

# Recommended Vapor–Liquid Equilibrium Data. Part 1: Binary *n*-Alkanol–*n*-Alkane Systems

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The recommended vapor–liquid equilibrium (VLE) data for 39 binary *n*-alcohol–*n*-alkane systems have been obtained after critical evaluation of all data (490 data sets) reported in the open literature up to the middle of 2001. The evaluation procedure consisted in combining the thermodynamic consistency tests, data correlation, comparison with enthalpy of mixing data, and comparison of VLE data for various mixtures. The data were correlated with equations based on the local compositions concept as well as with the equation of state appended with a chemical term (EoS<sub>C</sub>) proposed by Góral. The recommended data are presented in the form of individual pages containing tables of data, figures, and auxiliary information. Each page corresponds to one system and contains three isotherms (spaced by at least 15 K) and one isobar (preferably at 101.32 kPa). Experimental gaps were completed with the predicted data. © 2002 American Institute of Physics. [DOI: 10.1063/1.1480097]

Key words: alcohols; binary systems; hydrocarbons; predicted data; recommended data; vapor–liquid equilibria.

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## 1. Introduction

The objective of this paper is to provide selected and critically evaluated vapor–liquid equilibrium (VLE) data for binary *n*-alcohol–*n*-hydrocarbon systems, taken from the open literature up to the middle of 2001 and completed, when needed, with predicted data.

Properties of the binary 1-alkanol+*n*-alkane mixtures were the object of the International IUPAC Project sponsored by the IUPAC Commission on Thermodynamics Subcommittee on Thermodynamic Tables. The objective of this project was to develop a set of recommended data, mainly low-pressure vapor–liquid equilibrium and related properties for these systems. The First Workshop (on Vapor–Liquid Equilibria in 1-Alkanol+*n*-Alkane Mixtures) was held near Warsaw in 1984, followed by Workshops in Paris (1985), Budapest (1987), Thessaloniki (1988), Gradisca d’Isonzo (1989), and Liblice (1991). A technical report concerning the results of the international efforts was prepared by Dymond.<sup>1</sup> The results of the critical evaluation of vapor–liquid equilibrium data were published by Oracz.<sup>2</sup> The thermodynamic consistency test of VLE data for binary alcohol+hydrocarbon systems has also been carried out by Moon *et al.*<sup>3</sup> but among 224 data sets considered there only 44 belongs to *n*-alkanol+*n*-alkane. Góral<sup>4</sup> has successfully applied the cubic Equation of State with a Chemical term (EoSC) for an accurate description of VLE in alcohol+hydrocarbon systems. Using the EoSC coupled with classical methods, the extended critical evaluation has been done by Góral *et al.*<sup>5</sup> for all literature available for the alcohol+aliphatic hydrocarbon systems. In a recent paper by Góral<sup>6</sup> the EoSC has been proven to be applicable for completion and/or prediction of VLE for the systems with limited or no experimental data.

## 2. Evaluation of the Experimental VLE Data

All available data (below 0.5 MPa) for the considered systems were taken from the open literature up to the middle of 2001. This data consist of 490 data sets taken from 160 references, all of which are listed in the Appendix (Sec. 9).

All data were critically evaluated using a multistage procedure. The procedure consists of combining the thermodynamic consistency tests, data correlation, comparison with enthalpy of mixing data, and comparison of VLE data for various mixtures.

Thermodynamic consistency tests were applied to *P–T–x–y* data. They are:

- (1) overall area (area deficit) test of Redlich–Kister–Herington,<sup>7,8</sup>

- (2) point-to-point test of Van Ness and Mrazek<sup>9</sup> and Kojima *et al.*;<sup>10</sup>
- (3) extended pressure dependent area test of Oracz;<sup>2</sup>
- (4) infinite dilution test of Kojima *et al.*,<sup>10</sup> and
- (5) the so-called Van Ness–Fredenslund *y*’s test.<sup>11,12</sup>

These five tests have been united into a single procedure. The criterion numbers were taken from tests of Kojima *et al.*<sup>10</sup> and Oracz.<sup>2</sup> The highest quality data have to pass all the listed thermodynamic consistency tests.

If the vapor concentration is not measured, then the thermodynamic consistency cannot be checked. This problem occurs in more than half of the data sets. Therefore, several other methods were used for the verification. These methods are described briefly in the following paragraphs.

Various data sets, for the same system measured at different *P–T* conditions, were correlated simultaneously using the Wilson equation with an extended temperature dependence of the binary interaction parameters. The calculations, whenever possible, were based on a multiresponse maximum likelihood method. Graphical output of primary *P–T–x(–y)* data, with corresponding calculated curves, enabled a comparison of the different data sets in respect to a uniform set of the Wilson parameters. The enthalpy of mixing, calculated from the temperature dependent Wilson parameters and compared to experimental  $H^E$ , gave us the additional possibility of determining any systematic error of the data.

Another method consisted of a comparison of the different data sets, as represented by  $G^E/RT$ , obtained from a separate correlation of the data sets. The values of  $G^E/RT$  at arbitrary selected concentrations were plotted against  $1/T$ . From the Gibbs–Helmholtz equation, the slope of the resulting line should be equal to  $H^E/R$  at the selected concentration (see e.g., Oracz and Warycha).<sup>13</sup> The test was performed at several concentrations.

Finally a method of correlation was applied, which uses only one binary parameter  $\Theta$  in addition to a model for self-association of the alcohols. (The method of the correlation, EoSC, is described in Sec. 3.) The value of  $\Theta$ , adjusted to the experimental data set, can be easily compared with other values of  $\Theta$  obtained from other data sets. Such comparisons were done for a mixture represented by several data sets or for mixtures belonging to the same homologous series. It was also possible to compare the different mixtures in respect to the method of prediction described later. Examples of such comparisons are discussed in the paper by Góral.<sup>6</sup>

## 3. Correlation of VLE Data

The mixtures of alcohols with hydrocarbons exhibit large deviations from ideality; such deviations make any correlation of some systems difficult. We have tested several equations based on the activity coefficients concept. Among two-parameter equations, the best results for homogenous mixtures were obtained with the Wilson equation for  $G^E$ . Multiparameter equations are less suitable for evaluation of

the data because they are more likely to fit systematic error. Góral<sup>4</sup> has showed that equation of state appended with the chemical term (EoS<sub>C</sub>), having one adjustable binary parameter, is capable of correlating these systems as accurately as the two-parameter Wilson equation. Moreover, the binary parameter used in the EoS<sub>C</sub> can be predicted with good accuracy. Therefore, we have decided to use the EoS<sub>C</sub> for the correlation of the VLE data.

The chemical potential in the EoS<sub>C</sub> method is separated into the physical and the chemical contributions. In this work the Redlich–Kwong equation of state (RK EoS)<sup>14</sup> was used to calculate the physical contribution to the chemical potential. It yields the following formula for change of the chemical potential of the *k*th component with respect to the standard state (perfect gas at 1 kPa):

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

where *V* is molar volume determined with RK EoS at temperature *T*, pressure *P*, and mole fraction *x<sub>k</sub>* using parameters *b* and *a* calculated with the classical mixing rules

$$b = x_i b_i + x_j b_j, \quad (2)$$

$$a = x_i^2 a_{ii} + 2x_i x_j a_{ij} + x_j^2 a_{jj}. \quad (3)$$

*a<sub>ij</sub>* is related to the binary adjustable parameter  $\Theta_{ij}$  with the equation

$$a_{ij} = (a_{ii} a_{jj})^{0.5} (1 - \Theta_{ij}). \quad (4)$$

(*na/b*)' in the Eq. (1) denotes the differential of the expression in the parenthesis where *n* is the total number of moles and *a*, *b* are expressed with Eqs. (2) and (3). The differentiation is done with respect to number of moles of the *k*th component. Equation (1) is also applicable for pure components provided that the following constraints are used: *x<sub>k</sub>* = 1; *a* = *a<sub>kk</sub>*; and *b* = *b<sub>k</sub>*.

In the EoS<sub>C</sub> method, the equation of state of the pure self-associating component is not modified. The pure alcohol is treated in the same way as hydrocarbon using effective *a<sub>kk</sub>*, *b<sub>k</sub>* parameters. The excluded volume *b<sub>k</sub>* of a pure substance is assumed to be temperature independent and is calculated from relevant critical parameters *T<sub>c,k</sub>* and *P<sub>c,k</sub>* using the standard formula for RK EoS:

$$b_k = (RT_{c,k} / P_{c,k}) (2^{(1/3)} - 1) / 3. \quad (5)$$

The energetic parameter *a<sub>kk</sub>* is adjusted by iteration to the saturated vapor pressure of the pure compound *P<sub>k</sub><sup>0</sup>* in the following way: liquid and vapor molar volumes under *P<sub>k</sub><sup>0</sup>* are calculated from the RK EoS using a starting value of *a<sub>kk</sub>*. The calculated volumes are introduced into Eq. (1) to calculate chemical potentials of the pure component in the liquid and vapor phases. At equilibrium the chemical potentials in both phases should be equal. If this constraint is not fulfilled, an improved value of *a<sub>kk</sub>* is used in the next iteration. This procedure is applied both for alcohols and for hydrocarbons. In this way, correlation of VLE for the mixture is not af-

fectured by improper description of *P<sub>k</sub><sup>0</sup>*. Whenever available, the value of *P<sub>k</sub><sup>0</sup>* given by the author of the data was used. If the saturated vapor pressure of the pure *k*th compound was not reported or, in the case of isobaric data, then *P<sub>k</sub><sup>0</sup>* was calculated from Antoine's equation. The critical constants and the Antoine's constants used in this paper are given in Table 1. These constants were taken from the Thermodynamic Research Center.<sup>15</sup>

In mixtures Eq. (1) is supplemented with the chemical term *f<sub>k,chem</sub><sup>E</sup>*:

$$f_{k,chem}^E = f_{k,chem} - f_{k,chem}^0 + \Delta_k, \quad (6)$$

where *f<sub>k,chem</sub>* and *f<sub>k,chem</sub><sup>0</sup>* result from association in the mixture and in the pure component, respectively. The general expression for *f<sub>k,chem</sub>* applicable to various types of association is given in a paper of Góral.<sup>4</sup> The particular form used in this work results from the assumption that self-association of the alcohol can be described with the model of Mecke and Kempter.<sup>16</sup> For mixture of the alcohol C<sub>*i*</sub>H<sub>2*i*+1</sub>OH and the alkane C<sub>*j*</sub>H<sub>2*j*+2</sub>, this model leads to the following equations:

$$f_{i,chem} = RT \ln(1 + K_{ii} p_i^*) - (V_i - b_i) P_{chem}, \quad (7)$$

$$f_{j,chem} = -(V_j - b_j) P_{chem}, \quad (8)$$

where *V<sub>i</sub>*, *V<sub>j</sub>* are molar volumes of the pure components calculated with RK EoS, *K<sub>ii</sub>* is the constant of self-association of the *i*th alcohol, and *P<sub>chem</sub>* and *p<sub>i</sub><sup>\*</sup>* are defined as follows:

$$P_{chem} = (1/K_{ii}) \ln(1 + K_{ii} p_i^*) - p_i^*, \quad (9)$$

$$p_i^* = x_i RT / [x_i (V_i - b_i) + x_j (V_j - b_j)]. \quad (10)$$

For pure alcohol the term *f<sub>i,chem</sub><sup>0</sup>* is calculated with the same equations as *f<sub>i,chem</sub>* but using *x<sub>i</sub>* = 1. For hydrocarbon *f<sub>j,chem</sub><sup>0</sup>* is equal to zero by definition. The term  $\Delta_k$  in Eq. (6) is calculated with the formula

$$\Delta_k = (f_{i,chem}^0 / a_{ii}^{0.5}) (a_{ii}^{0.5} / b_i - a_{jj}^{0.5} / b_j) \times \partial [n_i n_j b_i b_j / (n_i b_i + n_j b_j)] / \partial n_k, \quad (11)$$

where *k* is equal to *i* or *j*. The temperature dependence of *K<sub>ii</sub>* is approximated with the van't Hoff equation

$$K_{ii} = K_{ii}^0 \exp[(-\Delta H_i / R)(1/T - 1/313.15)], \quad (12)$$

where *K<sub>ii</sub><sup>0</sup>* is the equilibrium constant at 313.15 K and  $\Delta H_i / R$  is enthalpy of the association divided by the gas constant. Values of *K<sub>ii</sub><sup>0</sup>* and  $\Delta H_i / R$  were the same as used in Góral.<sup>6</sup> They are given in Table 2. Excluded volumes of alcohols (*b<sub>i</sub>*) used in the chemical part, Eqs. (7)–(11) are shifted by some value  $\Delta b_i$  with respect to the excluded volume calculated with Eq. (5) and used in the physical part, Eq. (1). Values of the parameter  $\Delta b_i$  are also given in Table 2.

## 4. Prediction of VLE Data

EoS<sub>C</sub> uses one binary parameter  $\Theta_{ij}$ , defined by Eq. (4).  $\Theta_{ij}$  depends on both *i*th and *j*th components of the mixture,

TABLE 1. Properties of the pure substances: critical temperature ( $T_c$ ), critical pressure ( $P_c$ ), constants of Antoine's equation,  $\ln(P/\text{kPa})=A-B/(T/\text{K}-C)$ , and its temperature range ( $T_{\min}$ ,  $T_{\max}$ )

CAS	$T_c/\text{K}$	$P_c/\text{kPa}$	$A$	$B$	$C$	$T_{\min}$	$T_{\max}$	Name
67-56-1	512.64	8097	16.169 68	3394.19	44.02	258	356	Methanol
811-98-3	512.64	8097	16.034 89	3298.98	49.48	308	348	Methanol- $d_4$
1849-29-2	512.64	8097	15.919 60	3246.58	50.25	308	348	Methan- $d_3$ -ol
1455-13-6	512.64	8097	16.169 68	3394.19	44.02	258	356	Methanol- $d$
64-17-5	513.92	6148	17.145 03	3956.07	35.63	270	370	Ethanol
1516-08-1	513.92	6148	16.702 38	3661.64	48.68	293	353	Ethanol- $d_6$
1859-08-1	513.92	6148	16.662 60	3661.34	47.16	293	343	Ethan- $d_5$ -ol
71-23-8	536.78	5175	16.054 94	3452.06	68.51	287	389	1-propanol
71-36-3	563.05	4423	15.200 98	3137.02	94.38	305	411	1-butanol
71-41-0	588.15	3909	14.512 00	3026.89	105.04	318	433	1-pentanol
111-27-3	611.40	3510	16.084 37	4055.45	76.49	333	452	1-hexanol
111-70-6	631.90	3150	14.054 73	3042.01	127.17	337	450	1-heptanol
111-87-5	652.50	2860	14.297 70	3356.62	121.57	361	494	1-octanol
143-08-8	668.90	2600	16.009 19	4498.79	91.25	377	511	1-nonanol
112-30-1	684.40	2370	13.897 26	3446.97	131.45	385	532	1-decanol
112-53-8	711.70	1990	13.562 88	3462.24	150.64	426	550	1-dodecanol
112-72-1	735.00	1680	12.915 13	3253.34	177.78	424	569	1-tetradecanol
109-66-0	469.69	3365	13.818 33	2477.07	39.95	223	331	Pentane
110-54-3	507.50	3012	13.804 33	2691.08	48.94	248	365	Hexane
142-82-5	540.30	2736	13.858 69	2911.32	56.51	271	397	Heptane
111-65-9	568.83	2487	13.894 50	3108.08	63.77	292	425	Octane
111-84-2	594.70	2280	13.952 05	3291.45	71.33	344	426	Nonane
124-18-5	617.70	2100	14.019 64	3474.03	77.78	331	476	Decane
1120-21-4	639.00	1930	14.039 10	3614.07	85.45	348	499	Undecane
112-40-3	658.20	1780	14.098 39	3774.56	91.31	365	520	Dodecane
629-59-4	691.90	1520	14.133 04	4008.52	105.43	432	529	Tetradecane
629-62-9	706.80	1420	14.157 42	4121.51	111.77	447	546	Pentadecane
544-76-3	720.60	1320	14.169 12	4214.91	118.70	467	563	Hexadecane

whereas the self-association parameters given in Table 2 do not change in mixtures of the same alcohol with various hydrocarbons. Thus the problem of the VLE prediction for a mixture of  $n$ -alcohol  $\text{C}_i\text{H}_{2i+1}\text{OH}$  and  $n$ -alkane  $\text{C}_j\text{H}_{2j+2}$  is reduced to the prediction of  $\Theta_{ij}$ . Once it is known then VLE in the corresponding mixture can be calculated with the EoS. It was found that  $\Theta_{ij}$  is well approximated with the following formula derived by Góral:<sup>6</sup>

$$\Theta_{i,j} = 0.0227 + 5.6/T + 0.0080Z_i - 0.0035Z_j - 0.00203Z_iZ_j \quad (13)$$

The parameters  $Z_i$  and  $Z_j$  are calculated with the following equations:

$$Z_i = (i-3)(a_{ii}/a_{4,4})^{-0.5}, \quad (14)$$

$$Z_j = (j-6)(a_{jj}/a_{7,7})^{-0.5}, \quad (15)$$

where  $a_{4,4}$ ,  $a_{ii}$ ,  $a_{7,7}$ , and  $a_{jj}$  are energetic parameters of butanol, the  $i$ th alcohol, heptane, and the  $j$ th alkane, respectively. The particular form of Eqs. (14) and (15) results from the fact that propanol, butanol, hexane, and heptane were chosen as the reference substances.

Ratios  $(a_{ii}/a_{4,4})$  and  $(a_{jj}/a_{7,7})$  occurring in Eqs. (14) and (15) were assumed to be independent of temperature and were approximated with the formulas

$$(a_{ii}/a_{4,4})^{0.5} = 0.5656 + 0.0730i^{1.25}, \quad (16)$$

TABLE 2. Parameters of the self-association model of alcohols: self-2 enthalpy of self-association divided by gas constant ( $\Delta H/R$ ), constant of self-association at 313.15 K ( $K_{ii}^0$ ), and shift of the parameter  $b$  used in the association part with respect to  $b$  used in Redlich-Kwong equation of state ( $\Delta b$ ).

$-\Delta H/R$	$K_{ii}^0/\text{MPa}^{-1}$	$\Delta b/\text{cm}^3$	Alcohol
2700	0.90	2.1	methanol- $d$
2700	0.85	2.1	methanol- $d_4$ ; methan- $d_3$ -ol
2700	0.85	2.1	Methanol
2700	0.49	-3.3	ethan- $d_5$ -ol
2700	0.52	-3.3	ethanol- $d_6$
2700	0.47	-3.3	ethanol
2700	0.47	-10.0	propanol
2700	0.47	$-(i-2)9.0$	$n$ -alkanols $\text{C}_i\text{H}_{2i+1}\text{OH}$ ( $3 < i < 15$ )

$$(a_{jj}/a_{7,7})^{0.5} = 0.197 + 0.0774j^{1.20}. \quad (17)$$

The accuracy of the prediction with Eq. (13) was compared with the accuracy of the correlation in the paper.<sup>6</sup> To this end 183 isothermal data sets have been used, within the temperature range from 278 to 383 K. They were taken from the data collection<sup>5</sup> containing the verified VLE data. For all these mixtures both the prediction and correlation were done with parameters  $\Delta H_i/R$ ,  $K_{ii}$ , and  $\Delta b_i$  given in Table 2. In the case of the correlation  $\Theta_{ij}$  was adjusted to each data set individually, in the case of the prediction  $\Theta_{ij}$  was calculated by Eq. (13). Standard deviations of pressure  $\sigma$  resulting from the prediction and from the correlation were calculated by Eq. (18)

$$\sigma = \left[ \sum_{k=1}^{N-n} (P_{\text{exper.}} - P_{\text{calc.}})_k^2 / (N-n-m) \right]^{0.5}, \quad (18)$$

where  $P_{\text{exper.}}$  is experimental pressure,  $P_{\text{calc.}}$  is calculated pressure,  $N$  is total number of the experimental points in the data set,  $n$  is number of data points for pure substances, and  $m$  is number of the adjustable parameters. In the case of correlation  $m=1$ , in the case of prediction  $m=0$  was used.

Both isothermal and isobaric data were treated in a uniform way in the respect that the vapor pressure and vapor composition were adjusted to liquid composition and temperature via EoS. Hence accuracy of the VLE description for both types of data is characterized by the standard deviation of pressure calculated by Eq. (18).

The value of  $\sigma$  divided by average pressure in the corresponding data set and expressed in percent averaged for the 183 data sets was equal 0.87% in the case of the prediction and 0.66% for the correlation. The details are given in the paper by Góral.<sup>6</sup> This small difference between the correlation and the prediction indicates an excellent accuracy of the prediction as well as the absence of significant systematic errors in the data selected in the data collection.<sup>5</sup> This conclusion is based on the fact that the standard deviation of the correlation depends mainly on scattering of the data points, whereas the standard deviation of the prediction is additionally increased by systematic errors in the data and errors of the prediction. Thus the error of the prediction cannot be estimated from the standard deviation alone. One should rather consider the difference between the standard deviations of the prediction and the correlation.

## 5. Description of Tables Containing the Recommended Data

Each system is presented on a separate sheet, which includes a table of VLE data, the corresponding figures, and auxiliary information. The VLE data are presented in a series of tables—Tables 3.1–3.39—with each table being accompanied by two figures (pressure versus mole fraction and temperature versus mole fraction). In the tables and figures, 1 for the component refers to the first chemical species listed un-

der the subtitle “Components,” whereas 2 refers to the second chemical species listed under the subtitle “Components.”

The verification procedure, described above, discarded more than half of the investigated data sets. For some systems, however, the remaining amount of data is still too large and must undergo further selection. In such cases the following criteria were used:

- (1) In the table for a given system the highest and the lowest isotherms are printed. The third isotherm is selected in nearly half of the temperature intervals. The difference between isotherms should be at least 15 K. The fourth set selected is the isobaric data set, preferably at a pressure equal to 101.32 kPa.
- (2) In the case of replicate (or measured within small range) experimental data sets, which passed the verification, the set with the smallest standard deviation in pressure (as obtained from correlation with the EoS) is selected.
- (3) If the standard deviations are similar then data with reported compositions of the vapor phase are selected and/or with greater number of experimental points.

For many systems, however, there are not enough data to fill the corresponding table with the three isotherms and the isobaric data set. In such a case the table is completed with the predicted “artificial” data provided that at least one positively evaluated experimental data set is available for a given system. The artificial data sets are specified as “predicted.” The isobaric artificial data are calculated using the equation  $\Theta = \alpha + \beta/T$  where  $\alpha$  and  $\beta$  are determined on the basis of Eq. (13). The equations for  $\Theta_0$  are given below the data set. The isothermal predicted data set is accompanied by value of  $\Theta_0$  used for the prediction.

To estimate the accuracy of the prediction the experimental data sets are accompanied by the auxiliary parameters  $\Theta_1$ ,  $\sigma_1$ ,  $\Theta_0$ , and  $\sigma_0$ , where  $\Theta_0$  is calculated by Eq. (13),  $\Theta_1$  is adjusted to the experimental data set and  $\sigma_0$ ,  $\sigma_1$  are corresponding standard deviations of pressure calculated by Eq. (18). The same four parameters characterize the isobaric data. As was found in Góral,<sup>6</sup> the temperature dependence of  $\Theta$  can be ignored during the correlation of the isobaric data. In this case  $\Theta_1$  corresponds to some average temperature in the given data set. Consequently, a prediction is also made with constant  $\Theta$  calculated with Eq. (13) at an average temperature defined as the arithmetic mean of the experimental boiling temperatures reported for the given data set.

For all the mixtures both the prediction and the correlation were done with parameters  $\Delta H_i/R$ ,  $K_{ii}$ , and  $\Delta b_i$  given in Table 2.

If experimental vapor concentration  $y$  is not reported for the selected data set then the experimental data are appended with the calculated values of  $y$ . These values are not shown in the figures to differentiate them from the experimental points. The only points shown in the figures correspond to experimental values. The approximating lines are calculated from  $\Theta_1$  adjusted to the data. For the artificial data sets only the curves calculated with the predicted  $\Theta$  are shown.

## 6. Conclusions

The complete collection of data sets for the 39 systems given in this paper is internally consistent, because separate data sets for various mixtures are approximated very well within the same Eq. (13). This statement is supported by the good agreement of  $\Theta_1$  and  $\Theta_0$  given below each experimental data set. The values of  $\Theta_1$ , adjusted individually to the data, and  $\Theta_0$ , calculated with Eq. (13), describe the experimental data with similar accuracy as is shown by values of the corresponding standard deviations  $\sigma_1$  and  $\sigma_0$ . The good accuracy of the prediction demonstrated on the experimental data leads us to believe in a good accuracy for the predicted data used to fill the experimental gaps in the tables.

## 7. Acknowledgments

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3. Recommended VLE Data for *n*-alcohol+*n*-alkane Systems

 TABLE 3.1. Methanol-*d*<sub>4</sub>-hexane

Components			References								
Methanol- <i>d</i> <sub>4</sub> , CD <sub>4</sub> O [811-98-3]			<sup>1</sup> H. Wolff, O. Bauer, R. Goetz, H. Landeck, O. Schiller, and L. Schimpf,								
Hexane, C <sub>6</sub> H <sub>14</sub> [110-54-3]			J. Phys. Chem. <b>80</b> , 131 (1976).								
Reference vapor-liquid equilibrium data											
T/K=308.15, Ref. 1			T/K=323.15, Ref. 1			T/K=343.15, predicted			P/kPa=101.32, predicted		
P/kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	P/kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	P/kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	T/K	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
30.60	0.0000	0.0000	53.94	0.0000	0.0000	105.11	0.00	0.0000	342.11	0.00	0.0000
45.94	0.0146	0.3267	78.46	0.0146	0.3049	178.44	0.05	0.4139	326.13	0.05	0.4199
47.40	0.0187	0.3497	82.18	0.0187	0.3337	195.64	0.10	0.4715	324.49	0.10	0.4580
49.53	0.0281	0.3820	87.58	0.0281	0.3762	202.79	0.15	0.4949	323.96	0.15	0.4718
49.92	0.0306	0.3878	88.55	0.0306	0.3841	206.46	0.20	0.5078	323.71	0.20	0.4789
51.77	0.0497	0.4152	93.59	0.0497	0.4229	208.56	0.25	0.5161	323.59	0.25	0.4833
52.13	0.0594	0.4231	94.69	0.0594	0.4344	209.83	0.30	0.5219	323.52	0.30	0.4863
52.82	0.0691	0.4289	95.57	0.0691	0.4431	210.61	0.35	0.5263	323.48	0.35	0.4885
53.17	0.0794	0.4337	97.23	0.0794	0.4503	211.10	0.40	0.5298	323.46	0.40	0.4901
53.72	0.0965	0.4396	98.39	0.0965	0.4591	211.37	0.45	0.5327	323.46	0.45	0.4913
54.06	0.1150	0.4441	99.09	0.1150	0.4660	211.50	0.50	0.5352	323.45	0.50	0.4921
54.09	0.1200	0.4450	99.34	0.1200	0.4675	211.53	0.55	0.5373	323.46	0.55	0.4927
54.25	0.1340	0.4474	99.79	0.1340	0.4713	211.46	0.60	0.5393	323.46	0.60	0.4931
54.54	0.1460	0.4491	100.06	0.1460	0.4739	211.31	0.65	0.5413	323.46	0.65	0.4933
54.80	0.2350	0.4565	101.46	0.2350	0.4856	211.05	0.70	0.5434	323.46	0.70	0.4934
54.82	0.2480	0.4571	101.47	0.2480	0.4866	210.57	0.75	0.5464	323.48	0.75	0.4940
54.85	0.3700	0.4610	101.66	0.3700	0.4927	209.54	0.80	0.5514	323.54	0.80	0.4963
54.89	0.4850	0.4626	101.67	0.4850	0.4955	207.07	0.85	0.5617	323.76	0.85	0.5035
54.90	0.5450	0.4629	101.70	0.5450	0.4964	200.49	0.90	0.5863	324.53	0.90	0.5262
54.96	0.6040	0.4630	101.70	0.6040	0.4968	181.58	0.95	0.6581	327.26	0.95	0.6054
54.76	0.7180	0.4626	101.69	0.7180	0.4975	121.56	1.00	1.0000	338.46	1.00	1.0000
54.12	0.8670	0.4734	99.06	0.8670	0.5114						
41.29	0.9700	0.6252	76.67	0.9700	0.6667						
26.81	1.0000	1.0000	53.49	1.0000	1.0000						

$\Theta_1 = 0.0514$	$\sigma_1 = 0.32$ kPa	$\Theta_1 = 0.0521$	$\sigma_1 = 0.93$ kPa		
$\Theta_0 = 0.0520$	$\sigma_0 = 0.33$ kPa	$\Theta_0 = 0.0511$	$\sigma_0 = 0.98$ kPa	$\Theta_0 = 0.0501$	$\Theta_0 = 0.0338 + 5.6/T$

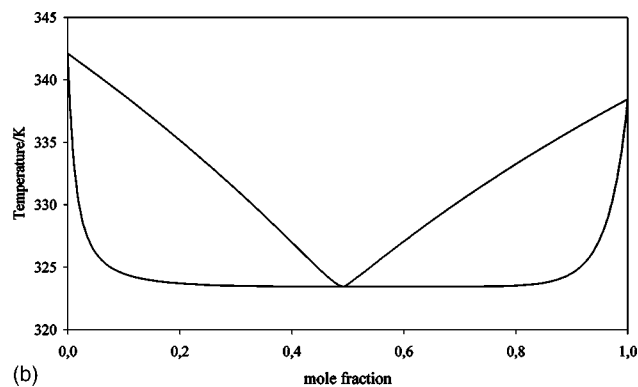
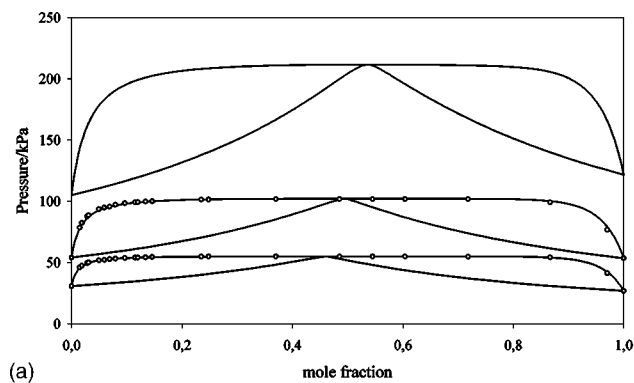


TABLE 3.2. Methan- $d_3$ -ol-hexane

Components			References								
Methan- $d_3$ -ol, CHD <sub>3</sub> O [1849-29-2]			<sup>1</sup> H. Wolff, O. Bauer, R. Goetz, H. Landeck, O. Schiller, and L. Schimpf,								
Hexane, C <sub>6</sub> H <sub>14</sub> [110-54-3]			J. Phys. Chem. <b>80</b> , 131 (1976).								
Reference vapor-liquid equilibrium data											
T/K=308.15, Ref. 1			T/K=323.15, Ref. 1			T/K=343.15, Ref. 1			P/kPa=101.32, predicted		
P/kPa	$x_1$	$y_{1,calc}$	P/kPa	$x_1$	$y_{1,calc}$	P/kPa	$x_1$	$y_{1,calc}$	T/K	$x_1$	$y_1$
30.61	0.0000	0.0000	54.01	0.0000	0.0000	105.06	0.0000	0.0000	342.13	0.00	0.0000
44.57	0.0108	0.3053	74.47	0.0108	0.2743	133.40	0.0108	0.2268	325.88	0.05	0.4254
46.60	0.0149	0.3391	79.33	0.0149	0.3144	141.91	0.0149	0.2707	324.22	0.10	0.4636
50.16	0.0277	0.3921	88.42	0.0277	0.3825	164.93	0.0277	0.3542	323.67	0.15	0.4774
51.45	0.0358	0.4090	91.65	0.0358	0.4058	174.31	0.0358	0.3856	323.42	0.20	0.4847
53.04	0.0509	0.4278	95.47	0.0509	0.4326	186.36	0.0509	0.4239	323.29	0.25	0.4892
53.22	0.0552	0.4314	96.06	0.0552	0.4379	188.48	0.0552	0.4319	323.21	0.30	0.4924
53.94	0.0689	0.4403	97.83	0.0689	0.4511	194.24	0.0689	0.4518	323.17	0.35	0.4948
54.33	0.0785	0.4449	98.78	0.0785	0.4579	197.16	0.0785	0.4624	323.15	0.40	0.4967
55.01	0.1000	0.4521	100.45	0.1000	0.4689	202.30	0.1000	0.4799	323.13	0.45	0.4982
55.26	0.1210	0.4567	101.19	0.1210	0.4761	204.78	0.1210	0.4917	323.13	0.50	0.4995
55.72	0.1700	0.4633	102.50	0.1700	0.4865	209.32	0.1700	0.5091	323.13	0.55	0.5006
55.86	0.2080	0.4664	103.14	0.2080	0.4914	211.18	0.2080	0.5176	323.14	0.60	0.5016
55.97	0.2240	0.4673	103.31	0.2240	0.4930	211.88	0.2240	0.5203	323.15	0.65	0.5026
56.02	0.2840	0.4700	103.60	0.2840	0.4974	213.14	0.2840	0.5283	323.17	0.70	0.5037
56.05	0.3380	0.4715	103.63	0.3380	0.5002	213.72	0.3380	0.5333	323.21	0.75	0.5055
56.06	0.4050	0.4728	103.70	0.4050	0.5026	214.17	0.4050	0.5379	323.31	0.80	0.5093
56.06	0.4650	0.4736	103.71	0.4650	0.5041	214.36	0.4650	0.5411	323.59	0.85	0.5186
56.09	0.5500	0.4741	103.74	0.5500	0.5058	214.36	0.5500	0.5449	324.41	0.90	0.5438
56.10	0.6100	0.4742	103.76	0.6100	0.5066	214.38	0.6100	0.5472	327.11	0.95	0.6247
56.08	0.6710	0.4741	103.71	0.6710	0.5074	214.12	0.6710	0.5496	337.62	1.00	1.0000
56.08	0.7260	0.4741	103.60	0.7260	0.5085	213.80	0.7260	0.5523			
56.06	0.7570	0.4745	103.50	0.7570	0.5095	213.38	0.7570	0.5544			
56.04	0.7750	0.4749	103.32	0.7750	0.5104	213.00	0.7750	0.5560			
55.89	0.8090	0.4767	103.07	0.8090	0.5132	211.81	0.8090	0.5603			
55.45	0.8560	0.4832	101.75	0.8560	0.5217	208.88	0.8560	0.5713			
53.49	0.9070	0.5055	97.90	0.9070	0.5470	200.56	0.9070	0.6001			
50.46	0.9370	0.5400	92.41	0.9370	0.5836	189.54	0.9370	0.6385			
47.18	0.9560	0.5836	86.75	0.9560	0.6279	179.00	0.9560	0.6824			
35.93	0.9870	0.7704	68.13	0.9870	0.8043	145.89	0.9870	0.8425			
28.13	1.0000	1.0000	55.86	1.0000	1.0000	125.59	1.0000	1.0000			
$\Theta_1 = 0.0536$	$\sigma_1 = 0.18$ kPa	$\Theta_1 = 0.0534$	$\sigma_1 = 0.64$ kPa	$\Theta_1 = 0.0524$	$\sigma_1 = 2.41$ kPa						
$\Theta_0 = 0.0520$	$\sigma_0 = 0.43$ kPa	$\Theta_0 = 0.0511$	$\sigma_0 = 0.98$ kPa	$\Theta_0 = 0.0501$	$\sigma_0 = 2.88$ kPa				$\Theta_0 = 0.0338 + 5.6/T$		

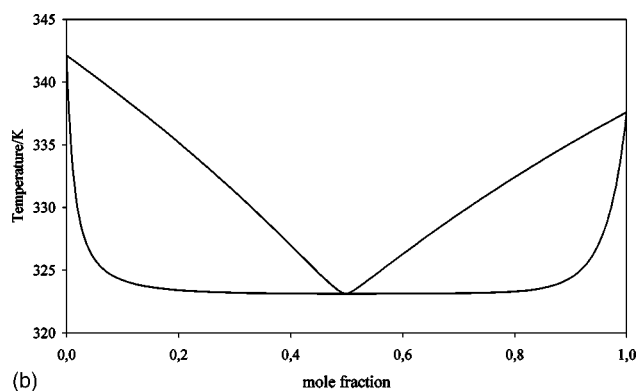
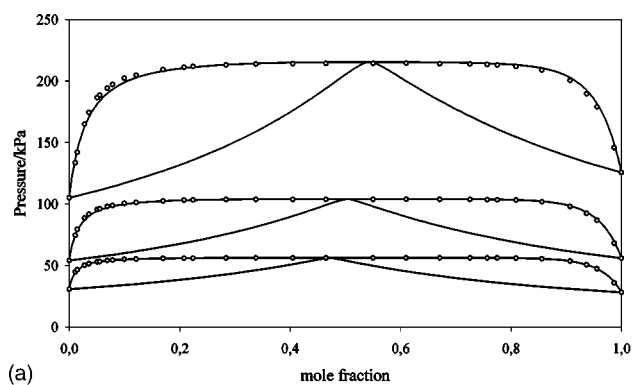




TABLE 3.3. Methanol-*d*-hexane

Components			References								
Methanol- <i>d</i> , CH <sub>3</sub> DO [1455-13-6]			<sup>1</sup> H. Wolff and H. E. Hoeppe, Ber. Bunsen Ges. Phys. Chem. <b>72</b> , 722 (1968).								
Hexane, C <sub>6</sub> H <sub>14</sub> [110-54-3]											
Reference vapor-liquid equilibrium data											
T/K=308.15, Ref. 1			T/K=323.15, Ref. 1			T/K=343.15, Ref. 1			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
30.637	0.0000	0.0000	54.049	0.0000	0.0000	105.32	0.00	0.0000	342.04	0.00	0.0000
42.463	0.0089	0.2740	71.327	0.0089	0.2443	178.03	0.05	0.4113	326.42	0.05	0.4122
45.676	0.0145	0.3246	77.900	0.0145	0.3036	194.39	0.10	0.4668	324.88	0.10	0.4488
47.569	0.0200	0.3531	83.153	0.0200	0.3396	201.14	0.15	0.4894	324.37	0.15	0.4621
48.676	0.0260	0.3731	85.953	0.0260	0.3662	204.61	0.20	0.5020	324.14	0.20	0.4691
50.343	0.0372	0.3957	90.499	0.0372	0.3974	206.62	0.25	0.5101	324.02	0.25	0.4734
51.222	0.0463	0.4070	92.726	0.0463	0.4136	207.84	0.30	0.5160	323.96	0.30	0.4764
52.169	0.0616	0.4192	94.952	0.0616	0.4315	208.62	0.35	0.5205	323.92	0.35	0.4787
52.196	0.0640	0.4206	95.006	0.0640	0.4337	209.10	0.40	0.5242	323.90	0.40	0.4804
52.836	0.0792	0.4279	96.605	0.0792	0.4446	209.39	0.45	0.5274	323.89	0.45	0.4817
53.316	0.0968	0.4337	97.699	0.0968	0.4534	209.52	0.50	0.5302	323.89	0.50	0.4828
54.009	0.1360	0.4415	99.232	0.1360	0.4655	209.54	0.55	0.5328	323.90	0.55	0.4836
54.222	0.1800	0.4465	100.125	0.1800	0.4733	209.45	0.60	0.5353	323.90	0.60	0.4842
54.382	0.2260	0.4498	100.338	0.2260	0.4785	209.24	0.65	0.5379	323.91	0.65	0.4846
54.409	0.2840	0.4526	100.765	0.2840	0.4829	208.89	0.70	0.5408	323.91	0.70	0.4850
54.422	0.3370	0.4544	100.778	0.3370	0.4858	208.26	0.75	0.5447	323.94	0.75	0.4859
54.422	0.4000	0.4562	100.858	0.4000	0.4886	207.03	0.80	0.5508	324.00	0.80	0.4883
54.436	0.4910	0.4581	100.858	0.4910	0.4916	204.29	0.85	0.5623	324.24	0.85	0.4958
54.422	0.5940	0.4597	100.872	0.5940	0.4945	197.47	0.90	0.5883	325.03	0.90	0.5187
54.396	0.6330	0.4602	100.805	0.6330	0.4955	178.61	0.95	0.6614	327.82	0.95	0.5988
54.342	0.7430	0.4620	100.725	0.7439	0.4992	120.18	1.00	1.0000	339.25	1.00	1.0000
54.302	0.7740	0.4632	100.485	0.7740	0.5012						
54.302	0.7760	0.4633	100.485	0.7760	0.5014						
53.316	0.8660	0.4757	98.192	0.8660	0.5174						
50.543	0.9170	0.5050	92.912	0.9170	0.5501						
47.449	0.9420	0.5404	87.433	0.9420	0.5874						
35.330	0.9820	0.7134	66.915	0.9820	0.7549						
26.544	1.0000	1.0000	53.302	1.0000	1.0000						
$\Theta_1 = 0.0515$	$\sigma_1 = 0.37$ kPa		$\Theta_1 = 0.0515$	$\sigma_1 = 0.97$ kPa							
$\Theta_0 = 0.0520$	$\sigma_0 = 0.38$ kPa		$\Theta_0 = 0.0511$	$\sigma_0 = 0.96$ kPa		$\Theta_0 = 0.0501$				$\Theta_0 = 0.0338 + 5.6/T$	

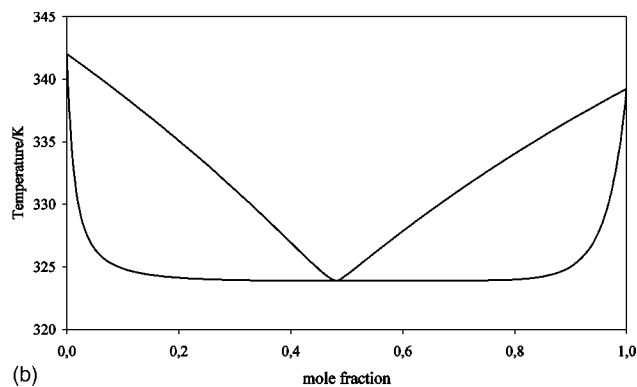
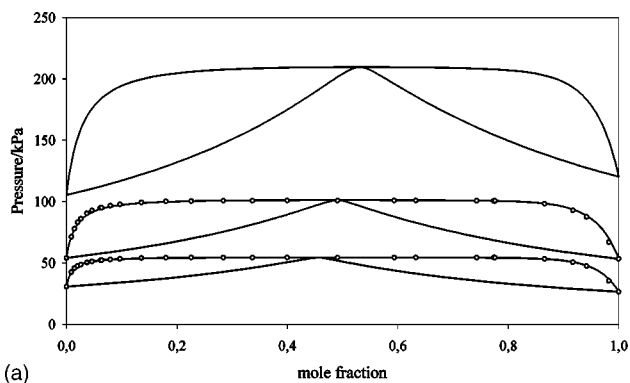


TABLE 3.4. Methanol–hexane

Components			References								
Methanol, CH <sub>4</sub> O [67-56-1]			<sup>1</sup> M. Goral, P. Oracz, and S. Warycha, Fluid Phase Equilib. <b>169</b> , 85 (2000).								
Hexane, C <sub>6</sub> H <sub>14</sub> [110-54-3]			<sup>2</sup> H. Wolff and H. E. Hoeppe, Ber. Bunsen Ges. Phys. Chem. <b>72</b> , 710 (1968).								
Reference vapor–liquid equilibrium data											
T/K=293.15, Ref. 1			T/K=313.15, Ref. 2			T/K=333.15, Ref. 2			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
16.159	0.000 00	0.0000	37.25	0.0000	0.0000	76.23	0.0000	0.0000	342.09	0.00	0.0000
16.187	0.000 03	0.0033	52.24	0.0106	0.2895	99.17	0.0106	0.2453	326.04	0.05	0.4213
16.341	0.000 27	0.0283	56.16	0.0154	0.3311	108.47	0.0154	0.2944	324.39	0.10	0.4594
16.587	0.000 76	0.0714	60.93	0.0286	0.3881	123.14	0.0286	0.3701	323.86	0.15	0.4732
21.082	0.006 09	0.2673	62.53	0.0365	0.4058	128.31	0.0365	0.3959	323.61	0.20	0.4804
22.369	0.008 29	0.2983	64.36	0.0513	0.4262	134.39	0.0513	0.4270	323.48	0.25	0.4849
25.534	0.024 43	0.3789	65.01	0.0583	0.4326	136.79	0.0583	0.4373	323.41	0.30	0.4879
26.508	0.041 42	0.4020	66.21	0.0809	0.4465	140.57	0.0809	0.4600	323.37	0.35	0.4901
27.415	0.071 20	0.4174	66.36	0.0817	0.4469	141.08	0.0817	0.4606	323.35	0.40	0.4918
27.496	0.085 99	0.4213	67.39	0.1200	0.4591	144.35	0.1200	0.4812	323.34	0.45	0.4931
27.647	0.102 28	0.4244	68.13	0.1650	0.4666	146.91	0.1650	0.4943	323.34	0.50	0.4941
27.971	0.148 30	0.4295	68.39	0.2080	0.4708	148.20	0.2080	0.5019	323.34	0.55	0.4948
27.871	0.859 20	0.4479	68.57	0.2680	0.4747	149.13	0.2680	0.5089	323.35	0.60	0.4953
27.171	0.900 70	0.4636	68.66	0.2940	0.4759	149.45	0.2940	0.5112	323.35	0.65	0.4957
25.459	0.934 90	0.4973	68.69	0.4080	0.4795	149.67	0.4080	0.5181	323.36	0.70	0.4962
24.069	0.950 20	0.5273	68.71	0.5490	0.4821	149.67	0.5490	0.5237	323.38	0.75	0.4971
20.873	0.972 00	0.6104	68.75	0.6200	0.4830	149.68	0.6200	0.5260	323.45	0.80	0.4998
16.588	0.989 89	0.7766	68.63	0.7440	0.4850	149.13	0.7440	0.5311	323.69	0.85	0.5076
15.020	0.994 30	0.8530	68.62	0.7680	0.4860	149.11	0.7680	0.5329	324.48	0.90	0.5310
13.874	0.997 13	0.9172	68.22	0.8100	0.4890	147.97	0.8100	0.5377	327.20	0.95	0.6107
13.350	0.998 95	0.9672	66.89	0.8840	0.5068	143.57	0.8840	0.5599	338.21	1.00	1.0000
13.306	0.999 20	0.9747	64.81	0.9170	0.5303	138.62	0.9170	0.5860			
13.158	0.999 62	0.9877	57.38	0.9550	0.5984	124.32	0.9550	0.6559			
13.004	1.000 00	1.0000	50.32	0.9750	0.6853	111.07	0.9750	0.7385			
			35.32	1.0000	1.0000	84.33	1.0000	1.0000			
$\Theta_1 = 0.0520$	$\sigma_1 = 0.35$ kPa	$\Theta_1 = 0.0519$	$\sigma_1 = 0.30$ kPa	$\Theta_1 = 0.0513$	$\sigma_1 = 1.49$ kPa						
$\Theta_0 = 0.0529$	$\sigma_0 = 0.38$ kPa	$\Theta_0 = 0.0517$	$\sigma_0 = 0.30$ kPa	$\Theta_0 = 0.0506$	$\sigma_0 = 1.50$ kPa	$\Theta_0 = 0.0338 + 5.6/T$					

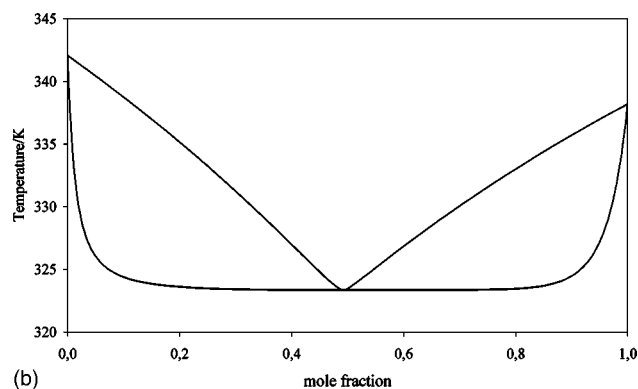
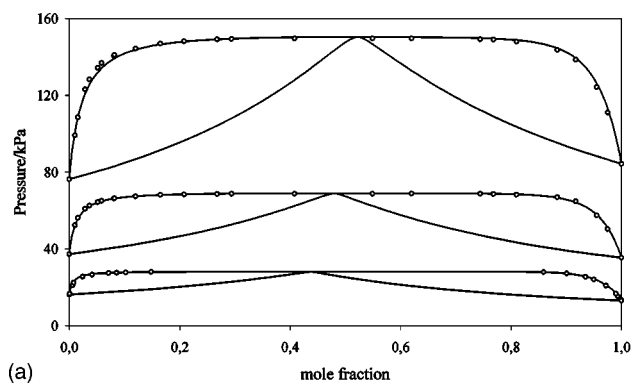


TABLE 3.5. Ethanol-*d*<sub>6</sub>-hexane

Components			References								
Ethanol- <i>d</i> <sub>6</sub> , C <sub>2</sub> D <sub>6</sub> O [1519-08-01]			<sup>1</sup> H. Wolff and R. Goetz, Z. Phys. Chem. (Frankfurt) <b>100</b> , 25 (1976).								
Hexane, C <sub>6</sub> H <sub>14</sub> [110-54-3]											
Reference vapor-liquid equilibrium data											
T/K=293.15, Ref. 1			T/K=313.15, Ref. 1			T/K=333.15, Ref. 1			P/kPa=101.32, predicted		
P/kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	P/kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	P/kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	T/K	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
16.13	0.0000	0.0000	37.25	0.0000	0.0000	76.29	0.0000	0.0000	342.06	0.00	0.0000
17.68	0.0050	0.0829	40.88	0.0050	0.0713	81.37	0.0050	0.0579	334.49	0.05	0.2362
18.56	0.0142	0.1410	43.93	0.0142	0.1403	88.57	0.0142	0.1272	332.97	0.10	0.2862
18.87	0.0200	0.1586	44.97	0.0200	0.1656	91.53	0.0200	0.1568	332.42	0.15	0.3077
19.07	0.0249	0.1687	45.50	0.0249	0.1813	93.79	0.0249	0.1767	332.18	0.20	0.3201
19.60	0.0516	0.1953	47.17	0.0516	0.2272	99.70	0.0516	0.2414	332.06	0.25	0.3285
19.73	0.0660	0.2018	47.70	0.0660	0.2396	101.41	0.0660	0.2609	332.02	0.30	0.3349
19.76	0.0689	0.2028	47.86	0.0689	0.2416	102.06	0.0689	0.2642	332.01	0.35	0.3403
19.87	0.0876	0.2080	48.28	0.0876	0.2518	103.18	0.0876	0.2812	332.03	0.40	0.3450
19.91	0.1063	0.2116	48.54	0.1063	0.2590	103.98	0.1063	0.2935	332.07	0.45	0.3497
19.97	0.1314	0.2150	49.01	0.1314	0.2658	105.18	0.1314	0.3056	332.14	0.50	0.3546
19.83	0.1575	0.2175	49.17	0.1575	0.2709	105.88	0.1575	0.3148	332.24	0.55	0.3600
19.92	0.1757	0.2189	49.09	0.1757	0.2737	106.19	0.1757	0.3199	332.40	0.60	0.3666
19.91	0.2088	0.2209	49.12	0.2088	0.2777	106.38	0.2088	0.3273	332.63	0.65	0.3749
19.89	0.2602	0.2234	49.14	0.2602	0.2822	106.82	0.2602	0.3357	332.97	0.70	0.3861
19.77	0.3011	0.2251	49.16	0.3011	0.2851	106.99	0.3011	0.3408	333.51	0.75	0.4019
19.80	0.3590	0.2272	49.41	0.3590	0.2884	107.14	0.3590	0.3467	334.37	0.80	0.4258
19.76	0.3807	0.2281	49.38	0.3807	0.2896	107.24	0.3807	0.3487	335.79	0.85	0.4641
19.67	0.5052	0.2337	48.56	0.5052	0.2965	106.24	0.5052	0.3594	338.23	0.90	0.5315
19.56	0.5608	0.2371	48.53	0.5608	0.3005	105.86	0.5608	0.3647	342.71	0.95	0.6664
19.55	0.5958	0.2399	48.40	0.5953	0.3035	105.34	0.5953	0.3686	351.71	1.00	1.0000
19.41	0.6111	0.2413	48.17	0.6111	0.3051	105.12	0.6111	0.3705			
19.20	0.7037	0.2533	47.00	0.7037	0.3182	102.92	0.7037	0.3861			
18.67	0.7501	0.2632	46.00	0.7501	0.3290	100.91	0.7501	0.3984			
18.00	0.7889	0.2752	44.86	0.7889	0.3419	98.70	0.7889	0.4128			
17.44	0.8192	0.2881	43.70	0.8192	0.3559	96.35	0.8192	0.4282			
17.20	0.8304	0.2941	43.25	0.8304	0.3624	95.17	0.8304	0.4352			
15.33	0.8904	0.3445	39.12	0.8904	0.4163	86.75	0.8904	0.4923			
13.87	0.9194	0.3905	35.80	0.9194	0.4642	80.01	0.9194	0.5413			
9.89	0.9680	0.5686	26.96	0.9680	0.6393	62.98	0.9680	0.7076			
5.64	1.0000	1.0000	17.45	1.0000	1.0000	46.04	1.0000	1.0000			

$\Theta_1 = 0.0466$	$\sigma_1 = 0.15$ kPa	$\Theta_1 = 0.0474$	$\sigma_1 = 0.37$ kPa	$\Theta_1 = 0.0462$	$\sigma_1 = 0.91$ kPa
$\Theta_0 = 0.0465$	$\sigma_0 = 0.15$ kPa	$\Theta_0 = 0.0453$	$\sigma_0 = 0.52$ kPa	$\Theta_0 = 0.0442$	$\sigma_0 = 1.13$ kPa
					$\Theta_0 = 0.0274 + 5.6/T$

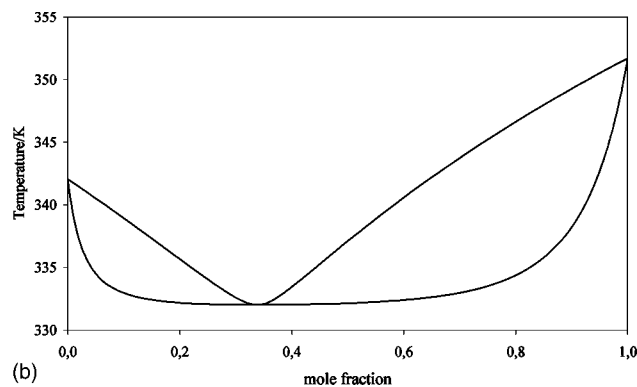
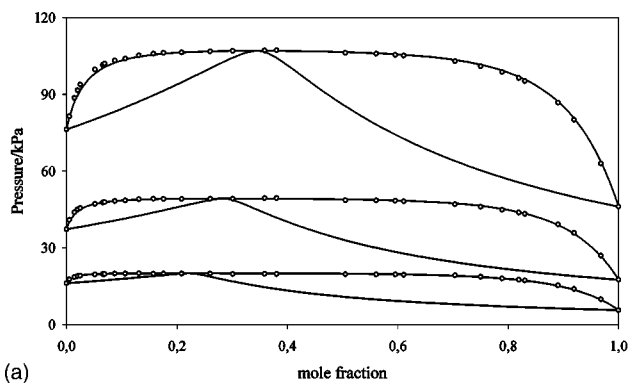


TABLE 3.6. Ethan- $d_5$ -of-hexane

Components			References								
Ethan- $d_5$ -ol, C <sub>2</sub> HD <sub>5</sub> O [1859-08-1]			<sup>1</sup> H. Wolff and R. Goetz, Z. Phys. Chem. (Frankfurt) <b>100</b> , 25 (1976).								
Hexane, C <sub>6</sub> H <sub>14</sub> [110-54-3]											
Reference vapor-liquid equilibrium data											
T/K=293.15, Ref. 1			T/K=313.15, Ref. 1			T/K=333.15, Ref. 1			P/kPa=101.32, predicted		
P/kPa	$x_1$	$y_{1,calc}$	P/kPa	$x_1$	$y_{1,calc}$	P/kPa	$x_1$	$y_{1,calc}$	T/K	$x_1$	$y_1$
16.13	0.0000	0.0000	37.25	0.0000	0.0000	76.29	0.0000	0.0000	342.06	0.00	0.0000
18.00	0.0059	0.0953	40.78	0.0059	0.0805	81.77	0.0059	0.0660	334.29	0.05	0.2415
18.13	0.0067	0.1027	41.24	0.0067	0.0883	82.57	0.0067	0.0732	332.66	0.10	0.2940
18.67	0.0108	0.1315	42.84	0.0108	0.1209	85.86	0.0108	0.1055	332.07	0.15	0.3165
19.27	0.0210	0.1691	45.25	0.0210	0.1713	92.25	0.0210	0.1622	331.81	0.20	0.3293
19.53	0.0290	0.1846	45.93	0.0290	0.1950	95.47	0.0290	0.1924	331.68	0.25	0.3379
19.65	0.0364	0.1941	46.89	0.0364	0.2106	97.74	0.0364	0.2138	331.63	0.30	0.3443
19.73	0.0449	0.2018	47.32	0.0449	0.2240	99.35	0.0449	0.2329	331.61	0.35	0.3496
19.91	0.0601	0.2109	47.93	0.0601	0.2405	101.69	0.0601	0.2580	331.63	0.40	0.3542
19.97	0.0712	0.2154	48.25	0.0712	0.2490	102.82	0.0712	0.2716	331.66	0.45	0.3585
20.04	0.0861	0.2198	48.68	0.0861	0.2575	104.10	0.0861	0.2856	331.72	0.50	0.3631
20.13	0.1021	0.2232	48.93	0.1021	0.2644	104.98	0.1021	0.2972	331.81	0.55	0.3681
20.13	0.1162	0.2256	49.13	0.1162	0.2690	105.79	0.1162	0.3054	331.95	0.60	0.3742
20.27	0.1651	0.2308	49.45	0.1651	0.2798	107.00	0.1651	0.3246	332.16	0.65	0.3819
20.34	0.1936	0.2328	49.60	0.1936	0.2839	107.50	0.1936	0.3321	332.47	0.70	0.3923
20.00	0.2975	0.2373	49.80	0.2975	0.2930	108.22	0.2975	0.3490	332.97	0.75	0.4073
19.96	0.3301	0.2384	49.70	0.3301	0.2950	108.14	0.3301	0.3527	333.78	0.80	0.4301
20.00	0.3609	0.2394	49.69	0.3609	0.2967	108.20	0.3609	0.3557	335.14	0.85	0.4671
19.93	0.4289	0.2416	49.60	0.4289	0.3003	108.08	0.4289	0.3616	337.52	0.90	0.5329
20.04	0.5234	0.2455	49.25	0.5234	0.3057	107.47	0.5234	0.3697	341.95	0.95	0.6661
19.87	0.6046	0.2506	48.73	0.6046	0.3121	106.56	0.6046	0.3781	350.99	1.00	1.0000
19.53	0.7053	0.2623	47.73	0.7053	0.3258	104.28	0.7053	0.3944			
18.96	0.7564	0.2729	46.70	0.7564	0.3378	102.18	0.7564	0.4080			
18.80	0.7737	0.2777	46.08	0.7737	0.3432	100.31	0.7737	0.4140			
18.48	0.8000	0.2868	45.12	0.8000	0.3534	99.39	0.8000	0.4252			
17.92	0.8229	0.2969	44.28	0.8229	0.3647	97.31	0.8229	0.4375			
15.69	0.8961	0.3573	39.14	0.8961	0.4304	87.07	0.8961	0.5066			
14.75	0.9140	0.3850	37.02	0.9140	0.4597	83.02	0.9140	0.5364			
11.24	0.9606	0.5284	29.17	0.9606	0.6036	68.01	0.9606	0.6748			
5.95	1.0000	1.0000	18.05	1.0000	1.0000	47.56	1.0000	1.0000			
$\Theta_1 = 0.0473$	$\sigma_1 = 0.20$ kPa	$\Theta_1 = 0.0462$	$\sigma_1 = 0.31$ kPa	$\Theta_1 = 0.0453$	$\sigma_1 = 1.15$ kPa						
$\Theta_0 = 0.0465$	$\sigma_0 = 0.21$ kPa	$\Theta_0 = 0.0453$	$\sigma_0 = 0.35$ kPa	$\Theta_0 = 0.0442$	$\sigma_0 = 1.19$ kPa					$\Theta_0 = 0.0274 + 5.6/T$	

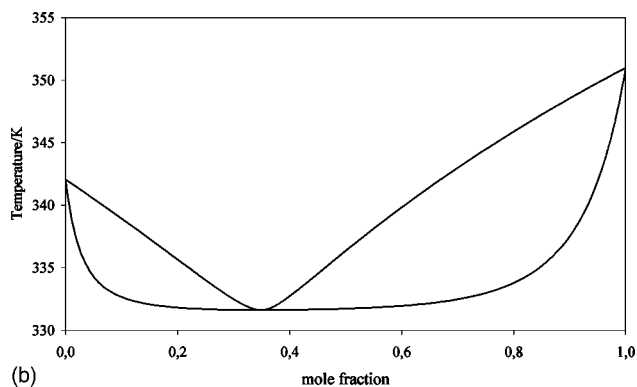
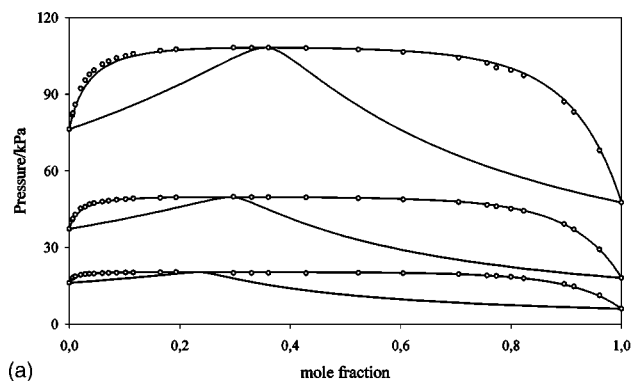


TABLE 3.7. Ethanol–butane

Components			References								
Ethanol, C <sub>2</sub> H <sub>6</sub> O [64-17-5]			<sup>1</sup> G. Dahlhoff, A. Pfennig, H. Hammer, and M. Van Oorschot, J. Chem. Eng. Data <b>45</b> , 887 (2000).								
Butane, C <sub>4</sub> H <sub>10</sub> [106-97-8]											
Reference vapor–liquid equilibrium data											
T/K=273.15, predicted			T/K=293.15, Ref. 1			T/K=313.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
103.27	0.00	0.0000	207.5	0.000	0.000	380.81	0.00	0.0000	272.80	0.00	0.0000
102.83	0.05	0.0098	205.7	0.123	0.025	381.19	0.05	0.0292	272.95	0.05	0.0083
102.39	0.10	0.0105	205.5	0.124	0.025	377.98	0.10	0.0354	273.06	0.10	0.0088
102.01	0.15	0.0108	203.7	0.241	0.026	375.24	0.15	0.0381	273.14	0.15	0.0091
101.61	0.20	0.0111	201.5	0.352	0.025	372.95	0.20	0.0397	273.21	0.20	0.0093
101.14	0.25	0.0113	201.2	0.355	0.025	370.98	0.25	0.0407	273.30	0.25	0.0094
100.57	0.30	0.0116	198.2	0.458	0.025	369.18	0.30	0.0414	273.40	0.30	0.0096
99.84	0.35	0.0118	192.7	0.561	0.025	367.40	0.35	0.0420	273.53	0.35	0.0098
98.92	0.40	0.0121	184.5	0.656	0.026	365.50	0.40	0.0426	273.71	0.40	0.0101
97.73	0.45	0.0124	170.0	0.747	0.030	363.28	0.45	0.0431	273.94	0.45	0.0104
96.21	0.50	0.0128	140.2	0.836	0.039	360.48	0.50	0.0438	274.24	0.50	0.0107
94.25	0.55	0.0133	135.2	0.848	0.042	356.73	0.55	0.0446	274.66	0.55	0.0112
91.70	0.60	0.0140	125.7	0.868	0.046	351.54	0.60	0.0457	275.24	0.60	0.0119
88.39	0.65	0.0148	85.0	0.919	0.067	344.16	0.65	0.0471	276.03	0.65	0.0129
84.04	0.70	0.0159	5.8	1.000	1.000	333.52	0.70	0.0492	277.15	0.70	0.0143
78.32	0.75	0.0175				317.98	0.75	0.0522	278.76	0.75	0.0164
70.71	0.80	0.0199				295.12	0.80	0.0570	281.14	0.80	0.0200
60.51	0.85	0.0239				261.20	0.85	0.0653	284.87	0.85	0.0267
46.71	0.90	0.0319				210.45	0.90	0.0822	291.26	0.90	0.0423
27.80	0.95	0.0553				133.90	0.95	0.1307	304.50	0.95	0.0989
1.59	1.00	1.0000				17.55	1.00	1.0000	352.16	1.00	1.0000
$\Theta_0 = 0.0122$			$\Theta_1 = 0.0121$		$\sigma_1 = 2.16$ kPa		$\Theta_0 = 0.0096$			$\Theta_0 = -0.0083 + 5.6/T$	
			$\Theta_0 = 0.0108$		$\sigma_0 = 2.41$ kPa						

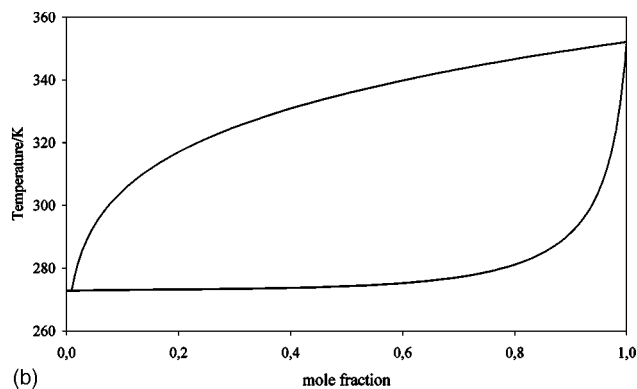
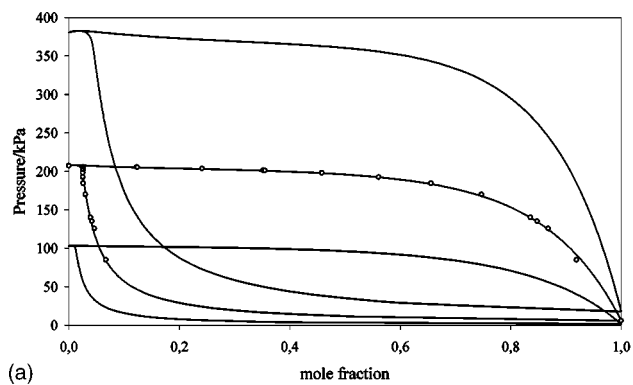


TABLE 3.8. Ethanol–Dentane

Components			References								
Ethanol, C <sub>2</sub> H <sub>6</sub> O [64-17-5]			<sup>1</sup> N. Ishii, J. Soc. Chem. Ind. Jap. <b>38</b> , 659 (1935).								
Pentane, C <sub>5</sub> H <sub>12</sub> [109-66-0]			<sup>2</sup> J. L. Reimers, V. R. Bhethanabotla, and S. W. Campbell, J. Chem. Eng. Data <b>37</b> , 127 (1992).								
Reference vapor–liquid equilibrium data											
T/K=273.15, Ref. 1			T/K=303.15, Ref. 2			T/K=323.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
29.60	0.00	0.0000	81.97	0.0000	0.0000	159.33	0.00	0.0000	309.37	0.00	0.0000
30.24	0.05	0.0366	86.46	0.0252	0.0605	171.01	0.05	0.0932	307.75	0.05	0.0764
30.30	0.10	0.0431	87.06	0.0608	0.0790	172.47	0.10	0.1154	307.69	0.10	0.0889
30.33	0.15	0.0449	87.02	0.0994	0.0865	172.44	0.15	0.1256	307.75	0.15	0.0943
30.34	0.20	0.0457	86.71	0.1613	0.0919	172.01	0.20	0.1316	307.83	0.20	0.0975
30.33	0.25	0.0462	86.31	0.2314	0.0951	171.44	0.25	0.1356	307.91	0.25	0.0998
30.30	0.30	0.0462	85.87	0.3033	0.0972	170.81	0.30	0.1386	308.00	0.30	0.1015
30.20	0.35	0.0464	85.37	0.3737	0.0989	170.14	0.35	0.1411	308.09	0.35	0.1031
30.05	0.40	0.0466	84.61	0.4587	0.1011	169.40	0.40	0.1432	308.20	0.40	0.1045
29.84	0.45	0.0470	84.51	0.4622	0.1012	168.56	0.45	0.1453	308.33	0.45	0.1061
29.61	0.50	0.0473	84.13	0.5017	0.1024	167.53	0.50	0.1475	308.49	0.50	0.1080
29.36	0.55	0.0477	83.98	0.5044	0.1025	166.20	0.55	0.1501	308.71	0.55	0.1103
28.96	0.60	0.0484	83.30	0.5519	0.1043	164.39	0.60	0.1532	309.03	0.60	0.1133
28.41	0.65	0.0490	83.18	0.5542	0.1044	161.84	0.65	0.1573	309.48	0.65	0.1176
27.64	0.70	0.0510	82.19	0.6026	0.1067	158.12	0.70	0.1631	310.17	0.70	0.1238
26.57	0.75	0.0530	82.11	0.6044	0.1068	152.58	0.75	0.1716	311.23	0.75	0.1333
25.06	0.80	0.0570	80.66	0.6533	0.1100	144.19	0.80	0.1848	312.89	0.80	0.1489
22.41	0.85	0.0660	78.47	0.7042	0.1147	131.32	0.85	0.2071	315.63	0.85	0.1764
17.88	0.90	0.0790	75.25	0.7554	0.1217	111.30	0.90	0.2504	320.43	0.90	0.2324
10.60	0.95	0.1510	70.45	0.8069	0.1331	79.75	0.95	0.3590	329.75	0.95	0.3783
1.64	1.00	1.0000	63.33	0.8571	0.1524	29.40	1.00	1.0000	351.61	1.00	1.0000
			55.33	0.8953	0.1792						
			48.24	0.9208	0.2098						
			38.89	0.9471	0.2665						
			30.33	0.9663	0.3474						
			10.51	1.0000	1.0000						
Θ <sub>1</sub> = 0.0341		σ <sub>1</sub> = 0.29 kPa		Θ <sub>1</sub> = 0.0326		σ <sub>1</sub> = 0.41 kPa					
Θ <sub>0</sub> = 0.0333		σ <sub>0</sub> = 0.31 kPa		Θ <sub>0</sub> = 0.0313		σ <sub>0</sub> = 0.64 kPa		Θ <sub>0</sub> = 0.0301		Θ <sub>0</sub> = 0.0128 + 5.6/T	

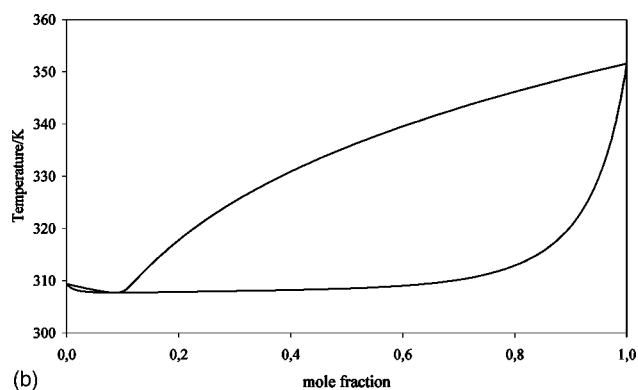
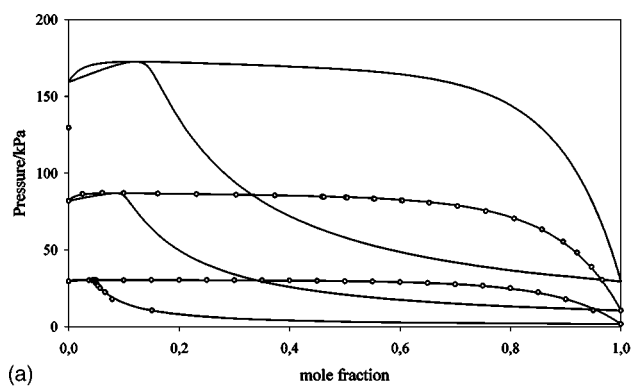


TABLE 3.9. Ethanol–hexane

Components			References								
Ethanol, C <sub>2</sub> H <sub>6</sub> O [64-17-5]			<sup>1</sup> L.-Z. Zhang, G.-H. Chen, Z.-H. Cao, and S.-J. Han, <i>Thermochim. Acta</i> <b>169</b> , 247 (1990).								
Hexane, C <sub>6</sub> H <sub>14</sub> [110-54-3]			<sup>2</sup> B. Janaszewski, P. Oracz, M. Goral, and S. Warycha, <i>Fluid Phase Equilib.</i> <b>9</b> , 295 (1982).								
			<sup>3</sup> H. Wolff and R. Goetz, <i>Z. Phys. Chem. (Frankfurt)</i> <b>100</b> , 25 (1976).								
			<sup>4</sup> L. S. Kudryavtseva and M. P. Susarev, <i>Zh. Prikl. Khim. (Leningrad)</i> <b>36</b> , 1471 (1963).								
Reference vapor–liquid equilibrium data											
T/K=298.15, Ref. 1			T/K=313.15, Ref. 2			T/K=333.15, Ref. 3			P/kPa=101.32, Ref. 4		
P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
25.56	0.1	0.232	37.27	0.0000	0.0000	76.29	0.0000	0.0000	341.90	0.0000	0.000
25.68	0.2	0.240	48.50	0.0944	0.2554	85.59	0.0115	0.1058	332.56	0.0916	0.285
25.68	0.3	0.245	49.15	0.1732	0.2760	89.31	0.0169	0.1372	331.68	0.1979	0.324
25.62	0.4	0.249	49.30	0.2463	0.2847	91.53	0.0224	0.1625	331.54	0.3070	0.329
25.47	0.5	0.254	49.32	0.3076	0.2896	94.87	0.0300	0.1897	331.67	0.4012	0.343
25.14	0.6	0.262	49.27	0.3725	0.2938	98.39	0.0430	0.2230	331.83	0.5001	0.354
24.44	0.7	0.277	49.12	0.4476	0.2983	100.44	0.0595	0.2513	332.17	0.6115	0.365
22.89	0.8	0.306	48.88	0.5054	0.3022	102.52	0.0822	0.2767	332.89	0.7035	0.386
19.09	0.9	0.384	48.55	0.5709	0.3074	103.55	0.0959	0.2877	334.16	0.8102	0.410
			48.09	0.6354	0.3145	103.72	0.1001	0.2906	338.21	0.9007	0.526
			47.31	0.7032	0.3255	104.80	0.1234	0.3039	351.45	1.0000	1.000
			46.23	0.7528	0.3377	105.59	0.1588	0.3179			
			43.96	0.8175	0.3641	106.66	0.2215	0.3335			
			31.00	0.9479	0.5554	107.06	0.2687	0.3413			
			17.90	1.0000	1.0000	107.51	0.3255	0.3484			
						107.35	0.3749	0.3534			
						106.70	0.4847	0.3631			
						105.67	0.5937	0.3739			
						104.11	0.6706	0.3850			
						103.08	0.7163	0.3944			
						101.24	0.7577	0.4062			
						98.06	0.8047	0.4255			
						91.49	0.8617	0.4649			
						81.59	0.9144	0.5359			
						73.01	0.9448	0.6125			
						46.84	1.0000	1.0000			
Θ <sub>1</sub> =0.0448	σ <sub>1</sub> =0.06 kPa	Θ <sub>1</sub> =0.0441	σ <sub>1</sub> =0.06 kPa	Θ <sub>1</sub> =0.0441	σ <sub>1</sub> =1.01 kPa	Θ <sub>1</sub> =0.0441	σ <sub>1</sub> =1.11 kPa				
Θ <sub>0</sub> =0.0462	σ <sub>0</sub> =0.18 kPa	Θ <sub>0</sub> =0.0453	σ <sub>0</sub> =0.25 kPa	Θ <sub>0</sub> =0.0442	σ <sub>0</sub> =0.99 kPa	Θ <sub>0</sub> =0.0443	σ <sub>0</sub> =1.05 kPa				

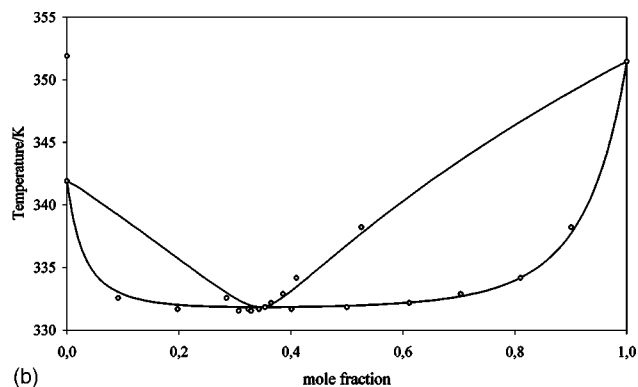
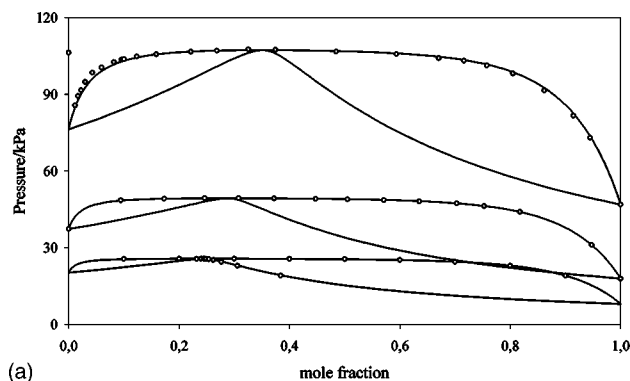


TABLE 3.10. Ethanol–heptane

Components			References								
Ethanol, C <sub>2</sub> H <sub>6</sub> O [64-17-5]			<sup>1</sup> M. Ronc and G. A. Ratcliff, Can. J. Chem. Eng. <b>54</b> , 326 (1976).								
Heptane, C <sub>7</sub> H <sub>16</sub> [142-82-5]			<sup>2</sup> H. C. Van Ness and M. M. Abbott, Int. DATA Ser., Sel. Data Mixtures, Ser. A <b>1</b> , 1 (1977).								
			<sup>3</sup> C. Berro, M. Rogalski, and A. Peneloux, Fluid Phase Equilib. <b>8</b> , 55 (1982).								
			<sup>4</sup> H. C. Van Ness, C. A. Soczek, and N. K. Kochar, J. Chem. Eng. Data <b>12</b> , 346 (1967).								
Reference vapor–liquid equilibrium data											
T/K=303.15, Ref. 1			T/K=323.15, Ref. 2			T/K=343.15, Ref. 3			P/kPa=101.32, Ref. 4		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
7.79	0.0000	0.0000	18.90	0.0000	0.0000	40.53	0.0000	0.0000	371.15	0.000	0.0000
14.78	0.0514	0.4781	31.12	0.0253	0.3896	83.87	0.0976	0.5344	365.22	0.010	0.1669
15.68	0.1556	0.5251	33.43	0.0378	0.4402	84.43	0.1013	0.5371	358.19	0.025	0.3371
15.97	0.2685	0.5364	35.31	0.0540	0.4779	88.77	0.1510	0.5655	351.96	0.050	0.4667
16.05	0.3548	0.5409	37.08	0.0762	0.5076	89.64	0.1666	0.5710	349.45	0.075	0.5110
16.11	0.4223	0.5439	38.13	0.0968	0.5245	91.04	0.1957	0.5807	348.16	0.100	0.5396
16.13	0.4770	0.5465	39.09	0.1244	0.5394	92.37	0.2344	0.5898	345.77	0.200	0.5853
16.13	0.5087	0.5482	39.92	0.1612	0.5520	92.94	0.2547	0.5943	344.99	0.300	0.6029
16.12	0.6036	0.5547	40.70	0.2170	0.5637	93.93	0.3003	0.6018	344.64	0.400	0.6140
16.20	0.6451	0.5588	41.30	0.2903	0.5731	94.15	0.3061	0.6043	344.43	0.500	0.6250
16.11	0.6695	0.5618	41.69	0.3745	0.5804	94.63	0.3419	0.6078	344.37	0.600	0.6302
16.14	0.6795	0.5631	41.93	0.4772	0.5879	94.67	0.3483	0.6089	344.40	0.700	0.6495
16.09	0.7167	0.5692	42.01	0.5523	0.5939	95.52	0.4248	0.6173	344.72	0.800	0.6834
16.07	0.7181	0.5694	42.03	0.6077	0.5993	95.61	0.4303	0.6182	345.80	0.900	0.7449
16.03	0.7516	0.5766	42.02	0.6512	0.6046	95.90	0.4698	0.6227	347.46	0.950	0.8214
15.97	0.7627	0.5795	41.98	0.6851	0.6097	95.98	0.4904	0.6241	348.93	0.975	0.8869
15.83	0.7966	0.5902	41.92	0.7133	0.6148	96.07	0.5046	0.6264	351.45	1.000	1.0000
15.49	0.8488	0.6155	41.90	0.7343	0.6193	96.18	0.5288	0.6282			
14.63	0.9108	0.6749	41.77	0.7569	0.6250	96.21	0.5356	0.6298			
13.70	0.9440	0.7366	41.60	0.7807	0.6321	96.33	0.5671	0.6326			
12.35	0.9743	0.8371	41.35	0.8061	0.6416	96.50	0.6116	0.6381			
11.37	0.9892	0.9178	40.97	0.8332	0.6544	96.42	0.6524	0.6436			
11.03	0.9936	0.9482	40.37	0.8620	0.6725	96.28	0.7116	0.6542			
10.47	1.0000	1.0000	39.39	0.8937	0.7005	96.07	0.7420	0.6613			
			37.77	0.9274	0.7459	95.54	0.7835	0.6735			
			35.24	0.9593	0.8165	94.98	0.8101	0.6833			
			32.69	0.9809	0.8936	94.18	0.8403	0.6985			
			31.71	0.9876	0.9255	92.09	0.8815	0.7267			
			30.98	0.9923	0.9511	88.25	0.9259	0.7767			
			30.30	0.9958	0.9721	80.83	0.9710	0.8742			
			29.92	0.9980	0.9864	79.09	0.9788	0.9001			
			29.73	0.9990	0.9931	75.16	0.9922	0.9569			
			29.59	1.0000	1.0000	74.22	0.9950	0.9713			
						73.51	0.9968	0.9812			
						72.34	1.0000	1.0000			
$\Theta_1 = 0.0555$	$\sigma_1 = 0.08$ kPa	$\Theta_1 = 0.0547$	$\sigma_1 = 0.18$ kPa	$\Theta_1 = 0.0562$	$\sigma_1 = 0.30$ kPa	$\Theta_1 = 0.0600$	$\sigma_1 = 1.72$ kPa				
$\Theta_0 = 0.0566$	$\sigma_0 = 0.11$ kPa	$\Theta_0 = 0.0555$	$\sigma_0 = 0.21$ kPa	$\Theta_0 = 0.0545$	$\sigma_0 = 0.63$ kPa	$\Theta_0 = 0.0544$	$\sigma_0 = 2.55$ kPa				

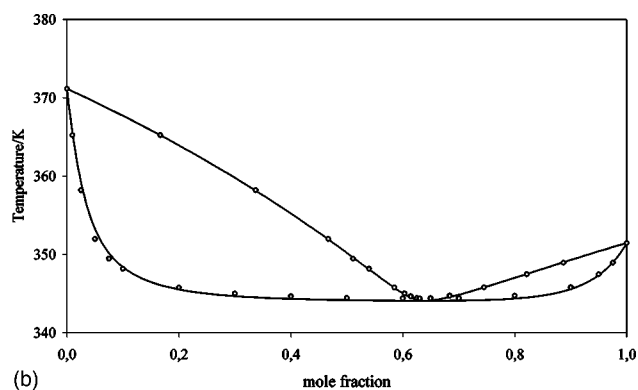
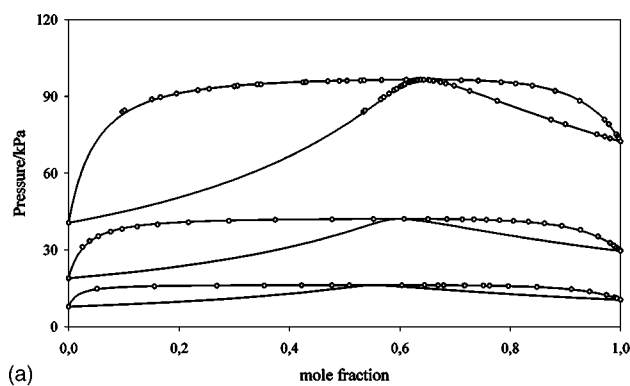




TABLE 3.11. Ethanol–octane

Components			References								
Ethanol, C <sub>2</sub> H <sub>6</sub> O [64-17-5]			<sup>1</sup> B. Janaszewski, P. Oracz, M. Goral, and S. Warycha, Fluid Phase Equilib. <b>9</b> , 295 (1982).								
Octane, C <sub>8</sub> H <sub>18</sub> [111-65-9]			<sup>2</sup> L. Boublikova and B. C.-Y. Lu, J. Appl. Chem. <b>19</b> , 89 (1969).								
Reference vapor–liquid equilibrium data											
T/K=313.15, Ref. 1			T/K=338.15, Ref. 2			T/K=348.15, Ref. 2			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
4.15	0.0000	0.0000	12.96	0.0000	0.0000	19.29	0.0000	0.0000	399.02	0.00	0.0000
16.96	0.0895	0.7645	16.07	0.0028	0.1758	24.30	0.0033	0.1907	368.90	0.05	0.6088
18.48	0.1990	0.7861	31.96	0.0280	0.6007	29.57	0.0103	0.3379	359.61	0.10	0.7227
18.77	0.2529	0.7900	48.21	0.0716	0.7396	48.42	0.0300	0.6054	356.05	0.15	0.7605
18.90	0.2980	0.7923	54.45	0.1372	0.7724	66.51	0.0659	0.7178	354.28	0.20	0.7789
19.13	0.3489	0.7943	57.72	0.2198	0.7897	81.57	0.1585	0.7762	353.24	0.25	0.7899
19.24	0.4247	0.7968	59.75	0.3202	0.7987	85.61	0.2290	0.7867	352.56	0.30	0.7973
19.34	0.4951	0.7991	60.58	0.3930	0.8051	88.26	0.3022	0.7993	352.09	0.35	0.8029
19.41	0.5616	0.8015	61.27	0.4760	0.8099	89.98	0.3734	0.8053	351.74	0.40	0.8075
19.49	0.6213	0.8044	61.87	0.5734	0.8150	91.63	0.4770	0.8126	351.46	0.45	0.8115
19.62	0.6852	0.8086	62.30	0.6553	0.8192	92.47	0.5557	0.8167	351.23	0.50	0.8152
19.62	0.7459	0.8145	62.75	0.7396	0.8292	93.47	0.6558	0.8224	351.02	0.55	0.8190
19.67	0.8011	0.8228	62.95	0.7890	0.8346	93.93	0.7163	0.8303	350.84	0.60	0.8230
19.64	0.8709	0.8422	63.10	0.8597	0.8522	94.57	0.7890	0.8409	350.67	0.65	0.8275
17.90	1.0000	1.0000	63.01	0.8846	0.8615	94.94	0.8639	0.8589	350.51	0.70	0.8329
			62.58	0.9254	0.8866	94.78	0.8909	0.8712	350.36	0.75	0.8397
			61.71	0.9556	0.9190	94.30	0.9245	0.8916	350.24	0.80	0.8489
			60.94	0.9712	0.9384	94.17	0.9292	0.8946	350.16	0.85	0.8621
			60.21	0.9833	0.9582	91.98	0.9721	0.9430	350.18	0.90	0.8831
			58.44	1.0000	1.0000	91.10	0.9832	0.9600	350.47	0.95	0.9208
						88.67	1.0000	1.0000	351.52	1.00	1.0000
Θ <sub>1</sub> =0.0621	σ <sub>1</sub> =0.08 kPa	Θ <sub>1</sub> =0.0651	σ <sub>1</sub> =0.60 kPa	Θ <sub>1</sub> =0.0665	σ <sub>1</sub> =0.85 kPa						
Θ <sub>0</sub> =0.0642	σ <sub>0</sub> =0.22 kPa	Θ <sub>0</sub> =0.0629	σ <sub>0</sub> =0.77 kPa	Θ <sub>0</sub> =0.0624	σ <sub>0</sub> =1.48 kPa	Θ <sub>0</sub> =0.0463+5.6/T					

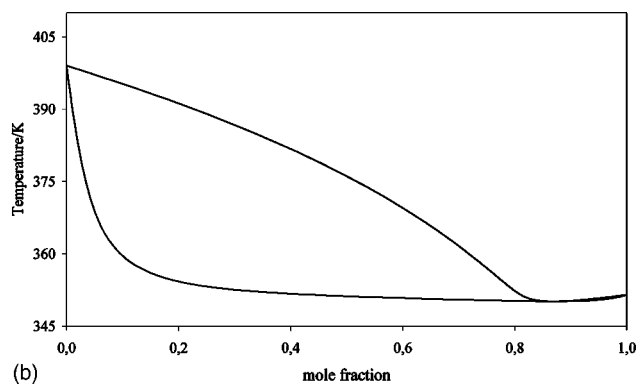
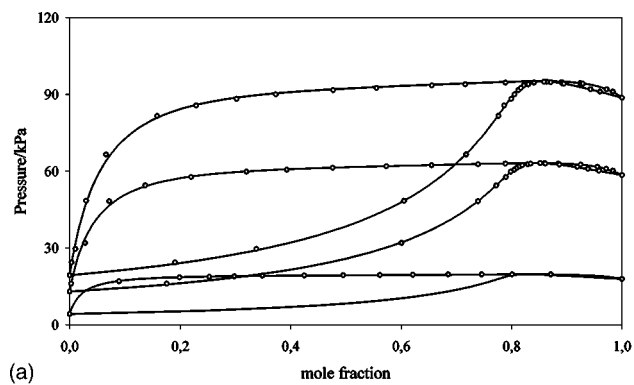


TABLE 3.12. Ethanol–nonane

Components			References								
Ethanol, C <sub>2</sub> H <sub>6</sub> O [64-17-5]			<sup>1</sup> C. Berro, M. Rogalski, and A. Peneloux, Fluid Phase Equilib. <b>8</b> , 55 (1982).								
Nonane, C <sub>9</sub> H <sub>20</sub> [111-84-2]											
Reference vapor–liquid equilibrium data											
T/K=343.15, Ref. 1			T/K=363.15, predicted			T/K=383.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
6.33	0.0000	0.0000	14.48	0.00	0.0000	29.84	0.00	0.0000	423.91	0.00	0.0000
50.49	0.0887	0.8788	69.99	0.05	0.7943	111.44	0.05	0.7316	378.92	0.05	0.7479
61.94	0.2161	0.9047	96.27	0.10	0.8526	159.99	0.10	0.8150	365.11	0.10	0.8511
64.67	0.2947	0.9101	111.18	0.15	0.8742	191.59	0.15	0.8477	360.22	0.15	0.8790
66.24	0.3735	0.9131	120.58	0.20	0.8856	213.45	0.20	0.8653	357.86	0.20	0.8915
67.51	0.4577	0.9158	126.96	0.25	0.8928	229.32	0.25	0.8766	356.50	0.25	0.8986
67.98	0.5076	0.9172	131.53	0.30	0.8978	241.32	0.30	0.8845	355.62	0.30	0.9032
68.83	0.5918	0.9191	134.99	0.35	0.9016	250.73	0.35	0.8906	355.01	0.35	0.9066
69.16	0.6292	0.9203	137.73	0.40	0.9048	258.38	0.40	0.8956	354.56	0.40	0.9093
69.53	0.6731	0.9218	140.00	0.45	0.9075	264.83	0.45	0.8999	354.19	0.45	0.9115
69.83	0.7140	0.9234	141.98	0.50	0.9100	270.48	0.50	0.9039	353.88	0.50	0.9136
70.20	0.7502	0.9251	143.78	0.55	0.9125	275.59	0.55	0.9077	353.61	0.55	0.9156
70.54	0.7808	0.9270	145.49	0.60	0.9151	280.37	0.60	0.9115	353.35	0.60	0.9178
70.69	0.7986	0.9283	147.16	0.65	0.9179	284.96	0.65	0.9156	353.11	0.65	0.9201
70.80	0.8079	0.9291	148.82	0.70	0.9212	289.47	0.70	0.9200	352.86	0.70	0.9228
70.91	0.8187	0.9301	150.52	0.75	0.9250	293.97	0.75	0.9251	352.61	0.75	0.9261
71.16	0.8410	0.9323	152.28	0.80	0.9299	298.50	0.80	0.9313	352.35	0.80	0.9303
71.53	0.8643	0.9354	154.11	0.85	0.9366	303.11	0.85	0.9391	352.08	0.85	0.9362
71.68	0.8781	0.9375	156.00	0.90	0.9465	307.77	0.90	0.9500	351.80	0.90	0.9455
71.92	0.8986	0.9415	157.77	0.95	0.9637	312.24	0.95	0.9672	351.55	0.95	0.9623
72.19	0.9187	0.9468	158.40	1.00	1.0000	315.14	1.00	1.0000	351.50	1.00	1.0000
72.39	0.9368	0.9529									
72.58	0.9531	0.9604									
72.65	0.9667	0.9686									
72.65	0.9788	0.9777									
72.58	0.9886	0.9869									
72.39	1.0000	1.0000									
$\Theta_1 = 0.0706$	$\sigma_1 = 0.10$ kPa										
$\Theta_0 = 0.0690$	$\sigma_0 = 0.37$ kPa	$\Theta_0 = 0.0681$				$\Theta_0 = 0.0672$					$\Theta_0 = 0.0526 + 5.6/T$

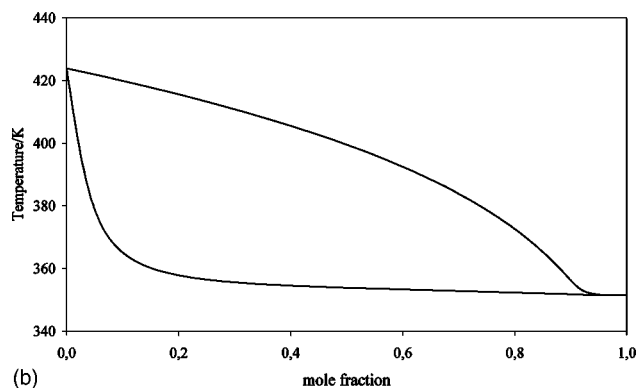
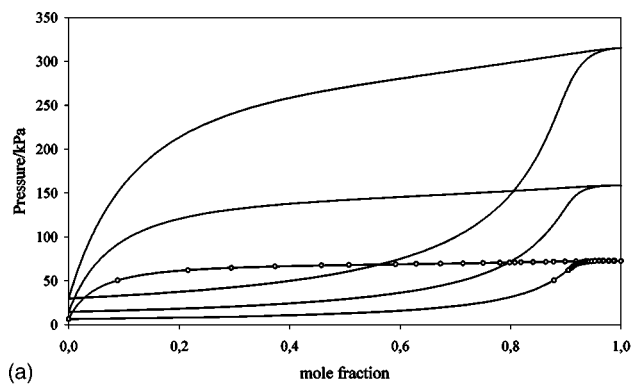


TABLE 3.13. Propanol-hexane

Components			References								
1-Propanol, C <sub>3</sub> H <sub>8</sub> O [71-23-8]			<sup>1</sup> M.V. Alekseeva and M. F. Moiseenko, Khim. Termodin. Rastvorov (Leningrad) 5, 179 (1982).								
Hexane, C <sub>6</sub> H <sub>14</sub> [110-54-3]			<sup>2</sup> J. Zielkiewicz, J. Chem. Thermodyn. 23, 605 (1991).								
Reference vapor-liquid equilibrium data											
T/K=298.15, Ref. 1			T/K=313.15, Ref. 2			T/K=333.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
20.19	0.0000	0.000	37.278	0.0000	0.0000	76.34	0.00	0.0000	342.04	0.00	0.0000
21.13	0.1052	0.079	39.775	0.0442	0.0849	82.68	0.05	0.1049	339.33	0.05	0.1115
21.04	0.2119	0.089	39.828	0.0572	0.0919	83.87	0.10	0.1346	338.77	0.10	0.1458
21.05	0.3091	0.098	39.974	0.0678	0.0962	84.08	0.15	0.1494	338.63	0.15	0.1634
20.82	0.3912	0.100	40.134	0.1071	0.1064	83.96	0.20	0.1588	338.64	0.20	0.1748
20.40	0.4995	0.106	39.900	0.1960	0.1175	83.68	0.25	0.1659	338.72	0.25	0.1835
19.41	0.6220	0.115	39.742	0.2138	0.1190	83.30	0.30	0.1717	338.84	0.30	0.1909
18.59	0.7049	0.123	39.659	0.2531	0.1220	82.83	0.35	0.1769	339.01	0.35	0.1976
15.24	0.8254	0.161	39.679	0.2538	0.1221	82.26	0.40	0.1820	339.21	0.40	0.2042
11.27	0.9102	0.239	39.525	0.2754	0.1236	81.55	0.45	0.1872	339.47	0.45	0.2111
2.84	1.0000	1.000	39.412	0.3136	0.1262	80.68	0.50	0.1928	339.78	0.50	0.2186
			39.119	0.3573	0.1290	79.57	0.55	0.1993	340.19	0.55	0.2273
			39.082	0.3742	0.1301	78.15	0.60	0.2068	340.72	0.60	0.2377
			38.734	0.4150	0.1329	76.29	0.65	0.2162	341.41	0.65	0.2507
			38.529	0.4469	0.1352	73.83	0.70	0.2284	342.36	0.70	0.2677
			38.329	0.4727	0.1372	70.52	0.75	0.2448	343.65	0.75	0.2909
			37.673	0.5444	0.1436	66.01	0.80	0.2685	345.50	0.80	0.3243
			36.665	0.6197	0.1524	59.75	0.85	0.3053	348.19	0.85	0.3758
			35.172	0.6856	0.1633	50.96	0.90	0.3697	352.31	0.90	0.4623
			34.167	0.7191	0.1707	38.43	0.95	0.5081	358.91	0.95	0.6270
			31.888	0.7787	0.1890	20.30	1.00	1.0000	370.20	1.00	1.0000
			29.028	0.8238	0.2103						
			21.141	0.9160	0.3102						
			16.218	0.9507	0.4116						
			6.987	1.0000	1.0000						
Θ <sub>1</sub> =0.0420		σ <sub>1</sub> =0.15 kPa	Θ <sub>1</sub> =0.0403		σ <sub>1</sub> =0.11 kPa						
Θ <sub>0</sub> =0.0415		σ <sub>0</sub> =0.15 kPa	Θ <sub>0</sub> =0.0406		σ <sub>0</sub> =0.11 kPa	Θ <sub>0</sub> =0.0395			Θ <sub>0</sub> =0.0227+5.6/T		

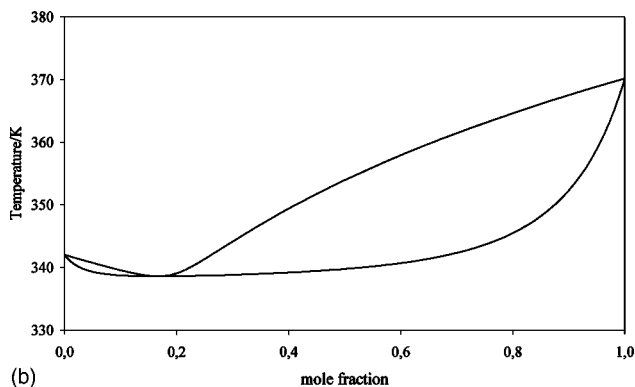
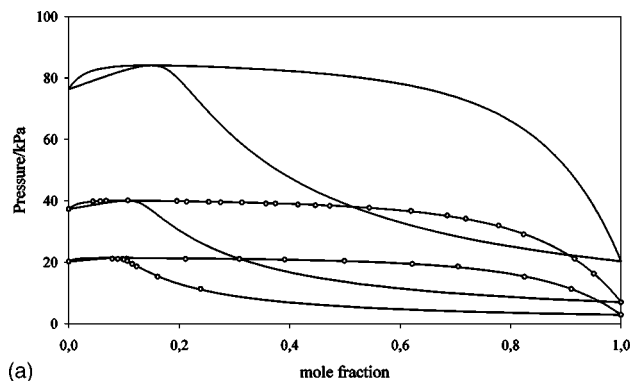


TABLE 3.14. Propanol–heptane

Components			References								
1-Propanol, C <sub>3</sub> H <sub>8</sub> O [71-23-8]			<sup>1</sup> J. T. Sipowska and S. A. Wieczorek, J. Chem. Thermodyn. <b>12</b> , 459 (1980).								
Heptane, C <sub>7</sub> H <sub>16</sub> [142-82-5]			<sup>2</sup> J. Zielkiewicz, J. Chem. Thermodyn. <b>24</b> , 455 (1992).								
			<sup>3</sup> H. C. Van Ness, C. A. Soczek, G. L. Peloquin, and R. L. Machado, J. Chem. Eng. Data <b>12</b> , 217 (1967).								
Reference vapor–liquid equilibrium data											
T/K=278.16, Ref. 1			T/K=313.15, Ref. 2			T/K=333.15, Ref. 3			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
2.07	0.0000	0.0000	12.345	0.0000	0.0000	28.13	0.0000	0.0000	371.57	0.00	0.0000
2.48	0.0643	0.1878	14.222	0.0139	0.1384	31.59	0.0126	0.1165	363.70	0.05	0.2361
2.51	0.1235	0.1981	15.121	0.0296	0.1953	33.84	0.0246	0.1755	360.80	0.10	0.3202
2.52	0.1794	0.2037	15.587	0.0449	0.2233	36.81	0.0627	0.2604	359.45	0.15	0.3622
2.50	0.2577	0.2098	16.077	0.0867	0.2589	39.02	0.1583	0.3250	358.72	0.20	0.3884
2.51	0.2920	0.2124	16.076	0.0878	0.2595	39.48	0.2156	0.3422	358.28	0.25	0.4071
2.50	0.4230	0.2222	16.222	0.1088	0.2688	39.74	0.2886	0.3579	358.01	0.30	0.4220
2.52	0.4733	0.2264	16.207	0.1109	0.2696	39.81	0.3867	0.3750	357.84	0.35	0.4348
2.47	0.5689	0.2358	16.303	0.1312	0.2763	39.66	0.4988	0.3942	357.75	0.40	0.4465
2.46	0.5895	0.2382	16.508	0.2642	0.3017	35.63	0.8168	0.5030	357.71	0.45	0.4579
2.37	0.7032	0.2561	16.509	0.3082	0.3076	30.75	0.9108	0.6155	357.73	0.50	0.4694
2.22	0.7964	0.2837	16.481	0.3884	0.3178	24.58	0.9723	0.8073	357.80	0.55	0.4817
2.17	0.8064	0.2881	16.436	0.4200	0.3218	20.33	1.0000	1.0000	357.93	0.60	0.4953
1.73	0.9065	0.3754	16.428	0.4443	0.3251				358.16	0.65	0.5110
1.67	0.9163	0.3927	16.372	0.4891	0.3313				358.49	0.70	0.5299
0.71	1.0000	1.0000	16.282	0.5353	0.3383				358.98	0.75	0.5537
			16.233	0.5568	0.3419				359.71	0.80	0.5852
			15.982	0.6340	0.3570				360.83	0.85	0.6292
			15.755	0.6734	0.3667				362.56	0.90	0.6951
			15.569	0.7122	0.3783				365.36	0.95	0.8028
			15.075	0.7689	0.4008				370.15	1.00	1.0000
			13.982	0.8401	0.4463						
			13.473	0.8636	0.4690						
			11.591	0.9230	0.5644						
			9.638	0.9628	0.6990						
			6.994	1.0000	1.0000						
Θ <sub>1</sub> = 0.0508	σ <sub>1</sub> = 0.02 kPa	Θ <sub>1</sub> = 0.0481	σ <sub>1</sub> = 0.03 kPa	Θ <sub>1</sub> = 0.0471	σ <sub>1</sub> = 0.10 kPa						
Θ <sub>0</sub> = 0.0508	σ <sub>0</sub> = 0.02 kPa	Θ <sub>0</sub> = 0.0486	σ <sub>0</sub> = 0.05 kPa	Θ <sub>0</sub> = 0.0475	σ <sub>0</sub> = 0.12 kPa	Θ <sub>0</sub> = 0.0307 + 5.6/T					

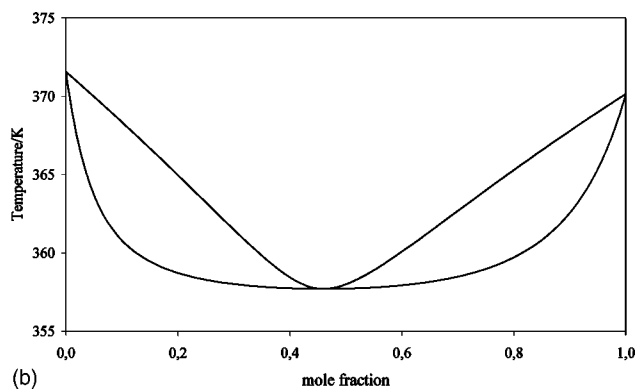
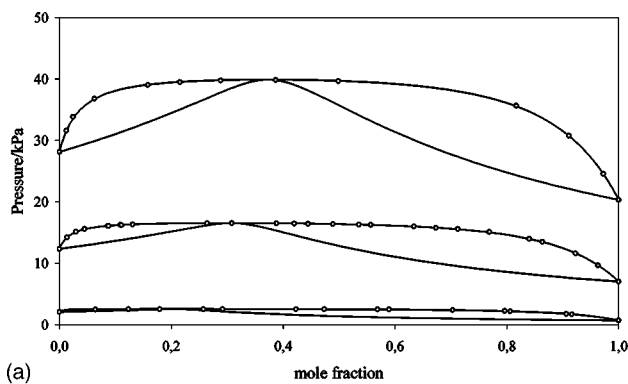


TABLE 3.15. Propanol–octane

Components			References								
1-Propanol, C <sub>3</sub> H <sub>8</sub> O [71-23-8]			<sup>1</sup> J. Zielkiewicz, J. Chem. Thermodyn. <b>24</b> , 455 (1992).								
Octane, C <sub>8</sub> H <sub>18</sub> [111-65-9]			<sup>2</sup> C. Berro, Int. DATA Ser., Sel. Data Mixtures, Ser. A <b>1</b> , 73 (1987).								
Reference vapor–liquid equilibrium data											
T/K=313.15, Ref. 1			T/K=363.15, Ref. 2			T/K=383.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
4.157	0.0000	0.0000	33.44	0.0000	0.0000	64.06	0.00	0.0000	398.93	0.00	0.0000
5.382	0.0074	0.2378	51.74	0.0368	0.3673	100.48	0.05	0.3782	383.68	0.05	0.3770
6.310	0.0160	0.3465	64.00	0.0801	0.5015	121.62	0.10	0.4992	376.94	0.10	0.5090
6.575	0.0191	0.3701	71.17	0.1280	0.5610	135.24	0.15	0.5604	373.64	0.15	0.5691
7.169	0.0305	0.4266	77.19	0.2027	0.6059	144.68	0.20	0.5984	371.75	0.20	0.6034
7.900	0.0594	0.4883	79.65	0.2520	0.6243	151.57	0.25	0.6252	370.53	0.25	0.6264
8.752	0.1694	0.5483	81.88	0.3120	0.6422	156.84	0.30	0.6457	369.68	0.30	0.6437
9.016	0.2544	0.5660	83.45	0.3680	0.6557	161.00	0.35	0.6626	369.05	0.35	0.6577
9.169	0.3480	0.5806	84.65	0.4230	0.6670	164.39	0.40	0.6772	368.56	0.40	0.6699
9.206	0.3929	0.5871	85.48	0.4708	0.6770	167.20	0.45	0.6905	368.17	0.45	0.6810
9.255	0.4501	0.5953	86.04	0.5073	0.6843	169.58	0.50	0.7031	367.84	0.50	0.6918
9.288	0.5308	0.6076	86.69	0.5601	0.6946	171.60	0.55	0.7156	367.58	0.55	0.7027
9.295	0.5790	0.6157	87.03	0.5942	0.7010	173.30	0.60	0.7283	367.36	0.60	0.7140
9.299	0.6599	0.6316	87.30	0.6255	0.7085	174.71	0.65	0.7419	367.19	0.65	0.7263
9.285	0.6831	0.6369	87.93	0.7028	0.7293	175.80	0.70	0.7568	367.07	0.70	0.7401
9.278	0.6971	0.6404	87.99	0.7499	0.7440	176.50	0.75	0.7739	367.01	0.75	0.7565
9.276	0.6978	0.6406	87.76	0.8004	0.7643	176.69	0.80	0.7946	367.04	0.80	0.7768
9.276	0.7139	0.6448	87.17	0.8432	0.7871	176.10	0.85	0.8209	367.21	0.85	0.8035
9.259	0.7265	0.6484	86.33	0.8785	0.8113	174.24	0.90	0.8569	367.61	0.90	0.8413
9.240	0.7414	0.6530	84.83	0.9156	0.8461	170.11	0.95	0.9104	368.44	0.95	0.8995
9.215	0.7572	0.6582	83.12	0.9422	0.8797	161.63	1.00	1.0000	370.14	1.00	1.0000
9.170	0.7835	0.6680	81.36	0.9631	0.9140						
9.118	0.8084	0.6790	78.93	0.9847	0.9593						
9.093	0.8185	0.6841	76.75	1.0000	1.0000						
9.056	0.8247	0.6874									
9.004	0.8428	0.6980									
8.980	0.8476	0.7011									
8.890	0.8651	0.7137									
8.751	0.8873	0.7331									
8.754	0.8881	0.7339									
8.640	0.9026	0.7494									
8.355	0.9295	0.7865									
8.323	0.9324	0.7913									
8.093	0.9490	0.8230									
7.805	0.9658	0.8645									
7.765	0.9710	0.8799									
7.667	0.9727	0.8852									
7.417	0.9840	0.9253									
6.994	1.0000	1.0000									

$\Theta_1 = 0.0527$	$\sigma_1 = 0.03$ kPa	$\Theta_1 = 0.0537$	$\sigma_1 = 0.23$ kPa		
$\Theta_0 = 0.0547$	$\sigma_0 = 0.08$ kPa	$\Theta_0 = 0.0522$	$\sigma_0 = 0.46$ kPa	$\Theta_0 = 0.0514$	$\Theta_0 = 0.0368 + 5.6/T$

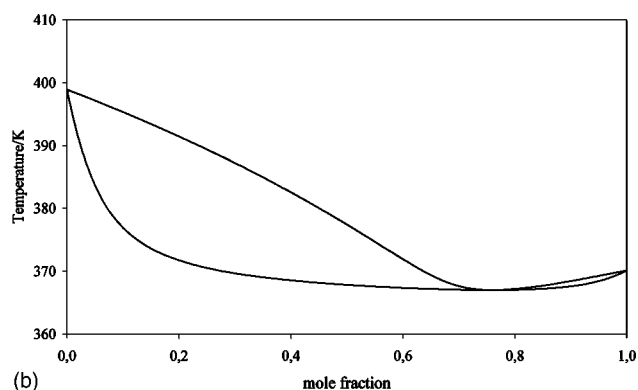
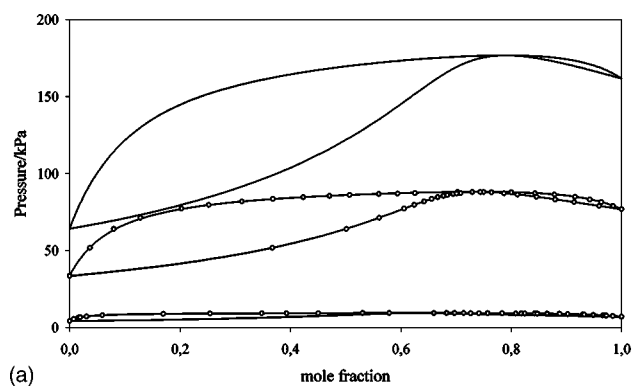


TABLE 3.16. Propanol–nonane

Components			References								
1-Propanol, C <sub>3</sub> H <sub>8</sub> O [71-23-8]			<sup>1</sup> C. Berro, J. Weclawski, and E. Neau, Int. DATA Ser., Sel. Data Mixtures, Ser. A 3, 221 (1986).								
Nonane, C <sub>9</sub> H <sub>20</sub> [111-84-2]											
Reference vapor–liquid equilibrium data											
T/K=333.15, Ref. 1			T/K=363.15, Ref. 1			T/K=383.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
3.97	0.0000	0.0000	14.48	0.0000	0.0000	29.85	0.00	0.0000	423.90	0.00	0.0000
13.79	0.0651	0.7200	43.66	0.0734	0.6817	67.42	0.05	0.5665	399.60	0.05	0.5110
16.18	0.1248	0.7668	54.16	0.1325	0.7512	89.49	0.10	0.6809	388.05	0.10	0.6704
17.38	0.1869	0.7859	58.81	0.1767	0.7748	103.94	0.15	0.7314	382.52	0.15	0.7330
17.94	0.2305	0.7940	63.32	0.2451	0.7963	114.15	0.20	0.7607	379.41	0.20	0.7654
18.63	0.3028	0.8051	66.03	0.3048	0.8090	121.78	0.25	0.7805	377.43	0.25	0.7856
18.92	0.3426	0.8095	67.50	0.3450	0.8155	127.77	0.30	0.7952	376.05	0.30	0.7999
19.23	0.4003	0.8159	69.47	0.4084	0.8245	132.66	0.35	0.8070	375.01	0.35	0.8110
19.48	0.4509	0.8205	70.99	0.4679	0.8320	136.79	0.40	0.8171	374.19	0.40	0.8202
19.67	0.4966	0.8246	71.82	0.5037	0.8372	140.37	0.45	0.8261	373.51	0.45	0.8284
19.85	0.5438	0.8287	72.59	0.5434	0.8416	143.56	0.50	0.8345	372.92	0.50	0.8359
20.08	0.6111	0.8352	73.40	0.5939	0.8465	146.45	0.55	0.8426	372.41	0.55	0.8432
20.12	0.6265	0.8369	74.19	0.6444	0.8530	149.12	0.60	0.8508	371.95	0.60	0.8506
20.24	0.6604	0.8414	74.96	0.6940	0.8600	151.60	0.65	0.8592	371.54	0.65	0.8582
20.41	0.7164	0.8484	75.47	0.7294	0.8656	153.93	0.70	0.8682	371.15	0.70	0.8665
20.58	0.7698	0.8584	76.00	0.7636	0.8719	156.13	0.75	0.8783	370.80	0.75	0.8757
20.68	0.8025	0.8654	76.75	0.8149	0.8838	158.18	0.80	0.8900	370.48	0.80	0.8867
20.76	0.8349	0.8741	77.12	0.8427	0.8918	160.04	0.85	0.9045	370.20	0.85	0.9006
20.83	0.8751	0.8884	77.58	0.8841	0.9070	161.60	0.90	0.9237	369.98	0.90	0.9196
20.84	0.9088	0.9052	77.81	0.9157	0.9225	162.47	0.95	0.9522	369.89	0.95	0.9487
20.77	0.9453	0.9312	77.49	0.9737	0.9661	161.63	1.00	1.0000	370.14	1.00	1.0000
20.62	0.9661	0.9518	76.75	1.0000	1.0000						
20.45	0.9851	0.9760									
20.35	0.9935	0.9888									
20.26	1.0000	1.0000									

$\Theta_1 = 0.0568$	$\sigma_1 = 0.08$ kPa	$\Theta_1 = 0.0589$	$\sigma_1 = 0.32$ kPa		
$\Theta_0 = 0.0583$	$\sigma_0 = 0.15$ kPa	$\Theta_0 = 0.0569$	$\sigma_0 = 0.59$ kPa	$\Theta_0 = 0.0561$	$\Theta_0 = 0.0415 + 5.6/T$

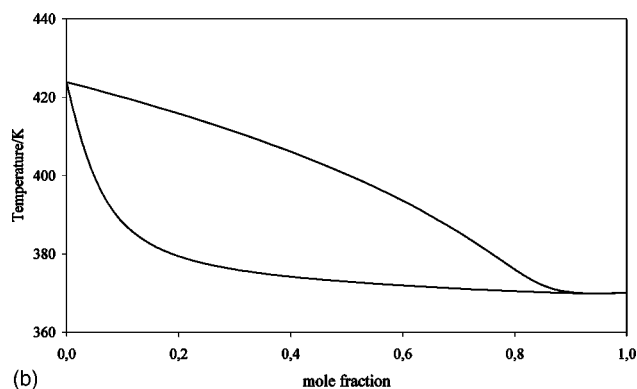
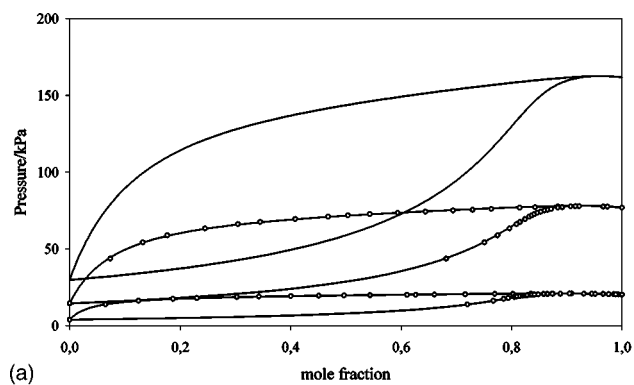


TABLE 3.17. Propanol–undecane

Components			References								
1-Propanol, C <sub>3</sub> H <sub>8</sub> O [71-23-8]			<sup>1</sup> J. Schmelzer, I. Lieberwirth, M. Krug, and R. Pfestorf, Fluid Phase Equilib.								
Undecane, C <sub>11</sub> H <sub>24</sub> [1120-21-4]			<b>11</b> , 187 (1983).								
Reference vapor–liquid equilibrium data											
T/K=333.15, Ref. 1			T/K=353.15, Ref. 2			T/K=383.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
0.55	0.000	0.000	1.71	0.000	0.000	6.67	0.00	0.0000	469.00	0.00	0.0000
11.95	0.082	0.955	15.79	0.032	0.902	45.50	0.05	0.8555	422.47	0.05	0.7302
14.91	0.200	0.975	27.24	0.080	0.942	68.53	0.10	0.9061	400.04	0.10	0.8777
15.57	0.250	0.965	33.66	0.165	0.953	83.94	0.15	0.9248	390.57	0.15	0.9165
15.91	0.267	0.968	37.32	0.250	0.968	94.96	0.20	0.9347	385.67	0.20	0.9328
16.43	0.310	0.970	39.90	0.335	0.968	103.32	0.25	0.9412	382.68	0.25	0.9417
16.89	0.378	0.975	40.94	0.372	0.960	109.96	0.30	0.9458	380.64	0.30	0.9474
17.20	0.452	0.968	42.05	0.438	0.964	115.46	0.35	0.9494	379.14	0.35	0.9516
17.52	0.540	0.972	43.37	0.540	0.971	120.17	0.40	0.9524	377.96	0.40	0.9549
18.01	0.638	0.970	43.93	0.581	0.970	124.33	0.45	0.9551	376.99	0.45	0.9576
18.13	0.656	0.974	45.17	0.658	0.968	128.09	0.50	0.9575	376.16	0.50	0.9601
18.40	0.720	0.978	45.80	0.720	0.977	131.58	0.55	0.9598	375.43	0.55	0.9623
18.47	0.732	0.972	46.21	0.742	0.978	134.86	0.60	0.9621	374.77	0.60	0.9644
18.73	0.790	0.980	46.86	0.788	0.977	137.99	0.65	0.9643	374.17	0.65	0.9665
19.00	0.838	0.980	47.36	0.810	0.990	141.03	0.70	0.9667	373.60	0.70	0.9686
19.42	0.892	0.990	48.70	0.897	0.978	144.00	0.75	0.9692	373.07	0.75	0.9709
20.38	1.000	1.000	50.83	1.000	1.000	146.95	0.80	0.9720	372.56	0.80	0.9734
						149.97	0.85	0.9753	372.05	0.85	0.9763
						153.19	0.90	0.9797	371.52	0.90	0.9802
						156.89	0.95	0.9866	370.91	0.95	0.9866
						161.55	1.00	1.0000	370.15	1.00	1.0000
Θ <sub>1</sub> = 0.0622	σ <sub>1</sub> = 0.17 kPa	Θ <sub>1</sub> = 0.0651	σ <sub>1</sub> = 0.47 kPa								
Θ <sub>0</sub> = 0.0650	σ <sub>0</sub> = 0.33 kPa	Θ <sub>0</sub> = 0.0641	σ <sub>0</sub> = 0.49 kPa	Θ <sub>0</sub> = 0.0628					Θ <sub>0</sub> = 0.0482 + 5.6/T		

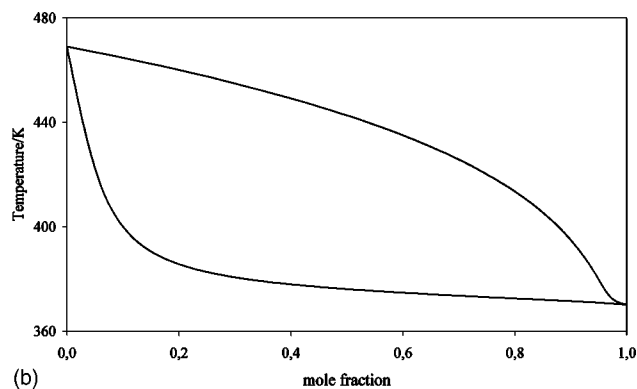
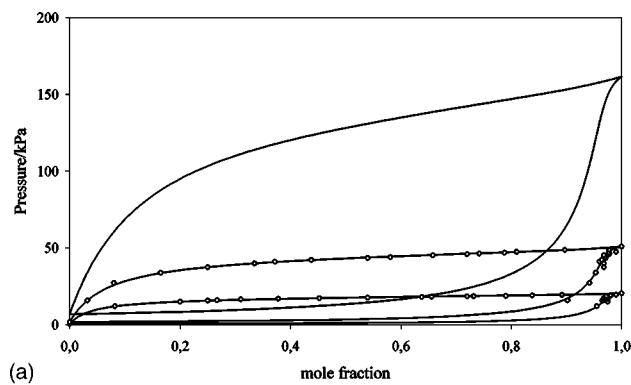


TABLE 3.18. Butanol–pentane

Components			References								
1-Butanol, C <sub>4</sub> H <sub>10</sub> O [71-36-3]			<sup>1</sup> M. Ronc and G. A. Ratcliff, Can. J. Chem. Eng. <b>54</b> , 326 (1976).								
Pentane, C <sub>5</sub> H <sub>12</sub> [109-66-0]											
Reference vapor–liquid equilibrium data											
T/K=303.15, Ref. 1			T/K=323.15, predicted			T/K=343.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
82.07	0.00	0.0000	159.52	0.00	0.0000	285.07	0.00	0.0000	309.32	0.00	0.0000
80.03	0.10	0.0090	156.55	0.05	0.0132	279.74	0.05	0.0195	309.74	0.05	0.0127
78.27	0.20	0.0100	154.37	0.10	0.0166	274.91	0.10	0.0270	310.08	0.10	0.0154
76.37	0.30	0.0108	152.63	0.15	0.0184	270.83	0.15	0.0310	310.37	0.15	0.0170
74.17	0.40	0.0116	151.06	0.20	0.0196	267.19	0.20	0.0338	310.67	0.20	0.0182
71.15	0.50	0.0128	149.49	0.25	0.0205	263.73	0.25	0.0359	311.01	0.25	0.0193
66.66	0.60	0.0145	147.80	0.30	0.0214	260.21	0.30	0.0377	311.40	0.30	0.0205
59.45	0.70	0.0174	145.86	0.35	0.0222	256.42	0.35	0.0394	311.87	0.35	0.0218
47.80	0.80	0.0232	143.57	0.40	0.0232	252.14	0.40	0.0412	312.45	0.40	0.0232
39.62	0.85	0.0291	140.78	0.45	0.0242	247.13	0.45	0.0431	313.16	0.45	0.0250
29.49	0.90	0.0407	137.34	0.50	0.0255	241.09	0.50	0.0453	314.04	0.50	0.0272
16.94	0.95	0.0740	133.09	0.55	0.0270	233.72	0.55	0.0479	315.15	0.55	0.0299
7.96	0.98	0.1616	127.80	0.60	0.0289	224.64	0.60	0.0511	316.55	0.60	0.0335
4.69	0.99	0.2758	121.22	0.65	0.0313	213.39	0.65	0.0552	318.35	0.65	0.0383
1.28	1.00	1.0000	113.06	0.70	0.0346	199.44	0.70	0.0607	320.68	0.70	0.0451
			102.94	0.75	0.0392	182.15	0.75	0.0684	323.78	0.75	0.0553
			90.45	0.80	0.0460	160.77	0.80	0.0797	328.03	0.80	0.0716
			75.05	0.85	0.0573	134.42	0.85	0.0981	334.10	0.85	0.1009
			56.14	0.90	0.0792	102.06	0.90	0.1329	343.39	0.90	0.1626
			33.00	0.95	0.1395	62.49	0.95	0.2234	359.04	0.95	0.3311
			4.76	1.00	1.0000	14.34	1.00	1.0000	388.37	1.00	1.0000
$\Theta_1 = 0.0302$	$\sigma_1 = 0.54$ kPa		$\Theta_0 = 0.0284$			$\Theta_0 = 0.0274$			$\Theta_0 = 0.0111 + 5.6/T$		
$\Theta_0 = 0.0295$	$\sigma_0 = 0.55$ kPa										

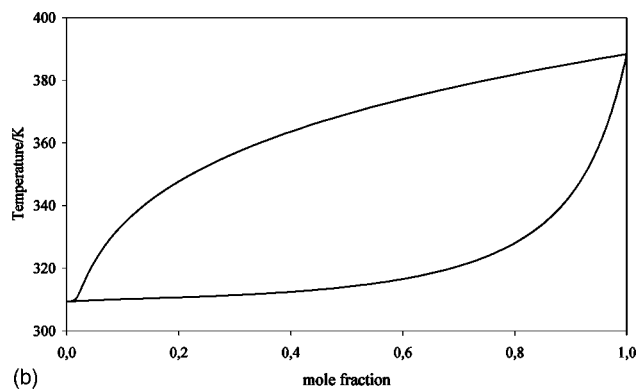
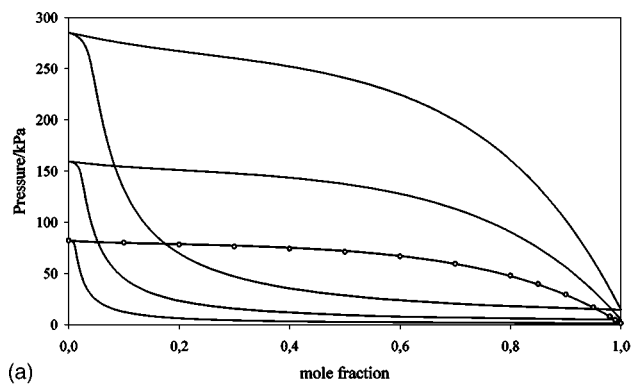




TABLE 3.19. Butanol-hexane

Components			References								
1-Butanol, C <sub>4</sub> H <sub>10</sub> O [71-36-3]			<sup>1</sup> M. Gracia, F. Gracia-Sanchez, P. Perez, J. Valero, and C. Gutierrez-Losa, J. Chem. Thermodyn. <b>24</b> , 463 (1992).								
Hexane, C <sub>6</sub> H <sub>14</sub> [110-54-3]			<sup>2</sup> C. Berro, M. Rogalski, and A. Peneloux, J. Chem. Eng. Data <b>27</b> , 352 (1982).								
Reference vapor-liquid equilibrium data											
T/K=288.15, Ref. 1			T/K=313.15, Ref. 1			T/K=333.15, Ref. 2			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
12.811	0.0000	0.0000	37.185	0.0000	0.0000	76.28	0.0000	0.0000	342.06	0.00	0.0000
12.927	0.0122	0.0108	37.404	0.0121	0.0152	76.78	0.0088	0.0120	341.56	0.05	0.0502
12.879	0.0291	0.0147	37.462	0.0291	0.0247	77.06	0.0164	0.0212	341.69	0.10	0.0684
12.834	0.0667	0.0175	37.313	0.0676	0.0334	77.32	0.0312	0.0333	341.93	0.15	0.0789
12.662	0.1226	0.0191	36.952	0.1254	0.0388	77.13	0.0563	0.0433	342.21	0.20	0.0865
12.435	0.2224	0.0209	36.202	0.2312	0.0437	76.72	0.0978	0.0521	342.53	0.25	0.0928
11.962	0.4024	0.0237	34.548	0.4156	0.0505	76.36	0.1291	0.0562	342.89	0.30	0.0986
11.374	0.5426	0.0268	32.711	0.5521	0.0573	75.05	0.2151	0.0646	343.30	0.35	0.1044
11.079	0.5878	0.0281	31.813	0.5976	0.0603	73.66	0.2937	0.0701	343.78	0.40	0.1103
10.186	0.6836	0.0322	29.168	0.6920	0.0694	73.25	0.3160	0.0717	344.36	0.45	0.1169
8.541	0.7914	0.0411	24.358	0.7992	0.0893	72.35	0.3597	0.0744	345.04	0.50	0.1243
5.977	0.8843	0.0617	16.941	0.8916	0.1353	71.86	0.3905	0.0766	345.89	0.55	0.1331
4.336	0.9278	0.0885	12.615	0.9321	0.1887	70.95	0.4251	0.0788	346.94	0.60	0.1439
1.637	0.9816	0.2548	5.642	0.9825	0.4510	69.68	0.4742	0.0824	348.28	0.65	0.1575
0.411	1.0000	1.0000	2.522	1.0000	1.0000	68.50	0.5114	0.0854	350.00	0.70	0.1755
						66.68	0.5628	0.0898	352.27	0.75	0.2002
						65.35	0.5928	0.0938	355.34	0.80	0.2364
						65.02	0.6017	0.0940	359.60	0.85	0.2928
						63.87	0.6238	0.0974	365.77	0.90	0.3895
						61.61	0.6668	0.1037	375.08	0.95	0.5771
						60.02	0.6911	0.1079	389.72	1.00	1.0000
						57.33	0.7257	0.1146			
						52.07	0.7810	0.1303			
						44.94	0.8378	0.1571			
						38.34	0.8785	0.1897			
						8.10	1.0000	1.0000			
$\Theta_1 = 0.0382$	$\sigma_1 = 0.05$ kPa	$\Theta_1 = 0.0378$	$\sigma_1 = 0.11$ kPa	$\Theta_1 = 0.0364$	$\sigma_1 = 0.18$ kPa						
$\Theta_0 = 0.0387$	$\sigma_0 = 0.06$ kPa	$\Theta_0 = 0.0371$	$\sigma_0 = 0.14$ kPa	$\Theta_0 = 0.0360$	$\sigma_0 = 0.20$ kPa	$\Theta_0 = 0.0192 + 5.6/T$					

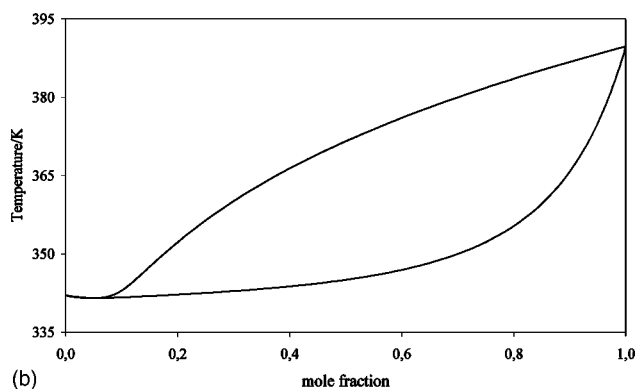
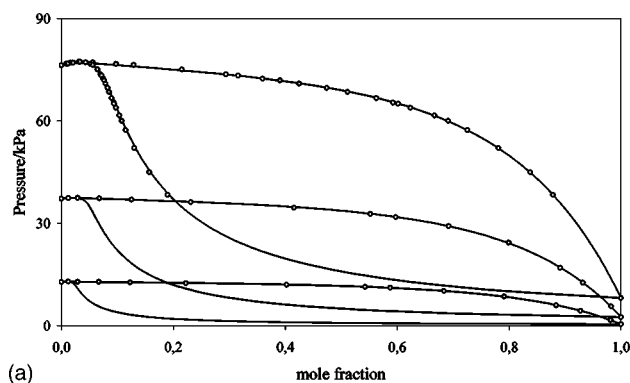


TABLE 3.20. Butanol–heptane

Components			References								
1-Butanol, C <sub>4</sub> H <sub>10</sub> O [71-36-3]			<sup>1</sup> J. Zielkiewicz, J. Chem. Thermodyn. <b>26</b> , 919 (1994).								
Heptane, C <sub>7</sub> H <sub>16</sub> [142-82-5]			<sup>2</sup> C. Berro and A. Peneloux, J. Chem. Eng. Data <b>29</b> , 206 (1984).								
Reference vapor–liquid equilibrium data											
T/K=313.15, Ref. 1			T/K=333.15, Ref. 2			T/K=363.15, Ref. 2			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
12.345	0.0000	0.0000	28.02	0.0000	0.0000	78.58	0.0000	0.0000	371.65	0.00	0.0000
12.857	0.0146	0.0494	30.52	0.0672	0.1163	83.54	0.0299	0.0815	368.74	0.05	0.1174
13.189	0.0655	0.0928	30.73	0.1288	0.1401	86.47	0.0610	0.1310	367.63	0.10	0.1713
13.205	0.1169	0.1063	30.72	0.1748	0.1513	88.50	0.1086	0.1716	367.17	0.15	0.2034
13.225	0.1478	0.1114	30.64	0.2211	0.1602	89.33	0.1637	0.1987	366.98	0.20	0.2259
13.136	0.2009	0.1182	30.53	0.2565	0.1662	89.49	0.1937	0.2097	366.95	0.25	0.2436
13.067	0.2552	0.1240	30.37	0.2978	0.1726	89.42	0.2507	0.2267	367.01	0.30	0.2589
12.930	0.3161	0.1299	30.11	0.3525	0.1805	89.08	0.3064	0.2410	367.14	0.35	0.2728
12.718	0.4068	0.1388	29.89	0.3943	0.1863	88.56	0.3556	0.2523	367.35	0.40	0.2863
12.612	0.4482	0.1431	29.64	0.4322	0.1915	87.85	0.4064	0.2641	367.62	0.45	0.3000
12.433	0.5004	0.1490	29.28	0.4829	0.1988	86.70	0.4716	0.2791	367.98	0.50	0.3143
12.076	0.5771	0.1592	28.56	0.5609	0.2118	85.85	0.5101	0.2884	368.42	0.55	0.3301
11.647	0.6488	0.1715	28.07	0.6030	0.2198	84.56	0.5589	0.3011	368.99	0.60	0.3478
10.598	0.7506	0.1984	27.53	0.6376	0.2275	83.02	0.6056	0.3150	369.72	0.65	0.3687
9.318	0.8251	0.2344	26.17	0.7060	0.2477	81.37	0.6476	0.3289	370.65	0.70	0.3941
8.804	0.8477	0.2511	24.77	0.7595	0.2698	78.76	0.6996	0.3500	371.88	0.75	0.4262
7.634	0.8896	0.2964	23.30	0.8014	0.2941	75.77	0.7465	0.3743	373.53	0.80	0.4687
7.187	0.9030	0.3172	21.15	0.8488	0.3345	74.80	0.7589	0.3816	375.78	0.85	0.5279
5.957	0.9348	0.3899	19.47	0.8776	0.3708	71.37	0.7992	0.4105	378.96	0.90	0.6155
4.388	0.9681	0.5448	16.96	0.9130	0.4366	64.76	0.8572	0.4710	383.59	0.95	0.7553
2.498	1.0000	1.0000	14.94	0.9372	0.5106	53.74	0.9245	0.5980	390.57	1.00	1.0000
			13.15	0.9555	0.5870	45.45	0.9608	0.7278			
			12.48	0.9620	0.6215	39.38	0.9830	0.8547			
			8.01	1.0000	1.0000	34.16	1.0000	1.0000			
$\Theta_1 = 0.0429$	$\sigma_1 = 0.05$ kPa	$\Theta_1 = 0.0424$	$\sigma_1 = 0.13$ kPa	$\Theta_1 = 0.0418$	$\sigma_1 = 0.18$ kPa						
$\Theta_0 = 0.0431$	$\sigma_0 = 0.05$ kPa	$\Theta_0 = 0.0420$	$\sigma_0 = 0.13$ kPa	$\Theta_0 = 0.0406$	$\sigma_0 = 0.36$ kPa				$\Theta_0 = 0.0252 + 5.6/T$		

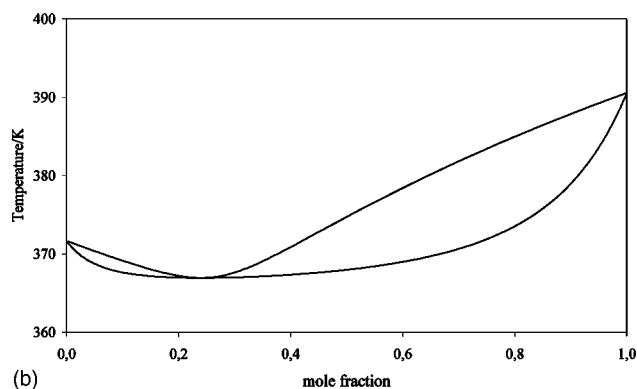
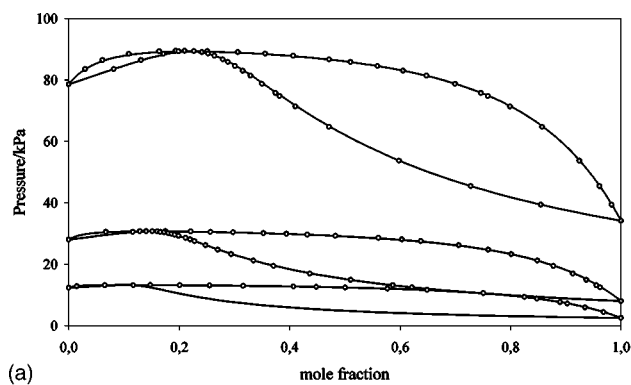


TABLE 3.21. Butanol–octane

Components			References								
1-Butanol, C <sub>4</sub> H <sub>10</sub> O [71-36-3]			<sup>1</sup> M. Gracia, F. Garcia-Sanchez, P. Perez, J. Valero, and C. Gutierrez-Losa, J. Chem. Thermodyn. <b>24</b> , 843 (1992).								
Octane, C <sub>8</sub> H <sub>18</sub> [111-65-9]			<sup>2</sup> P. Gierycz, J. Gregorowicz, and S. Malanowski, J. Chem. Thermodyn. <b>20</b> , 385 (1988).								
			V. V. Kogan, V. M. Fridman, and T. G. Romanova, Zh. Fiz. Khim. <b>33</b> , 1521 (1959).								
Reference vapor–liquid equilibrium data											
T/K=308.09, Ref. 1			T/K=323.18, Ref. 1			T/K=373.15, Ref. 2			P/kPa=101.32, Ref. 3		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
3.866	0.0307	0.1837	8.137	0.0297	0.1856	46.84	0.0000	0.0000	388.75	0.094	0.295
3.921	0.0395	0.1987	8.313	0.0384	0.2060	62.68	0.0980	0.3088	383.65	0.259	0.462
4.054	0.0792	0.2335	8.723	0.0780	0.2560	68.92	0.1938	0.3923	382.85	0.409	0.506
4.164	0.1363	0.2555	9.002	0.1357	0.2882	71.74	0.3019	0.4437	382.35	0.542	0.543
4.194	0.1768	0.2655	9.078	0.1758	0.3020	72.99	0.4011	0.4787	382.45	0.603	0.562
4.218	0.2730	0.2835	9.199	0.2726	0.3261	73.38	0.4941	0.5086	382.85	0.712	0.607
4.201	0.3265	0.2920	9.187	0.3263	0.3371	73.36	0.5500	0.5270	383.45	0.790	0.649
4.178	0.3986	0.3030	9.183	0.3986	0.3512	73.00	0.5987	0.5440	384.55	0.848	0.697
4.153	0.5025	0.3191	9.127	0.5028	0.3717	72.69	0.6461	0.5621	385.05	0.870	0.715
4.129	0.5695	0.3305	9.053	0.5698	0.3863	72.52	0.6517	0.5643	387.15	0.939	0.826
3.880	0.7329	0.3699	8.609	0.7335	0.4360	71.77	0.7021	0.5865			
3.181	0.8904	0.4797	7.230	0.8910	0.5601	68.95	0.8028	0.6458			
2.424	0.9619	0.6697	5.781	0.9621	0.7424	62.95	0.9038	0.7515			
						51.80	1.0000	1.0000			
Θ <sub>1</sub> = 0.0489	σ <sub>1</sub> = 0.03 kPa	Θ <sub>1</sub> = 0.0474	σ <sub>1</sub> = 0.02 kPa	Θ <sub>1</sub> = 0.0450	σ <sub>1</sub> = 0.39 kPa	Θ <sub>1</sub> = 0.0452	σ <sub>1</sub> = 0.48 kPa				
Θ <sub>0</sub> = 0.0479	σ <sub>0</sub> = 0.03 kPa	Θ <sub>0</sub> = 0.0470	σ <sub>0</sub> = 0.03 kPa	Θ <sub>0</sub> = 0.0447	σ <sub>0</sub> = 0.38 kPa	Θ <sub>0</sub> = 0.0443	σ <sub>0</sub> = 0.53 kPa				

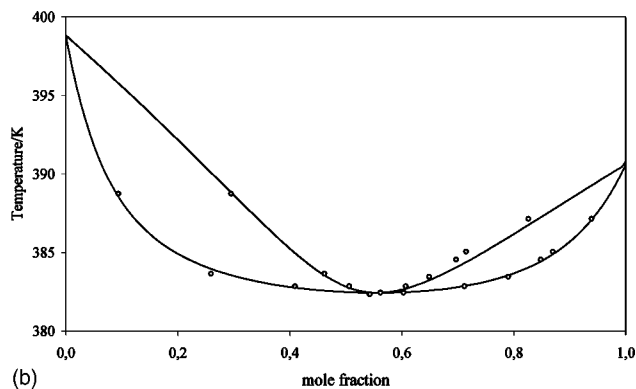
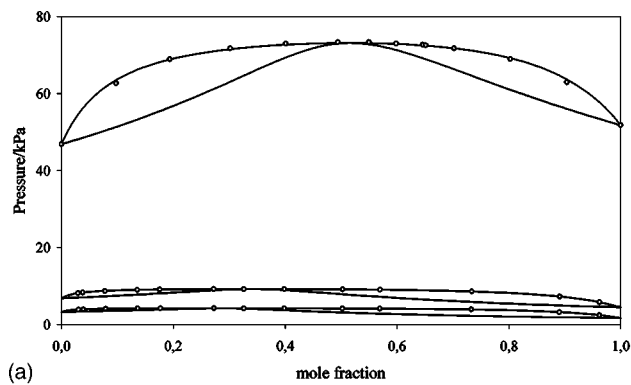


TABLE 3.22. Butanol–nonane

Components			References								
1-Butanol, C <sub>4</sub> H <sub>10</sub> O [71-36-3]			<sup>1</sup> V. V. Kogan, V. M. Fridman, and T. G. Romanova, Zh. Fiz. Khim. <b>33</b> , 1521 (1959).								
Nonane, C <sub>9</sub> H <sub>20</sub> [111-84-2]											
Reference vapor–liquid equilibrium data											
T/K = 373.15, predicted			T/K = 393.15, predicted			T/K = 413.15, predicted			P/kPa = 101.32, Ref. 1		
P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
21.05	0.00	0.0000	41.45	0.00	0.0000	75.40	0.00	0.0000	394.75	0.262	0.627
33.25	0.05	0.3882	61.66	0.05	0.3494	106.09	0.05	0.3103	391.75	0.417	0.692
39.62	0.10	0.5012	74.33	0.10	0.4766	128.03	0.10	0.4458	390.65	0.517	0.720
43.56	0.15	0.5577	82.99	0.15	0.5446	144.45	0.15	0.5236	390.75	0.522	0.715
46.26	0.20	0.5934	89.32	0.20	0.5885	157.19	0.20	0.5754	389.85	0.628	0.747
48.27	0.25	0.6192	94.18	0.25	0.6203	167.40	0.25	0.6134	389.55	0.715	0.766
49.83	0.30	0.6396	98.05	0.30	0.6452	175.78	0.30	0.6432	389.35	0.811	0.814
51.10	0.35	0.6568	101.24	0.35	0.6660	182.82	0.35	0.6680	389.35	0.879	0.857
52.17	0.40	0.6722	103.92	0.40	0.6842	188.83	0.40	0.6894	389.85	0.944	0.917
53.07	0.45	0.6865	106.22	0.45	0.7008	194.05	0.45	0.7088			
53.84	0.50	0.7002	108.21	0.50	0.7165	198.63	0.50	0.7268			
54.50	0.55	0.7138	109.95	0.55	0.7317	202.67	0.55	0.7440			
55.06	0.60	0.7276	111.46	0.60	0.7470	206.25	0.60	0.7611			
55.53	0.65	0.7422	112.76	0.65	0.7629	209.41	0.65	0.7784			
55.89	0.70	0.7580	113.85	0.70	0.7798	212.16	0.70	0.7965			
56.12	0.75	0.7759	114.70	0.75	0.7985	214.49	0.75	0.8161			
56.20	0.80	0.7972	115.26	0.80	0.8201	216.32	0.80	0.8381			
56.04	0.85	0.8240	115.43	0.85	0.8464	217.51	0.85	0.8640			
55.51	0.90	0.8600	114.97	0.90	0.8803	217.78	0.90	0.8962			
54.30	0.95	0.9130	113.48	0.95	0.9276	216.55	0.95	0.9387			
51.83	1.00	1.0000	110.08	1.00	1.0000	212.72	1.00	1.0000			

$\Theta_0 = 0.0483$	$\Theta_0 = 0.0475$	$\Theta_0 = 0.0468$	$\Theta_1 = 0.0492$	$\sigma_1 = 0.71$ kPa
			$\Theta_0 = 0.0476$	$\sigma_0 = 0.84$ kPa

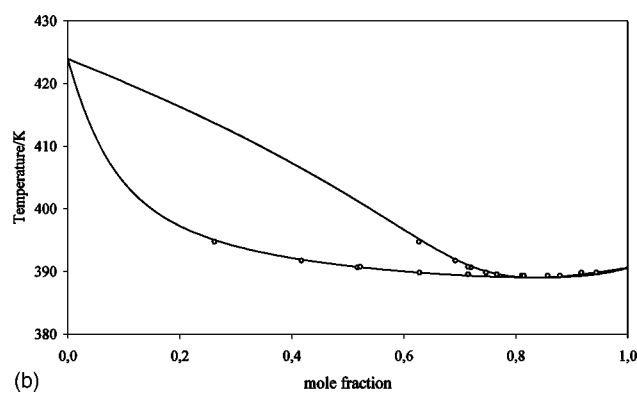
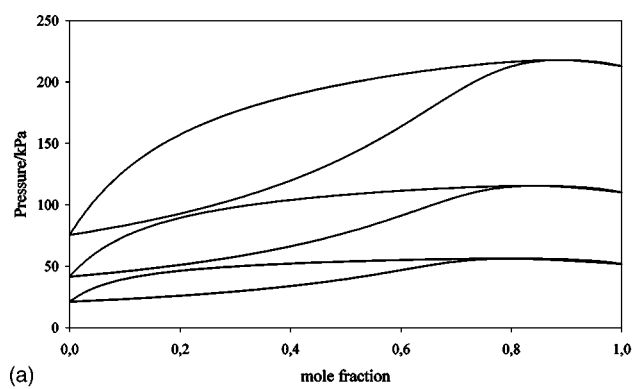


TABLE 3.23. Butanol–decane

Components			References								
1-Butanol, C <sub>4</sub> H <sub>10</sub> O [71-36-3]			<sup>1</sup> S. Bernatova, J. Linek, and I. Wichterle, Fluid Phase Equilib. <b>74</b> , 127 (1992).								
Decane, C <sub>10</sub> H <sub>22</sub> [124-18-5]											
Reference vapor–liquid equilibrium data											
T/K=358.15, Ref. 1			T/K=373.15, Ref. 1			T/K=388.15, Ref. 1			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
5.09	0.0000	0.0000	9.56	0.0000	0.0000	16.89	0.0000	0.0000	447.15	0.00	0.0000
14.08	0.0608	0.6580	28.35	0.0956	0.6925	51.76	0.1312	0.7155	428.39	0.05	0.4126
22.38	0.2928	0.8034	39.15	0.2550	0.7912	62.10	0.2181	0.7692	416.89	0.10	0.5943
24.23	0.4427	0.8291	45.14	0.4713	0.8355	78.70	0.4938	0.8414	410.08	0.15	0.6816
25.75	0.6287	0.8546	47.66	0.6163	0.8571	82.26	0.5967	0.8576	405.79	0.20	0.7307
26.41	0.7244	0.8709	49.39	0.7315	0.8780	86.57	0.7390	0.8846	402.86	0.25	0.7623
27.02	0.8209	0.8936	50.55	0.8163	0.8983	88.53	0.8106	0.9023	400.73	0.30	0.7848
27.29	0.8685	0.9098	51.18	0.8694	0.9160	90.12	0.8705	0.9218	399.08	0.35	0.8022
27.52	0.9161	0.9542	51.69	0.9144	0.9361	91.18	0.9117	0.9397	397.75	0.40	0.8165
27.60	0.9509	0.9319	52.00	0.9503	0.9576	91.74	0.9500	0.9609	396.65	0.45	0.8288
27.63	0.9706	0.9705	52.09	0.9702	0.9726	92.14	0.9695	0.9744	395.71	0.50	0.8399
27.60	0.9855	0.9847	52.15	0.9852	0.9859	92.34	0.9849	0.9871	394.88	0.55	0.8503
27.59	0.9957	0.9964	52.15	0.9958	0.9961	92.41	0.9956	0.9965	394.15	0.60	0.8603
27.58	1.0000	1.0000	52.15	1.0000	1.0000	92.48	1.0000	1.0000	393.49	0.65	0.8702
									392.90	0.70	0.8804
									392.35	0.75	0.8912
									391.85	0.80	0.9033
									391.38	0.85	0.9175
									390.97	0.90	0.9356
									390.63	0.95	0.9607
									390.48	1.00	1.0000
Θ <sub>1</sub> =0.0499	σ <sub>1</sub> =0.16 kPa	Θ <sub>1</sub> =0.0498	σ <sub>1</sub> =0.23 kPa	Θ <sub>1</sub> =0.0489	σ <sub>1</sub> =0.25 kPa						
Θ <sub>0</sub> =0.0517	σ <sub>0</sub> =0.20 kPa	Θ <sub>0</sub> =0.0511	σ <sub>0</sub> =0.28 kPa	Θ <sub>0</sub> =0.0505	σ <sub>0</sub> =0.39 kPa					Θ <sub>0</sub> =0.0361+5.6/T	

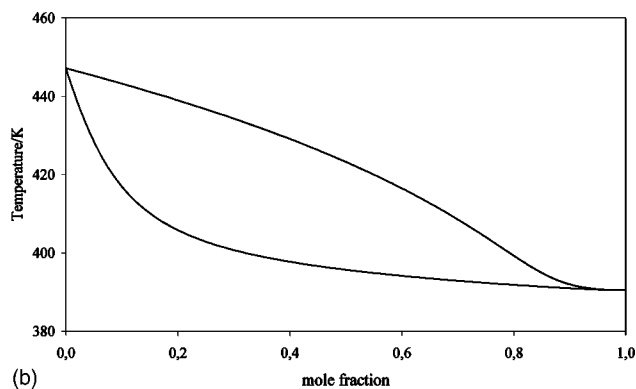
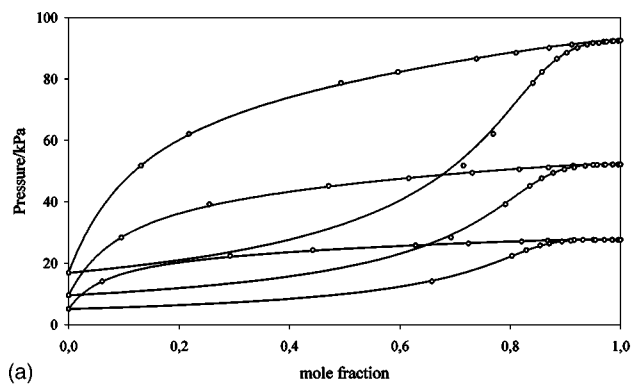


TABLE 3.24. Pentanol–pentane

Components			References								
Pentane, C <sub>5</sub> H <sub>12</sub> [109-66-0]			<sup>1</sup> M. Ronc and G. A. Ratcliff, Can. J. Chem. Eng. <b>54</b> , 326 (1976).								
1-Pentanol, C <sub>5</sub> H <sub>12</sub> O [71-41-0]											
Reference vapor–liquid equilibrium data											
T/K=303.15, Ref. 1			T/K=323.15, predicted			T/K=343.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
0.444	0.00	0.0000	1.89	0.00	0.0000	6.05	0.00	0.0000	410.96	0.00	0.0000
3.370	0.01	0.8645	26.02	0.05	0.9300	47.15	0.05	0.8753	371.68	0.05	0.7580
6.200	0.02	0.9268	46.68	0.10	0.9625	82.38	0.10	0.9310	351.29	0.10	0.9039
14.060	0.05	0.9687	64.43	0.15	0.9737	112.84	0.15	0.9511	339.69	0.15	0.9475
25.420	0.10	0.9835	79.55	0.20	0.9794	138.89	0.20	0.9614	332.26	0.20	0.9658
34.980	0.15	0.9885	92.38	0.25	0.9829	161.04	0.25	0.9677	327.11	0.25	0.9753
42.950	0.20	0.9910	103.20	0.30	0.9852	179.75	0.30	0.9719	323.35	0.30	0.9808
54.900	0.30	0.9936	112.29	0.35	0.9868	195.49	0.35	0.9749	320.52	0.35	0.9843
62.990	0.40	0.9948	119.87	0.40	0.9881	208.66	0.40	0.9772	318.34	0.40	0.9868
68.500	0.50	0.9956	126.18	0.45	0.9890	219.63	0.45	0.9790	316.63	0.45	0.9885
72.450	0.60	0.9961	131.41	0.50	0.9898	228.77	0.50	0.9804	315.27	0.50	0.9898
75.290	0.70	0.9964	135.73	0.55	0.9904	236.37	0.55	0.9816	314.18	0.55	0.9908
77.390	0.80	0.9967	139.29	0.60	0.9910	242.73	0.60	0.9826	313.31	0.60	0.9916
79.360	0.90	0.9971	142.25	0.65	0.9914	248.13	0.65	0.9836	312.60	0.65	0.9923
82.050	1.00	1.0000	144.72	0.70	0.9919	252.81	0.70	0.9844	312.01	0.70	0.9929
			146.85	0.75	0.9923	257.04	0.75	0.9853	311.53	0.75	0.9933
			148.75	0.80	0.9927	261.07	0.80	0.9862	311.12	0.80	0.9938
			150.58	0.85	0.9932	265.23	0.85	0.9874	310.76	0.85	0.9943
			152.56	0.90	0.9938	269.93	0.90	0.9890	310.41	0.90	0.9949
			155.07	0.95	0.9951	275.88	0.95	0.9921	310.02	0.95	0.9958
			159.48	1.00	1.0000	285.01	1.00	1.0000	309.33	1.00	1.0000
$\Theta_1 = 0.0291$	$\sigma_1 = 0.58$ kPa										
$\Theta_0 = 0.0290$	$\sigma_0 = 0.55$ kPa		$\Theta_0 = 0.0278$			$\Theta_0 = 0.0268$			$\Theta_0 = 0.0105 + 5.6/T$		

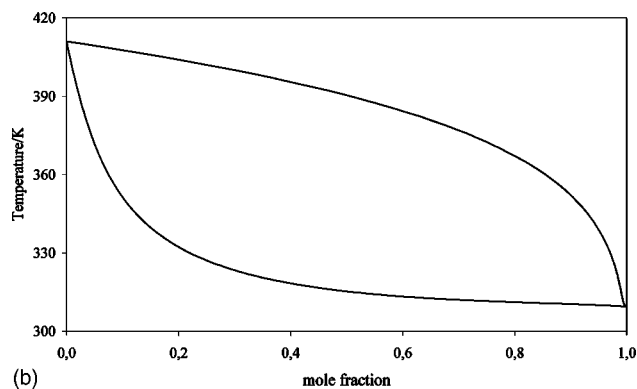
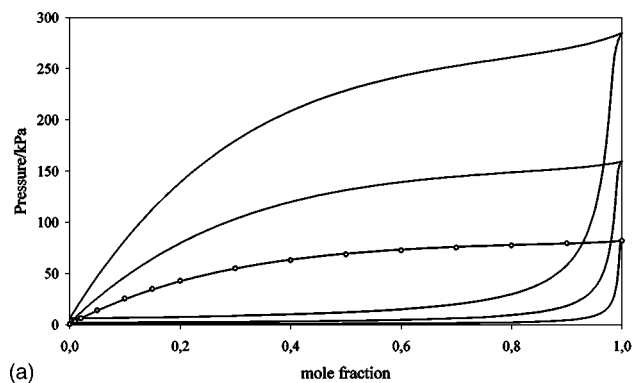


TABLE 3.25. Pentanol-hexane

Components			References								
1-Pentanol, C <sub>5</sub> H <sub>12</sub> O [71-41-0]			<sup>1</sup> M. Ronc and G. A. Ratcliff, Can. J. Chem. Eng. <b>54</b> , 326 (1976).								
Hexane, C <sub>6</sub> H <sub>14</sub> [110-54-3]											
Reference vapor-liquid equilibrium data											
T/K=303.15, Ref. 1			T/K=323.15, Ref. 1			T/K=343.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
24.97	0.00	0.0000	54.05	0.00	0.0000	105.32	0.00	0.0000	342.03	0.00	0.0000
24.37	0.10	0.0091	52.47	0.10	0.0160	103.32	0.05	0.0179	342.61	0.05	0.0188
23.79	0.20	0.0106	51.14	0.20	0.0193	101.54	0.10	0.0247	343.15	0.10	0.0262
23.12	0.30	0.0117	49.61	0.30	0.0217	99.98	0.15	0.0287	343.65	0.15	0.0307
22.36	0.40	0.0129	47.72	0.40	0.0241	98.51	0.20	0.0316	344.13	0.20	0.0342
21.35	0.50	0.0143	45.32	0.50	0.0270	97.04	0.25	0.0340	344.64	0.25	0.0373
19.87	0.60	0.0164	42.08	0.60	0.0311	95.49	0.30	0.0362	345.18	0.30	0.0402
17.61	0.70	0.0198	37.21	0.70	0.0377	93.79	0.35	0.0383	345.80	0.35	0.0432
14.16	0.80	0.0264	29.77	0.80	0.0504	91.88	0.40	0.0405	346.50	0.40	0.0465
11.76	0.85	0.0330	24.76	0.85	0.0629	89.69	0.45	0.0430	347.33	0.45	0.0502
8.78	0.90	0.0459	18.72	0.90	0.0869	87.13	0.50	0.0457	348.33	0.50	0.0545
5.08	0.95	0.0828	11.12	0.95	0.1521	84.12	0.55	0.0488	349.55	0.55	0.0599
2.42	0.98	0.1781	5.74	0.98	0.3018	80.52	0.60	0.0527	351.06	0.60	0.0666
1.46	0.99	0.2995	3.79	0.99	0.4606	76.21	0.65	0.0575	352.98	0.65	0.0756
0.44	1.00	1.0000	1.76	1.00	1.0000	71.01	0.70	0.0638	355.44	0.70	0.0879
						64.72	0.75	0.0724	358.69	0.75	0.1058
						57.07	0.80	0.0851	363.08	0.80	0.1336
						47.77	0.85	0.1054	369.23	0.85	0.1810
						36.42	0.90	0.1435	378.22	0.90	0.2717
						22.57	0.95	0.2406	391.97	0.95	0.4744
						5.65	1.00	1.0000	413.13	1.00	1.0000
$\Theta_1 = 0.0351$	$\sigma_1 = 0.06$ kPa	$\Theta_1 = 0.0339$	$\sigma_1 = 0.10$ kPa								
$\Theta_0 = 0.0350$	$\sigma_0 = 0.06$ kPa	$\Theta_0 = 0.0338$	$\sigma_0 = 0.09$ kPa	$\Theta_0 = 0.0328$					$\Theta_0 = 0.0165 + 5.6/T$		

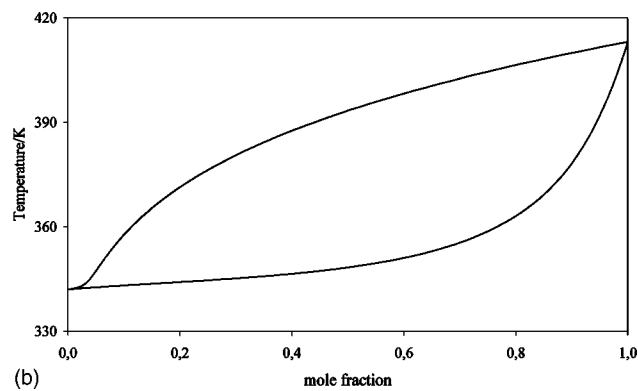
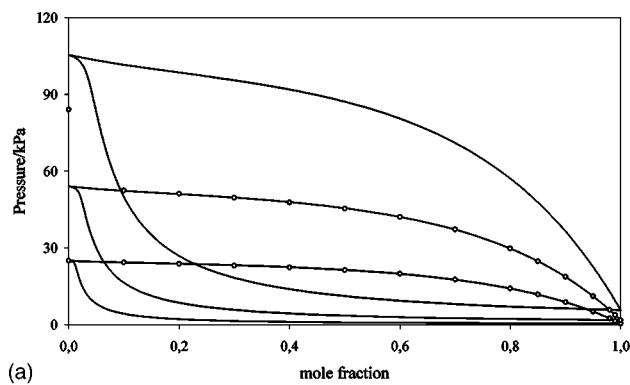


TABLE 3.26. Pentanol–heptane

Components			References								
1-Pentanol, C <sub>5</sub> H <sub>12</sub> O [71-41-0]			<sup>1</sup> J. M. Rhodes, V. R. Bhethanabotla, and S. W. Campbell, J. Chem. Eng. Data <b>42</b> , 731 (1997).								
Heptane, C <sub>7</sub> H <sub>16</sub> [142-82-5]			<sup>2</sup> I. Machova, J. Linek, and I. Wichterle, Fluid Phase Equilib. <b>4</b> , 257 (1988).								
Reference vapor–liquid equilibrium data											
T/K=313.15, Ref. 1			T/K=348.15, Ref. 2			T/K=368.15, Ref. 2			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
12.387	0.0000	0.0000	48.40	0.0000	0.0000	92.19	0.0000	0.0000	371.38	0.00	0.0000
12.442	0.0299	0.0236	48.55	0.0136	0.0183	92.31	0.0144	0.0189	370.92	0.05	0.0536
12.391	0.0600	0.0307	48.73	0.0343	0.0376	92.88	0.0339	0.0400	370.99	0.10	0.0818
12.312	0.1000	0.0355	48.79	0.0377	0.0400	92.98	0.0371	0.0432	371.24	0.15	0.1005
12.182	0.1501	0.0393	48.75	0.0570	0.0500	93.05	0.0548	0.0569	371.58	0.20	0.1148
12.054	0.2026	0.0423	48.68	0.0740	0.0562	93.08	0.0707	0.0665	371.98	0.25	0.1270
11.932	0.2508	0.0448	48.62	0.0888	0.0605	93.02	0.0874	0.0744	372.44	0.30	0.1380
11.780	0.3019	0.0473	48.60	0.0911	0.0612	92.18	0.1611	0.0977	372.95	0.35	0.1487
11.630	0.3504	0.0497	48.08	0.1636	0.0751	90.90	0.2348	0.1139	373.54	0.40	0.1594
11.447	0.4005	0.0522	47.36	0.2376	0.0851	86.92	0.3878	0.1392	374.22	0.45	0.1708
11.244	0.4507	0.0550	45.27	0.3894	0.1022	82.41	0.5210	0.1612	375.02	0.50	0.1833
11.006	0.5008	0.0580	43.13	0.5138	0.1156	76.94	0.6268	0.1821	375.97	0.55	0.1975
10.714	0.5506	0.0614	40.66	0.6062	0.1316	72.99	0.6847	0.2030	377.11	0.60	0.2141
10.631	0.5508	0.0614	38.28	0.6750	0.1445	64.95	0.7699	0.2435	378.51	0.65	0.2343
10.279	0.6009	0.0654	33.30	0.7692	0.1783	56.07	0.8382	0.2959	380.26	0.70	0.2598
9.821	0.6524	0.0706	28.53	0.8373	0.2183	44.32	0.9041	0.3965	382.49	0.75	0.2933
9.297	0.7000	0.0767	21.36	0.9086	0.3114	35.23	0.9436	0.5192	385.39	0.80	0.3394
8.583	0.7515	0.0856	16.41	0.9465	0.4263	29.15	0.9668	0.6420	389.25	0.85	0.4065
7.702	0.8015	0.0983	12.48	0.9703	0.5711	22.38	0.9906	0.8593	394.52	0.90	0.5105
6.765	0.8434	0.1146	8.78	0.9918	0.8414	19.37	1.0000	1.0000	401.89	0.95	0.6845
6.041	0.8704	0.1301	7.32	1.0000	1.0000				412.36	1.00	1.0000
3.673	0.9406	0.2236									
2.392	0.9701	0.3510									
0.891	1.0000	1.0000									
Θ <sub>1</sub> =0.0384	σ <sub>1</sub> =0.05 kPa	Θ <sub>1</sub> =0.0394	σ <sub>1</sub> =0.13 kPa	Θ <sub>1</sub> =0.0387	σ <sub>1</sub> =0.31 kPa						
Θ <sub>0</sub> =0.0388	σ <sub>0</sub> =0.05 kPa	Θ <sub>0</sub> =0.0370	σ <sub>0</sub> =0.35 kPa	Θ <sub>0</sub> =0.0361	σ <sub>0</sub> =0.66 kPa						Θ <sub>0</sub> =0.0209+5.6/T

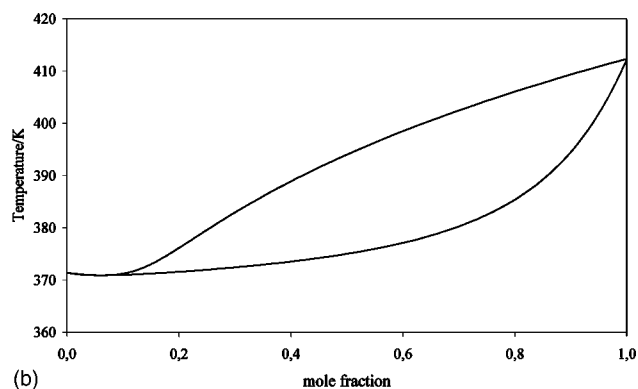
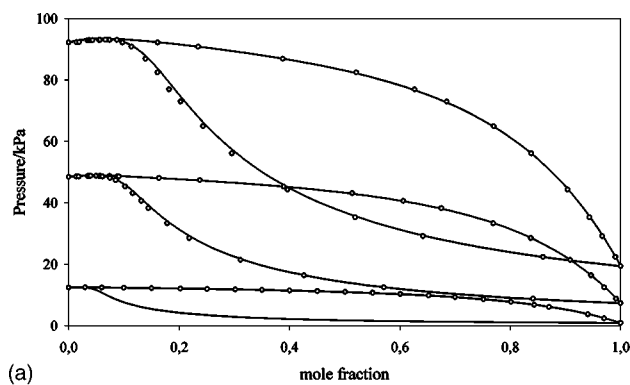




TABLE 3.27. Pentanol–octane

Components			References								
1-Pentanol, C <sub>5</sub> H <sub>12</sub> O [71-41-0]			<sup>1</sup> P. Oracz, thesis, Warsaw University, Warsaw, 1976.								
Octane, C <sub>8</sub> H <sub>18</sub> [111-65-9]			<sup>2</sup> T. Treszczanowicz and A. J. Treszczanowicz, Bull. Acad. Pol. Sci., Ser. Sci. Chim. <b>27</b> , 689 (1979).								
Reference vapor–liquid equilibrium data											
T/K=313.15, Ref. 1			T/K=373.32, Ref. 2			T/K=413.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
4.15	0.0000	0.0000	47.11	0.0000	0.0000	147.98	0.00	0.0000	398.87	0.00	0.0000
4.46	0.1323	0.1114	53.23	0.1305	0.1849	158.36	0.05	0.1039	396.29	0.05	0.1083
4.44	0.2041	0.1235	53.69	0.1871	0.2162	164.83	0.10	0.1718	394.96	0.10	0.1722
4.41	0.3015	0.1369	53.80	0.2068	0.2252	168.93	0.15	0.2212	394.24	0.15	0.2154
4.36	0.3690	0.1457	53.80	0.2717	0.2509	171.51	0.20	0.2597	393.86	0.20	0.2478
4.15	0.5121	0.1654	53.64	0.3086	0.2638	173.03	0.25	0.2915	393.67	0.25	0.2742
4.04	0.5825	0.1768	53.00	0.4108	0.2970	173.78	0.30	0.3191	393.63	0.30	0.2970
3.92	0.6390	0.1878	52.75	0.4352	0.3048	173.93	0.35	0.3439	393.69	0.35	0.3179
3.74	0.6944	0.2012	51.03	0.5505	0.3439	173.57	0.40	0.3672	393.84	0.40	0.3377
3.54	0.7454	0.2174	49.59	0.6152	0.3692	172.74	0.45	0.3896	394.07	0.45	0.3573
3.27	0.7951	0.2393	46.44	0.7130	0.4178	171.47	0.50	0.4119	394.38	0.50	0.3774
2.95	0.8421	0.2702	42.82	0.7946	0.4768	169.73	0.55	0.4348	394.80	0.55	0.3985
2.49	0.8936	0.3279	38.87	0.8565	0.5447	167.46	0.60	0.4590	395.32	0.60	0.4215
1.97	0.9366	0.4231	36.80	0.8841	0.5866	164.59	0.65	0.4855	395.99	0.65	0.4474
0.92	1.0000	1.0000	24.32	1.0000	1.0000	160.97	0.70	0.5153	396.83	0.70	0.4774
						156.41	0.75	0.5502	397.91	0.75	0.5136
						150.64	0.80	0.5928	399.31	0.80	0.5588
						143.26	0.85	0.6471	401.17	0.85	0.6179
						133.72	0.90	0.7205	403.69	0.90	0.6991
						121.21	0.95	0.8273	407.19	0.95	0.8170
						104.57	1.00	1.0000	412.17	1.00	1.0000
$\Theta_1 = 0.0422$	$\sigma_1 = 0.06$ kPa	$\Theta_1 = 0.0377$	$\sigma_1 = 0.50$ kPa								
$\Theta_0 = 0.0421$	$\sigma_0 = 0.05$ kPa	$\Theta_0 = 0.0392$	$\sigma_0 = 0.54$ kPa	$\Theta_0 = 0.0378$					$\Theta_0 = 0.0242 + 5.6/T$		

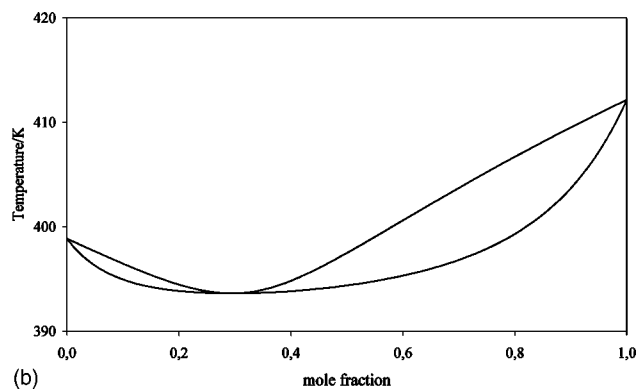
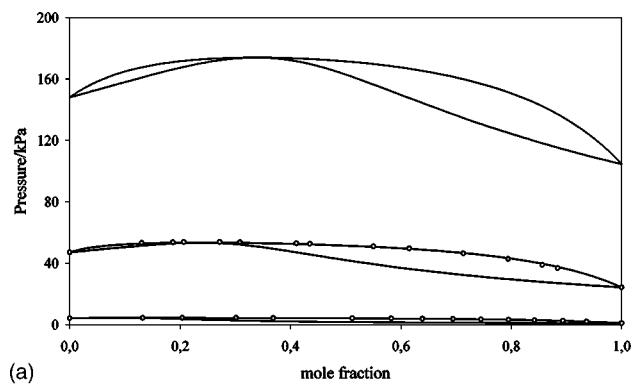


TABLE 3.28. Pentanol–decane

Components			References								
1-Pentanol, C <sub>5</sub> H <sub>12</sub> O [71-41-0]			<sup>1</sup> T. Treszczanowicz and A. J. Treszczanowicz, Bull. Acad. Pol. Sci., Ser. Sci. Chim. <b>27</b> , 689 (1979).								
Decane, C <sub>10</sub> H <sub>22</sub> [124-18-5]											
Reference vapor–liquid equilibrium data											
T/K=363.27, Ref. 1			T/K=383.15, predicted			T/K=403.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
6.38	0.0000	0.0000	14.09	0.00	0.0000	28.35	0.00	0.0000	447.08	0.00	0.0000
10.01	0.0657	0.4305	21.00	0.05	0.3544	39.82	0.05	0.3145	437.40	0.05	0.2521
13.31	0.1744	0.5650	24.99	0.10	0.4750	47.48	0.10	0.4449	430.83	0.10	0.3984
13.86	0.2112	0.5880	27.64	0.15	0.5391	52.99	0.15	0.5188	426.36	0.15	0.4890
15.67	0.4458	0.6805	29.55	0.20	0.5810	57.19	0.20	0.5682	423.21	0.20	0.5498
15.97	0.5159	0.7021	31.03	0.25	0.6120	60.52	0.25	0.6048	420.90	0.25	0.5939
15.98	0.5204	0.7035	32.23	0.30	0.6368	63.25	0.30	0.6339	419.13	0.30	0.6280
16.28	0.6021	0.7283	33.23	0.35	0.6579	65.55	0.35	0.6583	417.72	0.35	0.6560
16.48	0.6833	0.7546	34.07	0.40	0.6766	67.51	0.40	0.6798	416.59	0.40	0.6798
16.52	0.7030	0.7615	34.80	0.45	0.6938	69.22	0.45	0.6992	415.64	0.45	0.7011
16.58	0.7845	0.7938	35.44	0.50	0.7101	70.71	0.50	0.7174	414.85	0.50	0.7205
16.38	0.8916	0.8571	35.98	0.55	0.7259	72.01	0.55	0.7349	414.17	0.55	0.7390
15.43	1.0000	1.0000	36.46	0.60	0.7417	73.16	0.60	0.7521	413.59	0.60	0.7570
			36.86	0.65	0.7578	74.15	0.65	0.7696	413.10	0.65	0.7750
			37.19	0.70	0.7750	75.00	0.70	0.7879	412.68	0.70	0.7937
			37.43	0.75	0.7938	75.68	0.75	0.8076	412.34	0.75	0.8137
			37.59	0.80	0.8155	76.19	0.80	0.8299	412.09	0.80	0.8361
			37.60	0.85	0.8419	76.46	0.85	0.8563	411.93	0.85	0.8623
			37.41	0.90	0.8762	76.37	0.90	0.8894	411.90	0.90	0.8948
			36.87	0.95	0.9246	75.71	0.95	0.9341	412.10	0.95	0.9380
			35.67	1.00	1.0000	74.02	1.00	1.0000	412.67	1.00	1.0000
Θ <sub>1</sub> = 0.0417		σ <sub>1</sub> = 0.23 kPa		Θ <sub>0</sub> = 0.0435				Θ <sub>0</sub> = 0.0428		Θ <sub>0</sub> = 0.0289 + 5.6/T	
Θ <sub>0</sub> = 0.0443		σ <sub>0</sub> = 0.27 kPa									

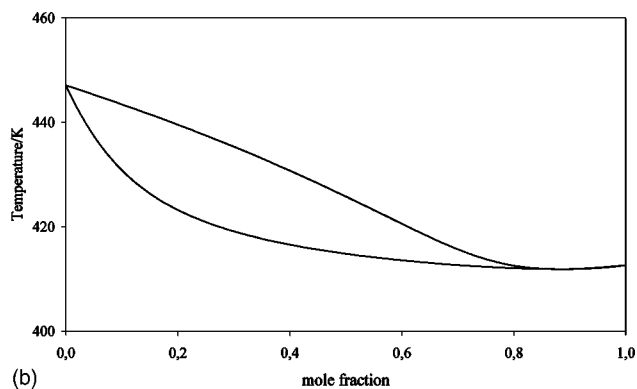
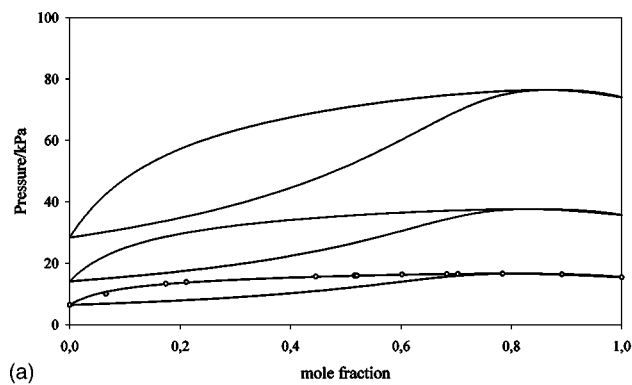


TABLE 3.29. Hexanol–hexane

Components			References								
Hexane, C <sub>6</sub> H <sub>14</sub> [110-54-3]			<sup>1</sup> S. A. Wiczorek and J. Stecki, J. Chem. Thermodyn. <b>10</b> , 177 (1978).								
1-Hexanol, C <sub>6</sub> H <sub>14</sub> O [111-27-3]											
Reference vapor–liquid equilibrium data											
T/K=298.23, Ref. 1			T/K=323.16, Ref. 1			T/K=342.82, Ref. 1			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
0.115	0.0000	0.0000	0.676	0.0000	0.0000	2.30	0.0000	0.0000	431.18	0.00	0.0000
5.870	0.0945	0.9821	14.740	0.0908	0.9574	26.83	0.0864	0.9194	405.05	0.05	0.5783
10.400	0.2005	0.9907	26.380	0.1955	0.9782	48.09	0.1888	0.9586	387.87	0.10	0.7834
13.030	0.2878	0.9931	33.250	0.2824	0.9838	61.25	0.2757	0.9697	376.66	0.15	0.8674
14.950	0.3759	0.9943	38.460	0.3711	0.9869	71.47	0.3652	0.9757	369.01	0.20	0.9083
16.800	0.5055	0.9954	43.670	0.5023	0.9896	82.00	0.4979	0.9808	363.52	0.25	0.9311
18.190	0.6599	0.9962	47.560	0.6531	0.9914	89.54	0.6434	0.9843	359.44	0.30	0.9453
19.170	0.8095	0.9969	50.520	0.8074	0.9930	96.09	0.8043	0.9875	356.31	0.35	0.9547
19.730	0.9128	0.9974	52.210	0.9125	0.9945	99.90	0.9118	0.9908	353.86	0.40	0.9614
19.920	0.9498	0.9977	52.850	0.9497	0.9955	101.43	0.9496	0.9930	351.90	0.45	0.9663
20.240	1.0000	1.0000	54.060	1.0000	1.0000	104.34	1.0000	1.0000	350.31	0.50	0.9701
									349.00	0.55	0.9732
									347.91	0.60	0.9757
									346.98	0.65	0.9778
									346.18	0.70	0.9798
									345.48	0.75	0.9816
									344.84	0.80	0.9833
									344.23	0.85	0.9853
									343.61	0.90	0.9876
									342.92	0.95	0.9913
									342.00	1.00	1.0000
Θ <sub>1</sub> = 0.0330	σ <sub>1</sub> = 0.06 kPa	Θ <sub>1</sub> = 0.0314	σ <sub>1</sub> = 0.16 kPa	Θ <sub>1</sub> = 0.0303	σ <sub>1</sub> = 0.26 kPa						
Θ <sub>0</sub> = 0.0331	σ <sub>0</sub> = 0.06 kPa	Θ <sub>0</sub> = 0.0317	σ <sub>0</sub> = 0.16 kPa	Θ <sub>0</sub> = 0.0307	σ <sub>0</sub> = 0.27 kPa	Θ <sub>0</sub> = 0.0143 + 5.6/T					

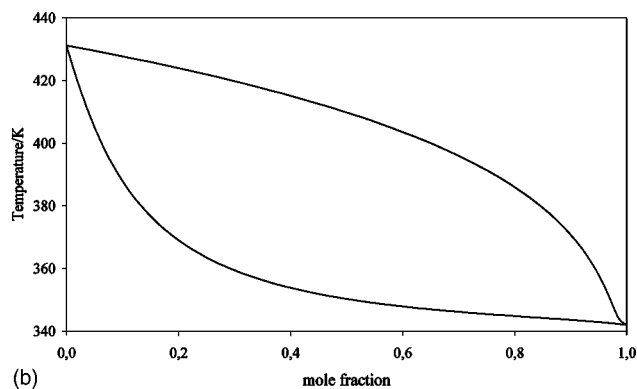
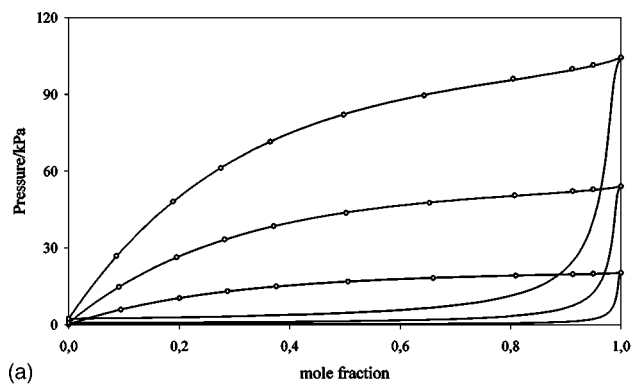


TABLE 3.30. Octanol-hexane

Components			References									
Hexane, C <sub>6</sub> H <sub>14</sub> [110-54-3]			<sup>1</sup> A. Heintz, E. Dolch, and R. N. Lichtenthaler, Fluid Phase Equilib. <b>27</b> , 61 (1986).									
1-Octanol, C <sub>8</sub> H <sub>18</sub> O [111-87-5]			<sup>2</sup> J. Schmelzer and H. Taummler, Karl Marx University, Leipzig, 1984 (unpublished data).									
Reference vapor-liquid equilibrium data												
T/K=313.15, Ref. 1			T/K=333.15, Ref. 2			T/K=373.15, predicted			P/kPa=101.32, predicted			
P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>	
8.89	0.0989	0.9945	14.37	0.0950	0.9793	2.60	0.00	0.0000	468.82	0.00	0.0000	
12.50	0.1487	0.9963	19.96	0.1225	0.9839	28.18	0.05	0.9107	429.02	0.05	0.7015	
18.00	0.2346	0.9976	25.75	0.1725	0.9884	51.44	0.10	0.9529	403.62	0.10	0.8852	
25.12	0.3834	0.9985	32.12	0.2175	0.9908	72.73	0.15	0.9678	388.00	0.15	0.9421	
27.10	0.4460	0.9987	35.92	0.2500	0.9919	92.04	0.20	0.9754	377.69	0.20	0.9651	
30.71	0.5780	0.9990	38.13	0.2775	0.9927	109.49	0.25	0.9801	370.40	0.25	0.9764	
33.41	0.7182	0.9992	42.89	0.3175	0.9936	125.19	0.30	0.9832	364.98	0.30	0.9828	
33.82	0.7435	0.9992	45.32	0.3390	0.9940	139.26	0.35	0.9855	360.82	0.35	0.9867	
34.83	0.8147	0.9993	46.68	0.3550	0.9943	151.82	0.40	0.9872	357.54	0.40	0.9894	
35.92	0.9120	0.9995	49.32	0.3800	0.9946	163.00	0.45	0.9886	354.91	0.45	0.9912	
			52.72	0.4175	0.9951	172.94	0.50	0.9897	352.76	0.50	0.9926	
			55.87	0.4700	0.9956	181.78	0.55	0.9906	350.99	0.55	0.9936	
			56.82	0.4900	0.9958	189.66	0.60	0.9914	349.51	0.60	0.9944	
			58.02	0.5175	0.9961	196.75	0.65	0.9922	348.27	0.65	0.9951	
			63.48	0.6250	0.9968	203.20	0.70	0.9929	347.21	0.70	0.9956	
			65.09	0.6775	0.9970	209.22	0.75	0.9935	346.29	0.75	0.9961	
			65.86	0.6980	0.9971	215.03	0.80	0.9942	345.48	0.80	0.9966	
			68.39	0.7750	0.9975	220.93	0.85	0.9950	344.73	0.85	0.9971	
			69.49	0.7875	0.9976	227.34	0.90	0.9960	343.99	0.90	0.9976	
			71.29	0.8500	0.9979	234.95	0.95	0.9974	343.17	0.95	0.9983	
			72.79	0.9100	0.9983	245.62	1.00	1.0000	342.02	1.00	1.0000	
			73.77	0.9375	0.9985							
			75.31	0.9750	0.9991							
			76.37	1.0000	1.0000							
$\Theta_1=0.0327$	$\sigma_1=0.09$ kPa	$\Theta_1=0.0289$	$\sigma_1=0.74$ kPa					$\Theta_0=0.0264$				
$\Theta_0=0.0292$	$\sigma_0=0.46$ kPa	$\Theta_0=0.0282$	$\sigma_0=0.75$ kPa						$\Theta_0=0.0113+5.6/T$			

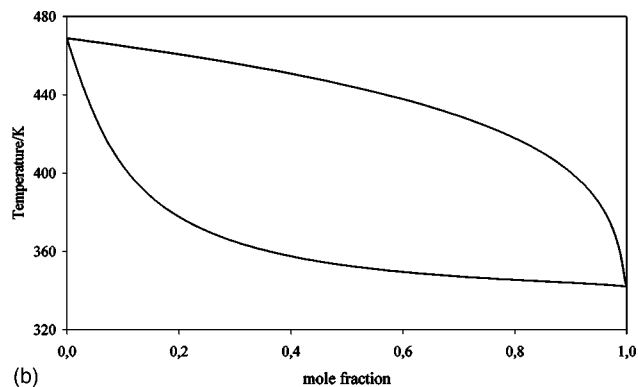
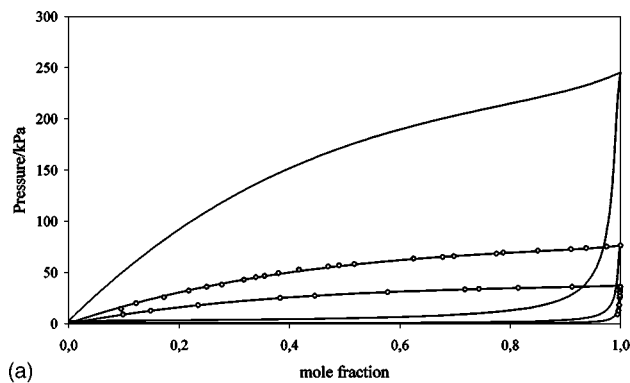


TABLE 3.31. Octanol–heptane

Components			References								
Heptane, C <sub>7</sub> H <sub>16</sub> [142-82-5]			<sup>1</sup> G. Geiseler, K. Quitzsch, H. G. Vogel, D. Pilz, and H. Sachse, Z. Phys. Chem. (Frankfurt) <b>56</b> , 288 (1967).								
1-Octanol, C <sub>8</sub> H <sub>18</sub> O [111-87-5]											
Reference vapor–liquid equilibrium data											
T/K=293.15, Ref. 1			T/K=313.15, Ref. 1			T/K=353.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
0.468	0.037	0.9644	1.35	0.037	0.9333	0.82	0.00	0.0000	468.82	0.00	0.0000
0.788	0.068	0.9800	2.23	0.068	0.9621	7.65	0.05	0.8973	446.05	0.05	0.4919
1.410	0.119	0.9882	3.60	0.119	0.9775	13.67	0.10	0.9450	429.18	0.10	0.7141
1.700	0.152	0.9906	4.34	0.152	0.9820	18.97	0.15	0.9621	417.06	0.15	0.8200
2.060	0.208	0.9929	5.62	0.208	0.9865	23.64	0.20	0.9708	408.21	0.20	0.8758
2.640	0.264	0.9943	6.66	0.264	0.9891	27.74	0.25	0.9762	401.58	0.25	0.9083
2.860	0.302	0.9949	7.21	0.302	0.9903	31.35	0.30	0.9798	396.47	0.30	0.9287
3.080	0.343	0.9955	7.76	0.343	0.9913	34.53	0.35	0.9825	392.42	0.35	0.9425
3.390	0.414	0.9961	8.77	0.414	0.9927	37.32	0.40	0.9845	389.17	0.40	0.9523
3.600	0.462	0.9965	9.31	0.462	0.9933	39.78	0.45	0.9861	386.49	0.45	0.9596
3.770	0.509	0.9968	9.72	0.509	0.9939	41.96	0.50	0.9874	384.27	0.50	0.9652
3.870	0.538	0.9970	9.92	0.538	0.9942	43.89	0.55	0.9885	382.38	0.55	0.9697
4.020	0.592	0.9972	10.34	0.592	0.9947	45.62	0.60	0.9895	380.77	0.60	0.9734
4.150	0.649	0.9975	10.79	0.649	0.9952	47.17	0.65	0.9904	379.37	0.65	0.9766
4.290	0.708	0.9977	11.07	0.708	0.9956	48.58	0.70	0.9912	378.13	0.70	0.9794
4.340	0.755	0.9979	11.33	0.755	0.9960	49.89	0.75	0.9920	377.01	0.75	0.9820
4.420	0.796	0.9980	11.64	0.796	0.9963	51.12	0.80	0.9928	375.97	0.80	0.9845
4.560	0.836	0.9982	11.72	0.836	0.9966	52.33	0.85	0.9937	374.98	0.85	0.9870
4.580	0.872	0.9983	11.78	0.872	0.9968	53.58	0.90	0.9948	373.99	0.90	0.9900
4.540	0.903	0.9985	11.94	0.903	0.9971	55.03	0.95	0.9965	372.92	0.95	0.9938
4.630	0.910	0.9985	12.09	0.910	0.9972	57.07	1.00	1.0000	371.64	1.00	1.0000
4.630	0.948	0.9987	12.14	0.948	0.9977						
4.670	0.965	0.9989	12.19	0.965	0.9980						
4.680	0.983	0.9991	12.31	0.983	0.9987						
$\Theta_1 = 0.0331$	$\sigma_1 = 0.05$ kPa		$\Theta_1 = 0.0337$	$\sigma_1 = 0.11$ kPa							
$\Theta_0 = 0.0319$	$\sigma_0 = 0.06$ kPa		$\Theta_0 = 0.0306$	$\sigma_0 = 0.17$ kPa		$\Theta_0 = 0.0286$				$\Theta_0 = 0.0128 + 5.6/T$	

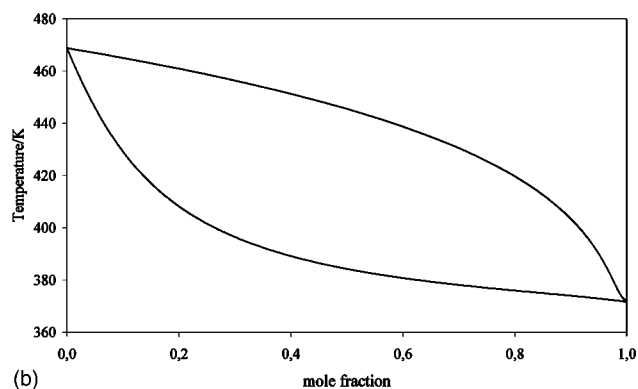
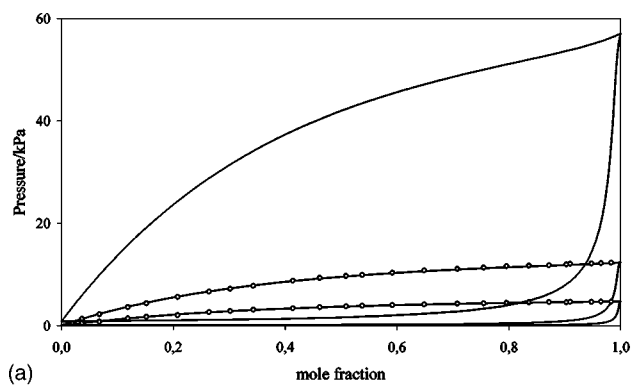


TABLE 3.32. Octanol–decane

Components			References								
1-Octanol, C <sub>8</sub> H <sub>18</sub> O [111-87-5]			<sup>1</sup> J. Schmelzer and H. Taummler, Karl Marx University, Leipzig, 1984 (unpublished data).								
Decane, C <sub>10</sub> H <sub>22</sub> [124-18-5]											
Reference vapor–liquid equilibrium data											
T/K=393.15, Ref. 1			T/K=413.15, Ref. 1			T/K=453.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
20.25	0.000	0.0000	39.30	0.000	0.0000	118.52	0.00	0.0000	446.80	0.00	0.0000
20.41	0.052	0.0579	39.49	0.052	0.0606	120.10	0.05	0.0592	446.26	0.05	0.0597
20.46	0.081	0.0800	39.62	0.081	0.0859	120.87	0.10	0.1075	446.01	0.10	0.1075
20.61	0.117	0.1022	39.85	0.117	0.1123	121.05	0.15	0.1486	445.96	0.15	0.1477
20.55	0.137	0.1128	39.78	0.137	0.1253	120.80	0.20	0.1850	446.05	0.20	0.1831
20.18	0.217	0.1487	39.37	0.217	0.1695	120.19	0.25	0.2181	446.26	0.25	0.2153
19.89	0.287	0.1752	39.04	0.287	0.2025	119.28	0.30	0.2491	446.57	0.30	0.2455
19.53	0.349	0.1973	38.16	0.349	0.2297	118.10	0.35	0.2789	446.96	0.35	0.2746
19.02	0.429	0.2256	37.45	0.429	0.2642	116.67	0.40	0.3080	447.45	0.40	0.3034
18.65	0.488	0.2474	36.77	0.488	0.2905	114.99	0.45	0.3372	448.02	0.45	0.3324
17.98	0.548	0.2713	35.48	0.548	0.3189	113.04	0.50	0.3670	448.70	0.50	0.3624
16.81	0.646	0.3174	33.56	0.646	0.3727	110.82	0.55	0.3980	449.48	0.55	0.3939
15.87	0.700	0.3492	31.86	0.700	0.4087	108.30	0.60	0.4309	450.38	0.60	0.4277
14.71	0.760	0.3934	30.08	0.760	0.4576	105.42	0.65	0.4666	451.43	0.65	0.4647
13.23	0.819	0.4522	27.62	0.819	0.5203	102.13	0.70	0.5062	452.66	0.70	0.5062
11.36	0.881	0.5439	24.79	0.881	0.6129	98.38	0.75	0.5513	454.11	0.75	0.5536
9.24	0.941	0.6940	21.02	0.941	0.7527	94.05	0.80	0.6041	455.83	0.80	0.6092
7.16	1.000	1.0000	16.98	1.000	1.0000	89.03	0.85	0.6679	457.89	0.85	0.6759
						83.17	0.90	0.7479	460.40	0.90	0.7583
						76.27	0.95	0.8531	463.46	0.95	0.8630
						68.09	1.00	1.0000	467.27	1.00	1.0000
Θ <sub>1</sub> = 0.0315	σ <sub>1</sub> = 0.23 kPa	Θ <sub>1</sub> = 0.0311	σ <sub>1</sub> = 0.23 kPa								
Θ <sub>0</sub> = 0.0296	σ <sub>0</sub> = 0.25 kPa	Θ <sub>0</sub> = 0.0289	σ <sub>0</sub> = 0.32 kPa	Θ <sub>0</sub> = 0.0277						Θ <sub>0</sub> = 0.0153 + 5.6/T	

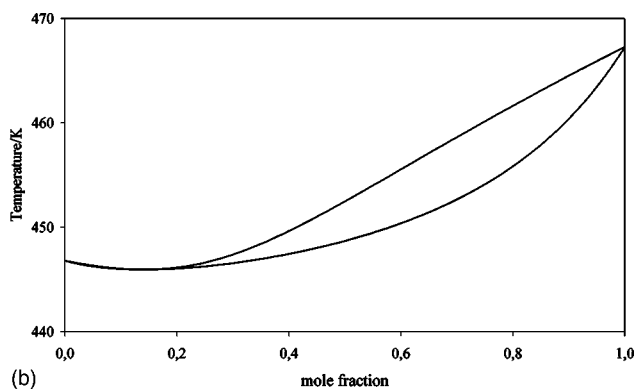
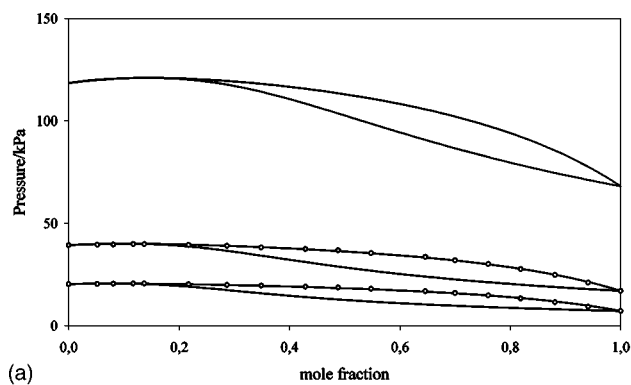


TABLE 3.33. Octanol–undecane

Components			References								
1-Octanol, C <sub>8</sub> H <sub>18</sub> O [111-87-5]			<sup>1</sup> J. Schmelzer and H. Taummler, Karl Marx University, Leipzig, 1984 (unpublished data).								
Undecane, C <sub>11</sub> H <sub>24</sub> [1120-21-4]											
Reference vapor–liquid equilibrium data											
T/K=393.15, Ref. 1			T/K=413.15, Ref. 1			T/K=453.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
10.31	0.000	0.0000	20.98	0.000	0.0000	69.64	0.00	0.0000	467.83	0.00	0.0000
10.79	0.045	0.0961	22.13	0.045	0.0936	73.48	0.05	0.0950	465.80	0.05	0.0919
11.40	0.130	0.1942	23.17	0.130	0.2015	76.37	0.10	0.1676	464.27	0.10	0.1649
11.65	0.215	0.2557	24.01	0.215	0.2728	78.57	0.15	0.2263	463.11	0.15	0.2250
11.69	0.293	0.3002	24.24	0.293	0.3249	80.27	0.20	0.2759	462.22	0.20	0.2760
11.75	0.371	0.3397	24.37	0.371	0.3708	81.56	0.25	0.3194	461.55	0.25	0.3208
11.65	0.452	0.3789	24.43	0.452	0.4159	82.54	0.30	0.3586	461.05	0.30	0.3611
11.57	0.523	0.4135	24.21	0.523	0.4553	83.23	0.35	0.3948	460.68	0.35	0.3984
11.43	0.585	0.4454	24.00	0.585	0.4910	83.69	0.40	0.4290	460.44	0.40	0.4335
11.13	0.656	0.4856	23.59	0.656	0.5352	83.94	0.45	0.4620	460.29	0.45	0.4673
10.72	0.734	0.5382	22.85	0.734	0.5914	83.97	0.50	0.4944	460.24	0.50	0.5004
10.40	0.777	0.5733	22.37	0.777	0.6277	83.81	0.55	0.5269	460.29	0.55	0.5336
9.84	0.836	0.6333	21.55	0.836	0.6875	83.44	0.60	0.5601	460.42	0.60	0.5675
9.17	0.891	0.7092	20.40	0.891	0.7594	82.85	0.65	0.5946	460.66	0.65	0.6027
8.41	0.945	0.8181	19.14	0.945	0.8553	82.02	0.70	0.6312	461.00	0.70	0.6400
7.19	1.000	1.0000	17.05	1.000	1.0000	80.91	0.75	0.6711	461.48	0.75	0.6805
						79.47	0.80	0.7157	462.10	0.80	0.7255
						77.62	0.85	0.7668	462.91	0.85	0.7768
						75.27	0.90	0.8276	463.96	0.90	0.8368
						72.25	0.95	0.9027	465.33	0.95	0.9094
						68.37	1.00	1.0000	467.13	1.00	1.0000
Θ <sub>1</sub> = 0.0306	σ <sub>1</sub> = 0.09 kPa	Θ <sub>1</sub> = 0.0290	σ <sub>1</sub> = 0.16 kPa					Θ <sub>0</sub> = 0.0282			
Θ <sub>0</sub> = 0.0301	σ <sub>0</sub> = 0.09 kPa	Θ <sub>0</sub> = 0.0294	σ <sub>0</sub> = 0.16 kPa						Θ <sub>0</sub> = 0.0158 + 5.6/T		

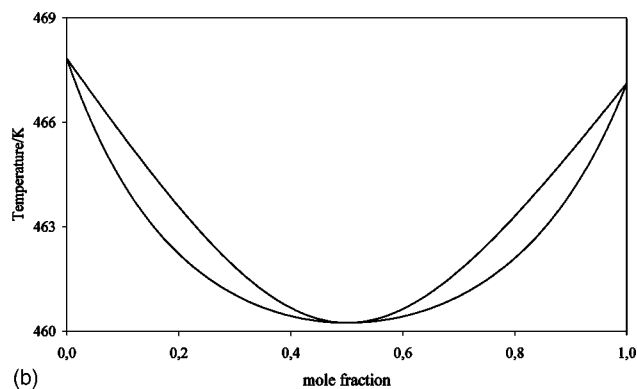
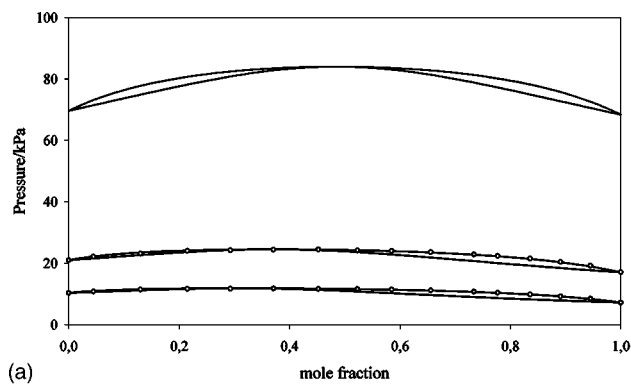


TABLE 3.34. Octanol–dodecane

Components			References								
1-Octanol, C <sub>8</sub> H <sub>18</sub> O [111-87-5]			<sup>1</sup> J. Schmelzer and H. Taummler, Karl Marx University, Leipzig, 1984 (unpublished data).								
Dodecane, C <sub>12</sub> H <sub>26</sub> [112-40-3]											
Reference vapor–liquid equilibrium data											
T/K=393.15, Ref. 1			T/K=413.15, Ref. 1			T/K=453.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
4.97	0.000	0.0000	10.91	0.000	0.0000	39.89	0.00	0.0000	488.71	0.00	0.0000
5.79	0.058	0.2170	12.51	0.058	0.1994	45.04	0.05	0.1530	484.63	0.05	0.1322
6.68	0.138	0.3482	14.37	0.138	0.3389	49.17	0.10	0.2576	481.35	0.10	0.2342
7.37	0.231	0.4347	15.87	0.231	0.4356	52.58	0.15	0.3355	478.69	0.15	0.3149
7.71	0.311	0.4884	16.85	0.311	0.4961	55.45	0.20	0.3971	476.51	0.20	0.3807
7.96	0.391	0.5331	17.40	0.391	0.5464	57.89	0.25	0.4482	474.71	0.25	0.4359
8.08	0.465	0.5703	17.85	0.465	0.5879	60.01	0.30	0.4920	473.20	0.30	0.4833
8.19	0.539	0.6055	18.12	0.539	0.6271	61.85	0.35	0.5308	471.92	0.35	0.5251
8.23	0.604	0.6364	18.40	0.604	0.6610	63.45	0.40	0.5659	470.84	0.40	0.5628
8.27	0.667	0.6676	18.50	0.667	0.6947	64.86	0.45	0.5985	469.91	0.45	0.5974
8.21	0.726	0.6994	18.59	0.726	0.7285	66.09	0.50	0.6292	469.12	0.50	0.6298
8.19	0.790	0.7392	18.50	0.790	0.7694	67.16	0.55	0.6588	468.45	0.55	0.6608
8.12	0.845	0.7811	18.44	0.845	0.8107	68.07	0.60	0.6878	467.87	0.60	0.6909
7.95	0.902	0.8373	18.16	0.902	0.8632	68.83	0.65	0.7168	467.39	0.65	0.7208
7.73	0.949	0.9004	17.85	0.949	0.9188	69.44	0.70	0.7464	467.01	0.70	0.7511
7.19	1.000	1.0000	17.05	1.000	1.0000	69.89	0.75	0.7773	466.71	0.75	0.7825
						70.16	0.80	0.8104	466.51	0.80	0.8159
						70.22	0.85	0.8470	466.42	0.85	0.8524
						70.01	0.90	0.8888	466.46	0.90	0.8935
						69.44	0.95	0.9384	466.68	0.95	0.9416
						68.37	1.00	1.0000	467.13	1.00	1.0000
Θ <sub>1</sub> =0.0323	σ <sub>1</sub> =0.09 kPa	Θ <sub>1</sub> =0.0297	σ <sub>1</sub> =0.17 kPa								
Θ <sub>0</sub> =0.0305	σ <sub>0</sub> =0.11 kPa	Θ <sub>0</sub> =0.0298	σ <sub>0</sub> =0.17 kPa	Θ <sub>0</sub> =0.0286					Θ <sub>0</sub> =0.0163+5.6/T		

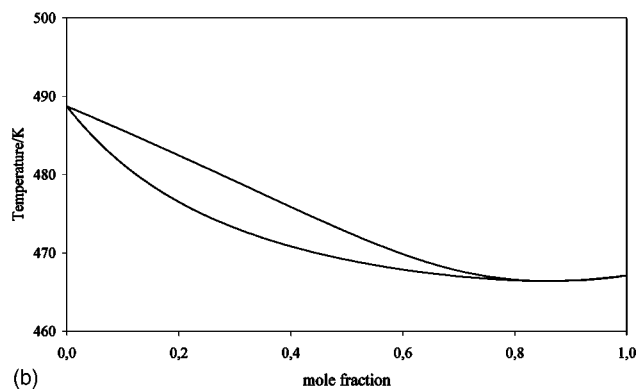
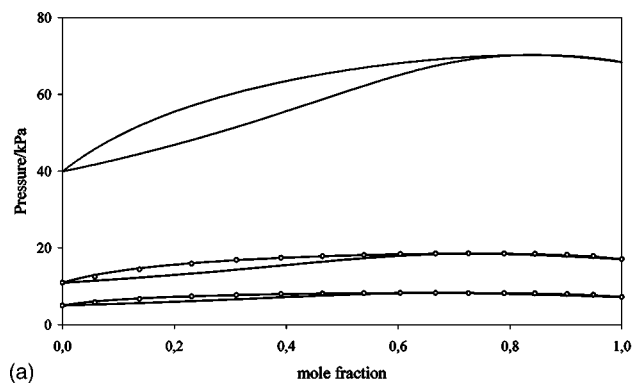




TABLE 3.35. Decanol-hexane

Components			References								
Hexane, C <sub>6</sub> H <sub>14</sub> [110-54-3]			<sup>1</sup> S. A. Wiczorek, J. Chem. Thermodyn. <b>11</b> , 239 (1979).								
1-Decanol, C <sub>10</sub> H <sub>22</sub> O [112-30-1]											
Reference vapor-liquid equilibrium data											
T/K=283.15, Ref. 1			T/K=303.15, Ref. 1			T/K=323.15, Ref. 1			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
2.65	0.1244	0.9997	6.30	0.1233	0.9990	0.024	0.0000	0.0000	502.98	0.00	0.0000
4.52	0.2316	0.9998	10.80	0.2301	0.9995	12.920	0.1213	0.9983	447.79	0.05	0.7994
5.98	0.3344	0.9999	14.36	0.3329	0.9997	22.410	0.2281	0.9991	414.69	0.10	0.9432
6.89	0.4135	0.9999	16.61	0.4125	0.9997	30.010	0.3309	0.9994	395.76	0.15	0.9761
7.81	0.5125	0.9999	18.91	0.5118	0.9998	34.950	0.4105	0.9995	383.63	0.20	0.9872
8.00	0.5358	0.9999	19.30	0.5301	0.9998	40.060	0.5104	0.9996	375.13	0.25	0.9921
8.72	0.6436	0.9999	21.20	0.6413	0.9998	40.390	0.5175	0.9996	368.81	0.30	0.9947
9.19	0.7339	1.0000	22.43	0.7326	0.9999	45.010	0.6364	0.9997	363.94	0.35	0.9961
9.62	0.8412	1.0000	23.52	0.8404	0.9999	47.810	0.7299	0.9998	360.07	0.40	0.9971
9.94	0.9525	1.0000	24.39	0.9525	0.9999	50.370	0.8387	0.9998	356.95	0.45	0.9977
10.09	1.0000	1.0000				52.520	0.9524	0.9999	354.38	0.50	0.9981
									352.26	0.55	0.9985
									350.49	0.60	0.9987
									349.00	0.65	0.9989
									347.73	0.70	0.9991
									346.65	0.75	0.9992
									345.71	0.80	0.9993
									344.87	0.85	0.9994
									344.07	0.90	0.9995
									343.21	0.95	0.9997
									342.02	1.00	1.0000
Θ <sub>1</sub> = 0.0301	σ <sub>1</sub> = 0.02 kPa	Θ <sub>1</sub> = 0.0296	σ <sub>1</sub> = 0.02 kPa	Θ <sub>1</sub> = 0.0272	σ <sub>1</sub> = 0.09 kPa						
Θ <sub>0</sub> = 0.0291	σ <sub>0</sub> = 0.05 kPa	Θ <sub>0</sub> = 0.0278	σ <sub>0</sub> = 0.18 kPa	Θ <sub>0</sub> = 0.0266	σ <sub>0</sub> = 0.14 kPa	Θ <sub>0</sub> = 0.0093 + 5.6/T					

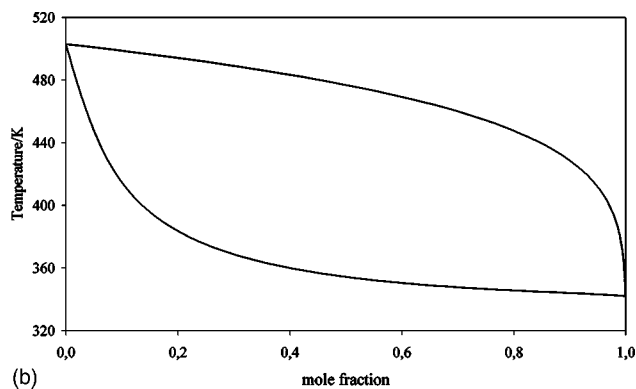
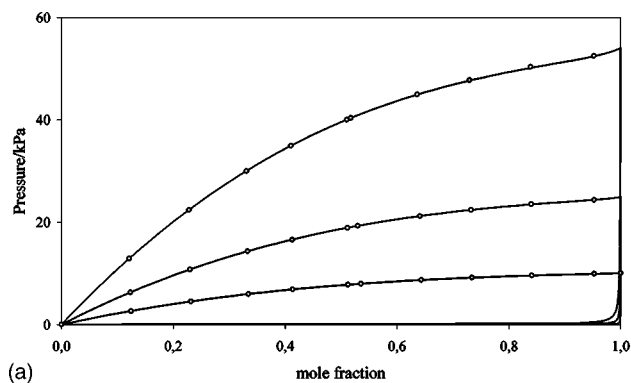


TABLE 3.36. Dodecanol–hexane

Components			References								
Hexane, C <sub>6</sub> H <sub>14</sub> [110-54-3]			<sup>1</sup> A. Heintz, E. Dolch, and R. N. Lichtenthaler, <i>Fluid Phase Equilib.</i> <b>27</b> , 61 (1986).								
1-Dodecanol, C <sub>12</sub> H <sub>26</sub> O [112-53-8]			<sup>2</sup> S. A. Wiczorek, <i>J. Chem. Thermodyn.</i> <b>10</b> , 187 (1978).								
Reference vapor–liquid equilibrium data											
T/K=298.15, Ref. 1			T/K=323.16, Ref. 2			T/K=342.82, Ref. 2			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
7.16	0.1999	0.9999	12.22	0.1269	0.9996	0.016	0.0000	0.0000	536.81	0.00	0.0000
11.96	0.3736	1.0000	21.55	0.2386	0.9998	22.210	0.1252	0.9993	462.25	0.05	0.8845
13.34	0.4332	1.0000	27.98	0.3277	0.9999	39.510	0.2357	0.9997	421.94	0.10	0.9774
16.31	0.5959	1.0000	34.49	0.4314	0.9999	48.580	0.3004	0.9997	400.68	0.15	0.9921
17.47	0.6767	1.0000	39.95	0.5352	0.9999	64.210	0.4289	0.9998	387.39	0.20	0.9963
17.70	0.6964	1.0000	44.10	0.6353	0.9999	74.820	0.5333	0.9999	378.13	0.25	0.9979
18.28	0.7468	1.0000	49.45	0.8069	1.0000	81.870	0.6193	0.9999	371.25	0.30	0.9987
18.57	0.7746	1.0000	51.48	0.9003	1.0000	93.480	0.8018	0.9999	365.92	0.35	0.9991
19.22	0.8470	1.0000	52.77	0.9618	1.0000	98.030	0.8990	0.9999	361.67	0.40	0.9994
19.65	0.9064	1.0000				101.170	0.9616	1.0000	358.22	0.45	0.9995
									355.37	0.50	0.9996
									353.01	0.55	0.9997
									351.04	0.60	0.9998
									349.38	0.65	0.9998
									347.98	0.70	0.9998
									346.79	0.75	0.9999
									345.78	0.80	0.9999
									344.89	0.85	0.9999
									344.07	0.90	0.9999
									343.21	0.95	0.9999
									342.02	1.00	1.0000
Θ <sub>1</sub> =0.0266	σ <sub>1</sub> =0.11 kPa	Θ <sub>1</sub> =0.0263	σ <sub>1</sub> =0.09 kPa	Θ <sub>1</sub> =0.0240	σ <sub>1</sub> =0.13 kPa						
Θ <sub>0</sub> =0.0270	σ <sub>0</sub> =0.11 kPa	Θ <sub>0</sub> =0.0256	σ <sub>0</sub> =0.16 kPa	Θ <sub>0</sub> =0.0246	σ <sub>0</sub> =0.21 kPa	Θ <sub>0</sub> =0.0082+5.6/T					

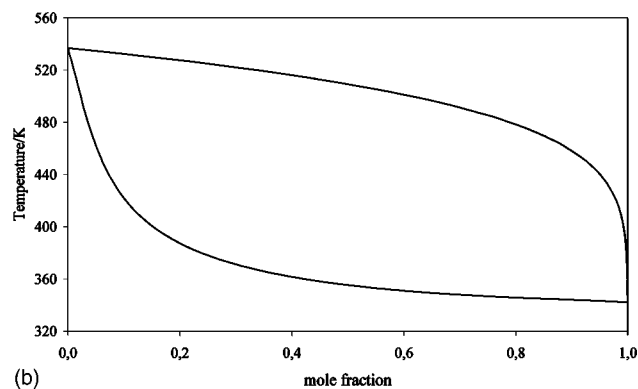
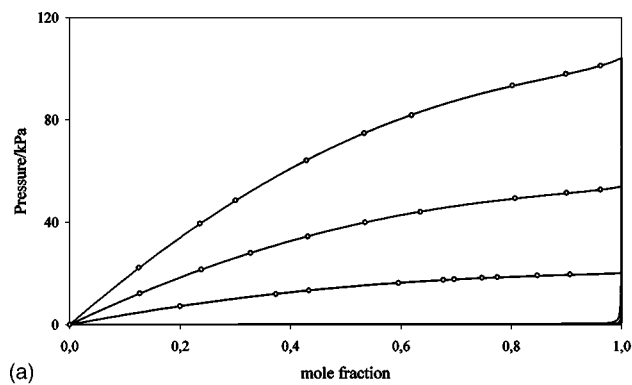


TABLE 3.37. Dodecanol–tridecane

Components			References								
1-Dodecanol, C <sub>12</sub> H <sub>26</sub> O [112-53-8]			<sup>1</sup> J. Schmelzer, V. Creutziger, I. Lieberwirth, and R. Pfestorf, Fluid Phase Equilib. <b>15</b> , 107 (1983).								
Tridecane, C <sub>13</sub> H <sub>28</sub> [629-50-5]											
Reference vapor–liquid equilibrium data											
T/K=413.15, predicted			T/K=453.15, Ref. 1			T/K=493.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
5.87	0.00	0.0000	23.77	0.000	0.0000	72.50	0.00	0.0000	507.37	0.00	0.0000
5.79	0.05	0.0325	23.40	0.076	0.0502	71.59	0.05	0.0371	507.87	0.05	0.0383
5.69	0.10	0.0576	22.24	0.222	0.1262	70.57	0.10	0.0710	508.45	0.10	0.0738
5.58	0.15	0.0792	21.33	0.304	0.1651	69.45	0.15	0.1028	509.10	0.15	0.1077
5.47	0.20	0.0988	20.42	0.381	0.2020	68.25	0.20	0.1332	509.81	0.20	0.1404
5.34	0.25	0.1176	19.73	0.455	0.2393	66.97	0.25	0.1628	510.57	0.25	0.1726
5.21	0.30	0.1360	18.40	0.536	0.2842	65.60	0.30	0.1921	511.40	0.30	0.2047
5.07	0.35	0.1546	17.33	0.604	0.3271	64.16	0.35	0.2215	512.30	0.35	0.2371
4.93	0.40	0.1738	15.72	0.708	0.4082	62.63	0.40	0.2515	513.27	0.40	0.2704
4.77	0.45	0.1940	14.76	0.764	0.4641	61.01	0.45	0.2825	514.32	0.45	0.3049
4.60	0.50	0.2156	12.67	0.847	0.5748	59.29	0.50	0.3150	515.46	0.50	0.3412
4.42	0.55	0.2392	10.84	0.920	0.7214	57.46	0.55	0.3495	516.70	0.55	0.3796
4.22	0.60	0.2656	8.61	1.000	1.0000	55.50	0.60	0.3867	518.05	0.60	0.4210
4.01	0.65	0.2958				53.41	0.65	0.4276	519.53	0.65	0.4660
3.77	0.70	0.3311				51.16	0.70	0.4731	521.15	0.70	0.5156
3.52	0.75	0.3740				48.73	0.75	0.5248	522.96	0.75	0.5708
3.23	0.80	0.4277				46.09	0.80	0.5848	524.96	0.80	0.6332
2.92	0.85	0.4982				43.22	0.85	0.6561	527.20	0.85	0.7046
2.56	0.90	0.5965				40.07	0.90	0.7434	529.71	0.90	0.7873
2.15	0.95	0.7452				36.61	0.95	0.8539	532.55	0.95	0.8844
1.69	1.00	1.0000				32.77	1.00	1.0000	535.76	1.00	1.0000

$\Theta_0 = 0.0203$	$\Theta_1 = 0.0197$	$\sigma_1 = 0.17$ kPa	$\Theta_0 = 0.0181$	$\Theta_0 = 0.0068 + 5.6/T$
	$\Theta_0 = 0.0191$	$\sigma_0 = 0.16$ kPa		

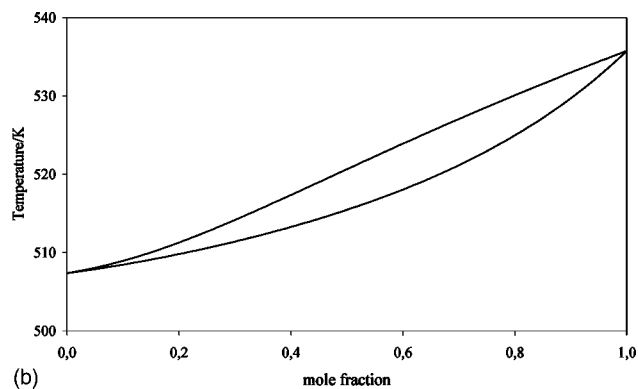
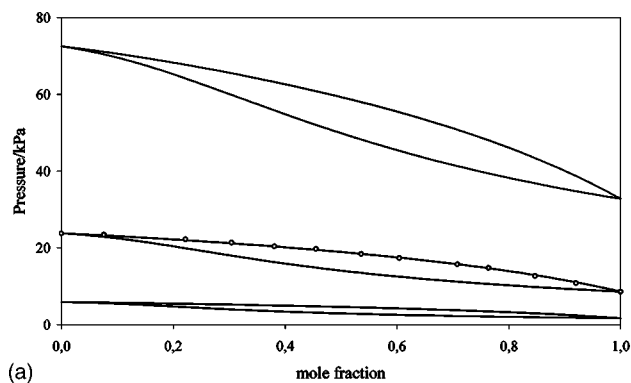


TABLE 3.38. Dodecanol–pentadecane

Components			References									
1-Dodecanol, C <sub>12</sub> H <sub>26</sub> O [112-53-8]			<sup>1</sup> J. Schmelzer, V. Creutziger, I. Lieberwirth, and R. Pfestorf, Fluid Phase Equilib. <b>15</b> , 107 (1983).									
Pentadecane, C <sub>15</sub> H <sub>32</sub> [629-62-9]												
Reference vapor–liquid equilibrium data												
T/K=433.15, predicted			T/K=473.15, Ref. 1			T/K=493.15, predicted			P/kPa=101.32, predicted			
P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>	
4.04	0.00	0.0000	16.19	0.000	0.0000	29.44	0.00	0.0000	542.93	0.00	0.0000	
4.24	0.05	0.0926	16.91	0.049	0.0853	30.62	0.05	0.0839	541.44	0.05	0.0774	
4.39	0.10	0.1613	17.64	0.123	0.1864	31.58	0.10	0.1543	540.17	0.10	0.1462	
4.49	0.15	0.2169	18.56	0.230	0.2996	32.39	0.15	0.2153	539.08	0.15	0.2081	
4.57	0.20	0.2643	18.88	0.330	0.3869	33.07	0.20	0.2695	538.14	0.20	0.2646	
4.63	0.25	0.3064	19.40	0.488	0.5082	33.64	0.25	0.3187	537.34	0.25	0.3166	
4.67	0.30	0.3450	19.32	0.624	0.6090	34.11	0.30	0.3642	536.65	0.30	0.3652	
4.70	0.35	0.3811	19.17	0.725	0.6886	34.50	0.35	0.4068	536.06	0.35	0.4110	
4.72	0.40	0.4155	18.67	0.835	0.7884	34.81	0.40	0.4475	535.57	0.40	0.4547	
4.72	0.45	0.4490	17.91	0.926	0.8912	35.05	0.45	0.4867	535.16	0.45	0.4968	
4.71	0.50	0.4821	17.34	1.000	1.0000	35.22	0.50	0.5250	534.84	0.50	0.5378	
4.70	0.55	0.5153				35.32	0.55	0.5629	534.58	0.55	0.5781	
4.67	0.60	0.5493				35.36	0.60	0.6009	534.40	0.60	0.6182	
4.63	0.65	0.5847				35.33	0.65	0.6395	534.30	0.65	0.6585	
4.58	0.70	0.6223				35.23	0.70	0.6793	534.26	0.70	0.6995	
4.51	0.75	0.6631				35.05	0.75	0.7210	534.31	0.75	0.7417	
4.43	0.80	0.7088				34.78	0.80	0.7655	534.44	0.80	0.7859	
4.32	0.85	0.7612				34.41	0.85	0.8138	534.66	0.85	0.8327	
4.18	0.90	0.8234				33.92	0.90	0.8675	534.99	0.90	0.8831	
4.01	0.95	0.9003				33.28	0.95	0.9286	535.44	0.95	0.9384	
3.79	1.00	1.0000				32.46	1.00	1.0000	536.05	1.00	1.0000	
$\Theta_0=0.0195$			$\Theta_1=0.0177$		$\sigma_1=0.09$ kPa		$\Theta_0=0.0180$			$\Theta_0=0.0066+5.6/T$		
			$\Theta_0=0.0184$		$\sigma_0=0.09$ kPa							

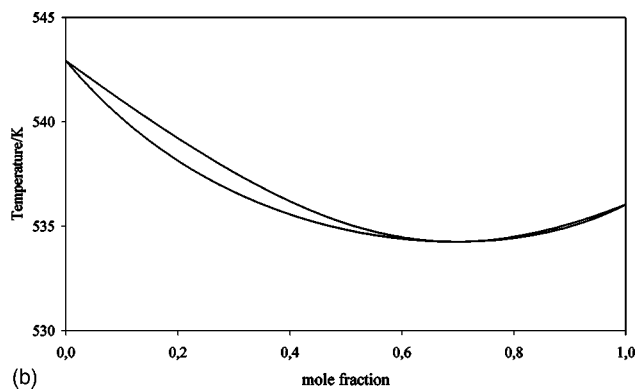
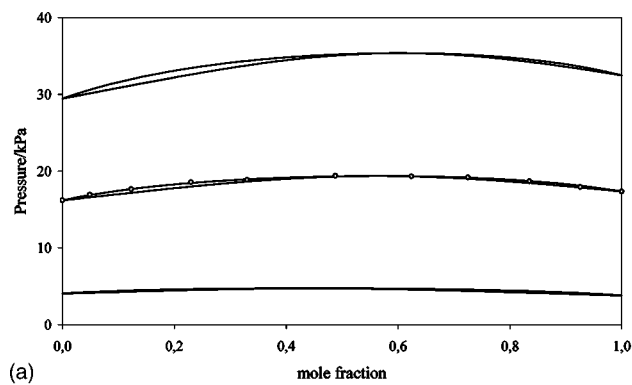
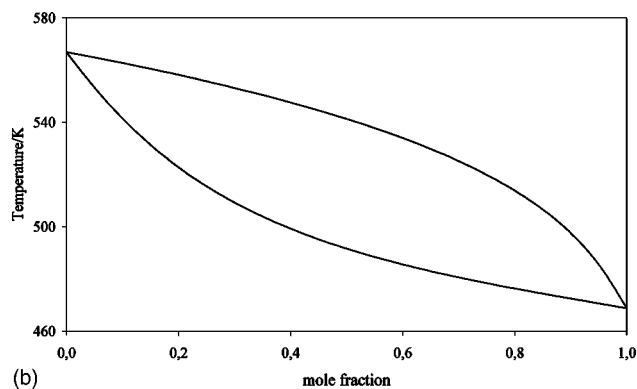
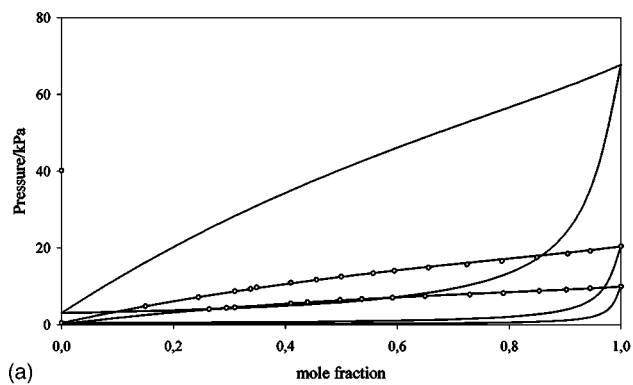


TABLE 3.39. Tetradecanol–undecane

Components			References								
Undecane, C <sub>11</sub> H <sub>24</sub> [1120-21-4]			<sup>1</sup> J. Schmelzer, I. Lieberwirth, M. Krug, and R. Pfestorf, Fluid Phase Equilib. <b>11</b> , 187 (1983).								
1-Tetradecanol, C <sub>14</sub> H <sub>30</sub> O [112-72-1]											
Reference vapor–liquid equilibrium data											
T/K=393.15, Ref. 1			T/K=413.15, Ref. 1			T/K=453.15, predicted			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
0.12	0.000	0.0000	0.43	0.000	0.0000	3.01	0.00	0.0000	566.90	0.00	0.0000
4.00	0.264	0.9769	4.80	0.150	0.9224	7.63	0.05	0.6235	553.31	0.05	0.2975
4.35	0.295	0.9795	7.13	0.245	0.9533	12.03	0.10	0.7722	541.47	0.10	0.4977
4.47	0.310	0.9806	8.67	0.310	0.9641	16.22	0.15	0.8390	531.36	0.15	0.6320
5.52	0.410	0.9859	9.33	0.338	0.9675	20.20	0.20	0.8771	522.76	0.20	0.7236
5.84	0.440	0.9871	9.71	0.349	0.9687	23.99	0.25	0.9018	515.47	0.25	0.7873
6.40	0.498	0.9890	10.93	0.410	0.9744	27.60	0.30	0.9193	509.24	0.30	0.8329
6.65	0.537	0.9900	11.73	0.456	0.9778	31.03	0.35	0.9323	503.89	0.35	0.8664
7.05	0.592	0.9914	12.49	0.500	0.9805	34.31	0.40	0.9424	499.26	0.40	0.8917
7.40	0.650	0.9926	13.37	0.557	0.9834	37.45	0.45	0.9506	495.20	0.45	0.9113
7.83	0.730	0.9941	14.01	0.595	0.9852	40.45	0.50	0.9574	491.63	0.50	0.9268
8.17	0.790	0.9952	14.85	0.656	0.9876	43.33	0.55	0.9632	488.44	0.55	0.9393
8.73	0.854	0.9963	15.68	0.725	0.9901	46.11	0.60	0.9682	485.58	0.60	0.9497
9.07	0.902	0.9973	16.57	0.787	0.9921	48.81	0.65	0.9728	482.99	0.65	0.9584
9.45	0.945	0.9983	17.52	0.850	0.9942	51.44	0.70	0.9769	480.62	0.70	0.9659
9.90	1.000	1.0000	18.47	0.905	0.9960	54.03	0.75	0.9807	478.42	0.75	0.9726
			19.19	0.945	0.9975	56.61	0.80	0.9844	476.36	0.80	0.9785
			20.40	1.000	1.0000	59.20	0.85	0.9880	474.40	0.85	0.9841
						61.87	0.90	0.9917	472.51	0.90	0.9894
						64.67	0.95	0.9956	470.65	0.95	0.9946
						67.71	1.00	1.0000	468.76	1.00	1.0000
Θ <sub>1</sub> = 0.0221	σ <sub>1</sub> = 0.10 kPa	Θ <sub>1</sub> = 0.0172	σ <sub>1</sub> = 0.24 kPa								
Θ <sub>0</sub> = 0.0201	σ <sub>0</sub> = 0.11 kPa	Θ <sub>0</sub> = 0.0194	σ <sub>0</sub> = 0.26 kPa	Θ <sub>0</sub> = 0.0182						Θ <sub>0</sub> = 0.0058 + 5.6/T	



## 9. Appendix: Bibliography of VLE for *n*-Alkanol–*n*-Alkane Systems

All references cited in Tables 3.1–3.29 are repeated in this Appendix; additional references, which were not used in the final critical evaluation, are also included.

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