}$ |
| | | | | 549.8 | 7074 | $4.57\times10^{-1}$ (Ref. 1) | $4.8\times10^{-1}$ |

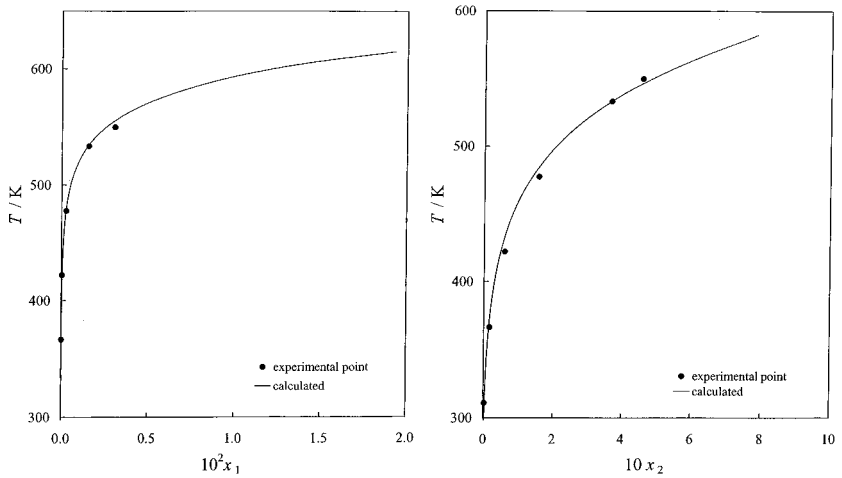


Table 4.15. 1-Ethyl–2-methylbenzene–water

| **Components** | **References** |
|---|---|
| (1) 1-Ethyl-2-methylbenzene; $C_9H_{12}$; [611-14-3]<br>(2) Water; $H_2O$; [7732-18-5] | [1]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982). |

Reference liquid–liquid equilibrium data

| | Water rich phase | | Hydrocarbon rich phase |
|---|---|---|---|
| $T$/K | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $x_{2,\mathrm{calc}}$ |
| 298.2 | $1.12\times10^{-5}$ (Ref. 1) | $1.0\times10^{-5}$ | $2.5\times10^{-3}$ |

Table 4.16. 1-Methyl-4-(1-methylethyl)benzene–water

| **Components** | **References** |
|---|---|
| (1) 1-Methyl-4-(1-methylethyl)benzene; $C_{10}H_{14}$;[99-87-6]<br>(2) Water; $H_2O$; [7732-18-5] | [1]B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).<br>[2]D. J. Miller and S. B. Hawthorne, J. Chem. Eng. Data **45**, 78 (2000). |

Reference liquid–liquid equilibrium data

| Water rich phase | | | Hydrocarbon rich phase | | |
|---|---|---|---|---|---|
| $T$ (K) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $T$ (K) | $x_{2,\mathrm{exp}}$ | $x_{2,\mathrm{calc}}$ |
| 423.0 | $4.30\times10^{-5}$ (Ref. 2) | $3.7\times10^{-5}$ | 283.2 | $1.66\times10^{-3}$ (Ref. 1) | $1.6\times10^{-3}$ |
| 473.0 | $2.00\times10^{-4}$ (Ref. 2) | $1.9\times10^{-4}$ | 293.2 | $2.27\times10^{-3}$ (Ref. 1) | $2.2\times10^{-3}$ |
| | | | 303.2 | $3.08\times10^{-3}$ (Ref. 1) | $2.9\times10^{-3}$ |

**Other references:**
[3]S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).
[4]H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).

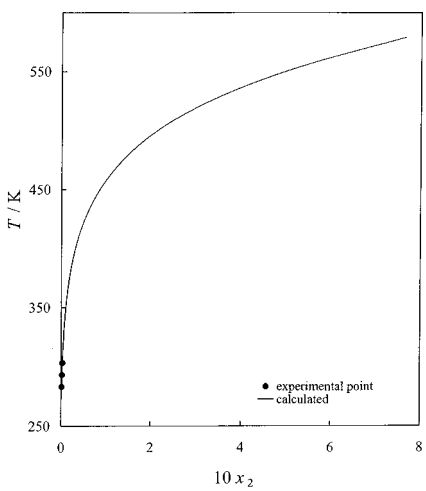


Table 4.17. 1,4-Bis(1-methylethyl)benzene–water

**Components**
(1) 1,4-Bis(1-methylethyl)benzene; $C_{12}H_{18}$; [100-18-5]
(2) Water; $H_2O$; [7732-18-5]

**References**
[1]I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).

Reference liquid–liquid equilibrium data

| Water rich phase | | | | Hydrocarbon rich phase | | | |
|---|---|---|---|---|---|---|---|
| $T$ (K) | $P$ (kPa) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $T$ (K) | $P$ (kPa) | $x_{2,\mathrm{exp}}$ | $x_{2,\mathrm{calc}}$ |
| 477.6 | 1799.5 | $5.80\times10^{-5}$ (Ref. 1) | $5.0\times10^{-5}$ | 310.9 | | $3.45\times10^{-3}$ (Ref. 1) | $3.3\times10^{-3}$ |
| 533.2 | 5081 | $4.50\times10^{-4}$ (Ref. 1) | $4.5\times10^{-4}$ | 366.5 | | $1.57\times10^{-2}$ (Ref. 1) | $1.3\times10^{-2}$ |
| 549.8 | 7460 | $7.10\times10^{-4}$ (Ref. 1) | $8.6\times10^{-4}$ | 533.2 | 5081 | $3.64\times10^{-1}$ (Ref. 1) | $3.3\times10^{-1}$ |
| | | | | 549.8 | 7460 | $4.62\times10^{-1}$ (Ref. 1) | $4.3\times10^{-1}$ |

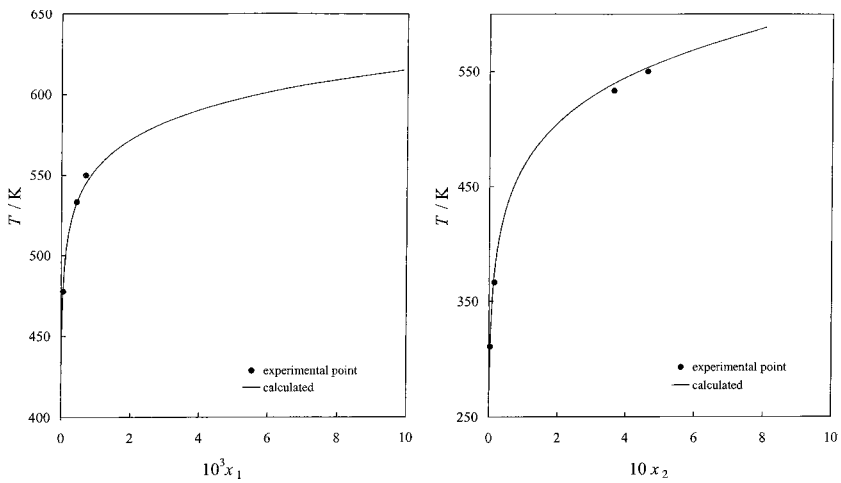


Table 4.18. 1,2,3-Trimethylbenzene–water

| **Components** | **References** |
|---|---|
| (1) 1,2,3-Trimethylbenzene; $C_9H_{12}$; [526-73-8] | [1]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982). |
| (2) Water; $H_2O$; [7732-18-5] | [2]C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975). |

Reference liquid–liquid equilibrium data

| | Water rich phase | | Hydrocarbon rich phase |
|---|---|---|---|
| $T$ (K) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $x_{2,\mathrm{calc}}$ |
| 288.2 | $8.97\times10^{-6}$ (Ref. 1) | $1.2\times10^{-5}$ | $1.9\times10^{-3}$ |
| 298.2 | $1.13\times10^{-5}$ (Ref. 2) | $1.2\times10^{-5}$ | $2.5\times10^{-3}$ |
| 308.2 | $1.08\times10^{-5}$ (Ref. 1) | $1.3\times10^{-5}$ | $3.2\times10^{-3}$ |
| 318.2 | $1.28\times10^{-5}$ (Ref. 1) | $1.4\times10^{-5}$ | $4.1\times10^{-3}$ |

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

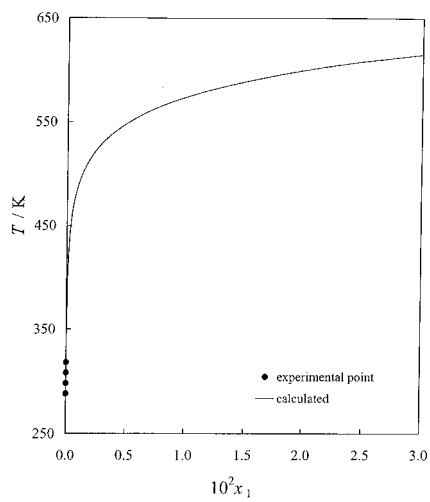


Table 4.19. 1,2,4-Trimethylbenzene–water

| **Components** | **References** |
|---|---|
| (1) 1,2,4-Trimethylbenzene; $C_9H_{12}$; [95-63-6] | [1]C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966). |
| (2) Water; $H_2O$; [7732-18-5] | [2]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982). |

Reference liquid–liquid equilibrium data

| | Water rich phase | | Hydrocarbon rich phase |
|---|---|---|---|
| $T$ (K) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $x_{2,\mathrm{calc}}$ |
| 288.2 | $7.84\times10^{-6}$ (Ref. 2) | $8.2\times10^{-6}$ | $1.9\times10^{-3}$ |
| 298.2 | $8.50\times10^{-6}$ (Ref. 1) | $8.3\times10^{-6}$ | $2.5\times10^{-3}$ |
| 308.2 | $9.32\times10^{-6}$ (Ref. 2) | $8.9\times10^{-6}$ | $3.3\times10^{-3}$ |
| 318.2 | $1.04\times10^{-5}$ (Ref. 2) | $9.9\times10^{-6}$ | $4.3\times10^{-3}$ |

**Other references:**
[3]L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[4]C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).

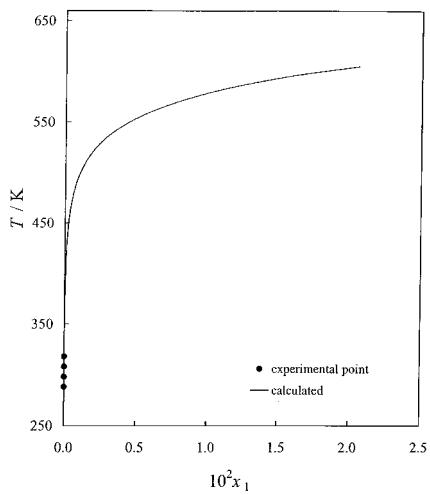


Table 4.20. 1,3,5-Trimethylbenzene–water

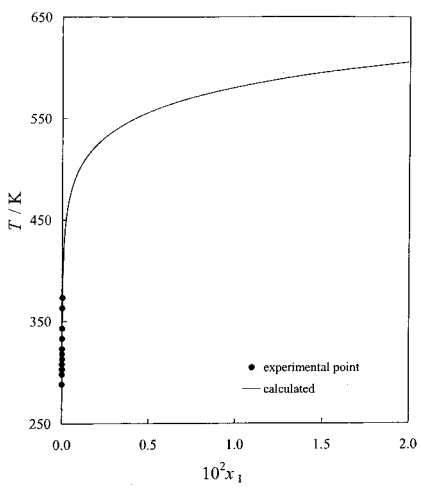
**Components**
(1) 1,3,5-Trimethylbenzene; $C_9H_{12}$; [108-67-8]
(2) Water; $H_2O$; [7732-18-5]

**References**
[1]H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 679 (1994).
[2]B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[3]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Chem. Lett. 225 (1981).
[4]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).
[5]C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
[6]A. Vesala, Acta Chem. Scand., Ser. A **28**, 839 (1974).

Reference liquid–liquid equilibrium data

| Water rich phase | | | Hydrocarbon rich phase | | |
|---|---|---|---|---|---|
| $T$ (K) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $T$ (K) | $x_{2,\mathrm{exp}}$ | $x_{2,\mathrm{calc}}$ |
| 288.2 | $6.90\times10^{-6}$ (Ref. 4) | $7.2\times10^{-6}$ | 293.2 | $1.94\times10^{-3}$ (Ref. 2) | $2.2\times10^{-3}$ |
| 298.0 | $5.91\times10^{-6}$ (Ref. 6) | $7.3\times10^{-6}$ | 303.2 | $2.62\times10^{-3}$ (Ref. 2) | $3.0\times10^{-3}$ |
| 298.2 | $7.22\times10^{-6}$ (Ref. 5) | $7.3\times10^{-6}$ | 313.2 | $3.50\times10^{-3}$ (Ref. 1) | $3.9\times10^{-3}$ |
| 303.2 | $9.58\times10^{-6}$ (Ref. 1) | $7.5\times10^{-6}$ | 323.2 | $4.88\times10^{-3}$ (Ref. 1) | $5.1\times10^{-3}$ |
| 308.2 | $8.11\times10^{-6}$ (Ref. 3) | $7.8\times10^{-6}$ | 333.2 | $6.09\times10^{-3}$ (Ref. 1) | $6.7\times10^{-3}$ |
| 313.2 | $1.00\times10^{-5}$ (Ref. 1) | $8.2\times10^{-6}$ | 343.2 | $7.97\times10^{-3}$ (Ref. 1) | $8.5\times10^{-3}$ |
| 318.2 | $8.83\times10^{-6}$ (Ref. 4) | $8.7\times10^{-6}$ | 353.2 | $1.06\times10^{-2}$ (Ref. 1) | $1.1\times10^{-2}$ |
| 323.2 | $1.11\times10^{-5}$ (Ref. 1) | $9.3\times10^{-6}$ | 363.2 | $1.40\times10^{-2}$ (Ref. 1) | $1.4\times10^{-2}$ |
| 333.2 | $1.36\times10^{-5}$ (Ref. 1) | $1.1\times10^{-5}$ | 373.2 | $1.90\times10^{-2}$ (Ref. 1) | $1.7\times10^{-2}$ |
| 343.2 | $1.66\times10^{-5}$ (Ref. 1) | $1.3\times10^{-5}$ | | | |
| 363.2 | $2.45\times10^{-5}$ (Ref. 1) | $2.0\times10^{-5}$ | | | |
| 373.2 | $2.91\times10^{-5}$ (Ref. 1) | $2.5\times10^{-5}$ | | | |

**Other references:**
[7]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
[8]H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).
[9]A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **18**, 76 (1963).



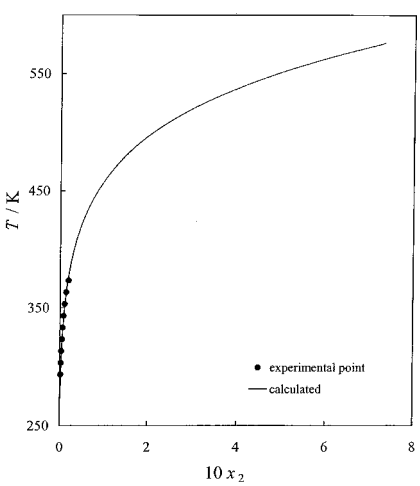
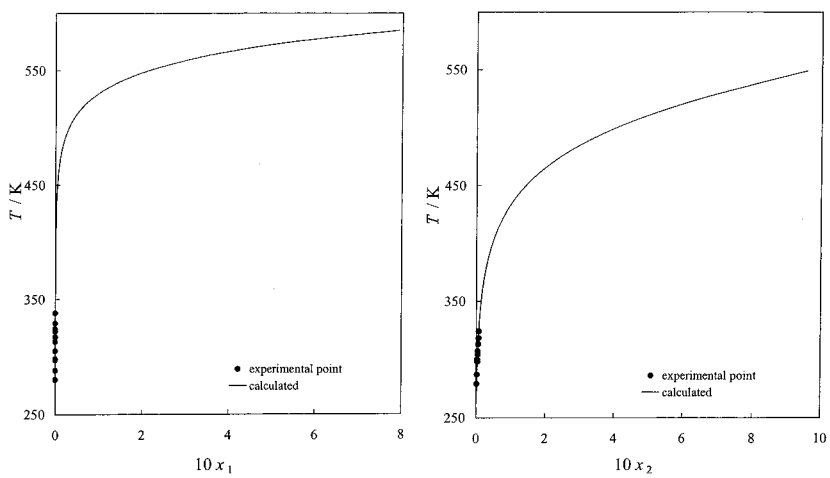



Table 4.21. Ethenylbenzene–water

| **Components** | **References** |
|---|---|
| (1) Ethenylbenzene; $C_8H_8$; [100-42-5] | [1]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950). |
| (2) Water; $H_2O$; [7732-18-5] | [2]W. H. Lane, Ind. Eng. Chem., Anal. Ed. **18**, 295 (1946). |

Reference liquid–liquid equilibrium data

| Water rich phase | | | Hydrocarbon rich phase | | |
|---|---|---|---|---|---|
| $T$ (K) | $x_{1,\mathrm{exp}}$ | $x_{1,\mathrm{calc}}$ | $T$ (K) | $x_{2,\mathrm{exp}}$ | $x_{2,\mathrm{calc}}$ |
| 280.2 | $5.00\times10^{-5}$ (Ref. 2) | $5.2\times10^{-5}$ | 279.2 | $1.8\times10^{-3}$ (Ref. 2) | $2.1\times10^{-3}$ |
| 288.2 | $4.30\times10^{-5}$ (Ref. 2) | $5.0\times10^{-5}$ | 287.2 | $2.3\times10^{-3}$ (Ref. 2) | $2.6\times10^{-3}$ |
| 297.2 | $5.70\times10^{-5}$ (Ref. 2) | $5.1\times10^{-5}$ | 298.2 | $3.8\times10^{-3}$ (Ref. 2) | $3.5\times10^{-3}$ |
| 298.2 | $5.19\times10^{-5}$ (Ref. 1) | $5.1\times10^{-5}$ | 300.2 | $3.5\times10^{-3}$ (Ref. 2) | $3.7\times10^{-3}$ |
| 305.2 | $6.20\times10^{-5}$ (Ref. 2) | $5.4\times10^{-5}$ | 304.2 | $4.8\times10^{-3}$ (Ref. 2) | $4.1\times10^{-3}$ |
| 313.2 | $6.90\times10^{-5}$ (Ref. 2) | $5.9\times10^{-5}$ | 307.2 | $4.6\times10^{-3}$ (Ref. 2) | $4.5\times10^{-3}$ |
| 317.2 | $6.90\times10^{-5}$ (Ref. 2) | $6.3\times10^{-5}$ | 313.2 | $5.7\times10^{-3}$ (Ref. 2) | $5.2\times10^{-3}$ |
| 322.2 | $7.80\times10^{-5}$ (Ref. 2) | $6.9\times10^{-5}$ | 318.2 | $6.9\times10^{-3}$ (Ref. 2) | $6.0\times10^{-3}$ |
| 324.2 | $7.80\times10^{-5}$ (Ref. 2) | $7.1\times10^{-5}$ | 324.2 | $7.1\times10^{-3}$ (Ref. 2) | $7.0\times10^{-3}$ |
| 329.2 | $8.60\times10^{-5}$ (Ref. 2) | $7.9\times10^{-5}$ | | | |
| 338.2 | $1.00\times10^{-4}$ (Ref. 2) | $9.7\times10^{-5}$ | | | |

**Other references:**

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