Recommended Vapor–Liquid Equilibrium Data. Part 4. Binary Alkanol–Alkene/Alkyne Systems

Marian Góral[a] **and Andrzej Bok**
Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

Teresa Kasprzycka–Gutman and Paweł Oracz
Department of Chemistry, University of Warsaw, Warsaw, Poland

(Received 20 February 2006; revised manuscript received 7 July 2006; accepted 14 July 2006; published online 19 October 2006)

The recommended vapor–liquid equilibrium (VLE) data for binary mixtures of alkanols with alkenes and alkynes have been selected after critical evaluation of all data reported in the open literature up to the end of 2003. 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 Wilson equation as well as with equation of state appended with chemical term (EoSC) proposed by Góral. The recommended data for 18 systems 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. © *2006 American Institute of Physics*.
[DOI: 10.1063/1.2336783]

Key words: alkanols; alkenes; alkynes; binary systems; predicted data; recommended data; vapor–liquid equilibria.

CONTENTS

List of Tables

List of Figures

1. Introduction

The objective of this paper is to provide selected and critically evaluated vapor–liquid equilibrium (VLE) data for binary mixtures of alkanols with alkenes and alkynes.

All available data (below 0.5 MPa) for considered systems, were taken from the open literature up to the end of 2003. They consist of 12 isothermal and 79 isobaric data sets taken from 26 references.

The data were critically evaluated using multistage procedure. The procedure was described in Part 1.[1] The critical evaluation of the data was difficult. Thermodynamic consistency tests can be performed only for 34 data sets because the remaining 57 sets do not contain concentrations of the vapor phase. Enthalpy of mixing, used as auxiliary data, is

[a]Author to whom correspondence should be addressed; electronic mail: mgoral@ichf.edu.pl

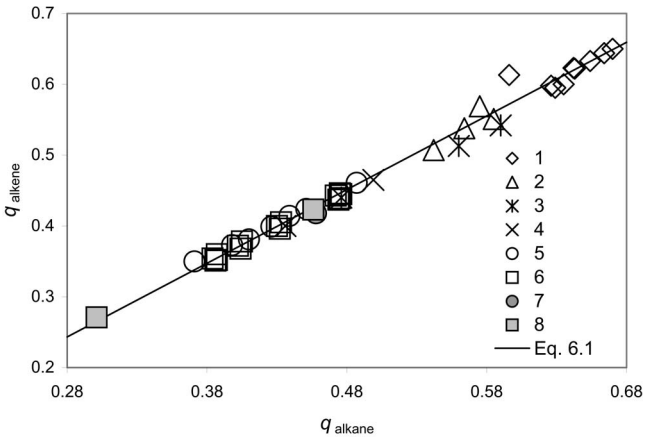


FIG. 1. Values of q for alkenes (q_{alkene}) and for alkanes (q_{alkane}) in the corresponding mixtures.The points correspond to the following mixtures: alkenes with methanol (1), with ethanol (2), with 1-propanol (3), with 2-propanol (4). Cykloalkenes with butanol (5). Izomers of oktene with butanol (6), with 2-butanol (7), with tert-butanol (8).

reported only for a few systems. Number of available VLE data sets was less than in systems investigated previously in papers.[1–3] For many systems only data measured by one laboratory are reported.

2. Correlation of VLE Data

Correlation of the data was done with equation of state with chemical term (EoSC) method developed by Góral.[1,4] It uses Redlich–Kwong equation of state (RK EoS) appended with association term. The physical part of EoSC has one adjustable binary parameter. The chemical part depends on association. The model of self association of the alkanols is the same as that used in the previous papers of this series.[1–3]

It was found that a weak cross association between the alkanols and the π bonds of the unsaturated hydrocarbons must be taken into account. The model of the cross-association and the relevant equations were described by Góral.[4] In the first stage of this investigation the constant of the coassociation, K_{ij}, was treated as adjustable parameter in EoSC. Analysis of K_{ij} fitted individually to each VLE data set showed that it can be approximated with Eq. (1)

$$K_{ij} = (\alpha K_{ii})^{0.5}, \tag{1a}$$

where K_{ii} is a constant of autoassociation of ith alkanol at given temperature. In further calculations the following values were used:
alkenes

$$\alpha = 0.06\ \text{GPa}^{-1}, \tag{1b}$$

alkynes

$$\alpha = 0.60\ \text{GPa}^{-1}. \tag{1c}$$

The same equation for K_{ij} but with $\alpha = 0.80\ \text{GPa}^{-1}$ was used in the previous paper[3] for coassociation of alkanols with alkylbenzenes.

Having K_{ij} defined by Eqs. (1a)–(1c) EoSC uses only one binary parameter (Θ) for correlation of VLE. This parameter Θ is used in the mixing rule for energetic parameter in RK equation of state. EoSC was successfully used in the previous papers[1–3] for correlation of VLE data in systems of alkanols with hydrocarbons. The results of the correlation were as good as in the case of the two-parameter equation for G^E proposed by Wilson. The same is true for mixtures investigated in this paper with the exception of the data reported by Kudryavtseva and co-workers. They measured azeotropic systems at isobaric conditions. Many of their data sets show systematic deviations from the approximating line calculated by EoSC, whereas the data for the same or similar system measured in another laboratory are well approximated by EoSC. Taking into account this fact and some other tests we assumed that the mentioned deviations are caused by systematic error of the data. The deviations occur near the limits of the concentration range. In this region the measurements are more vulnerable to systematic error of the concentration. This kind of error has negligible influence on the boiling temperature in the vicinity of the azeotropic point. Therefore, some of the mentioned data sets were used in Figs. 1 and 2 after removing one or two of the deviating points from the given data sets.

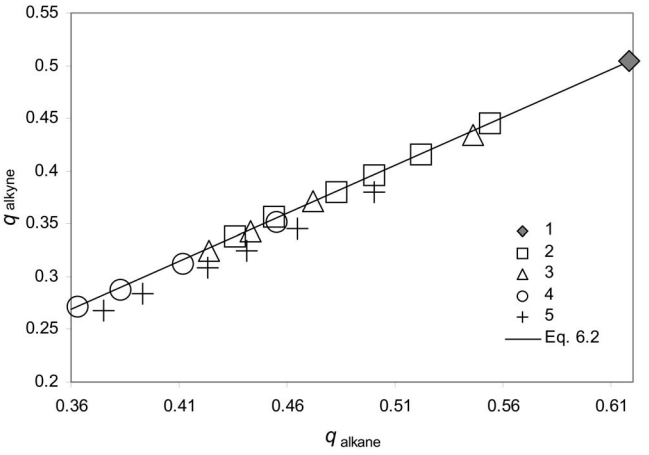


FIG. 2. Values of q for alkynes (q_{alkyne}) and for alkanes (q_{alkane}) in the corresponding mixtures.The points correspond to the following mixtures: hexyne+metanol (1), octyne+1-propanol (2), nonyne+1-propanol (3), 2-octyne+1-butanol (4), 1-octyne+1-butanol (5).

3. Prediction of VLE Data

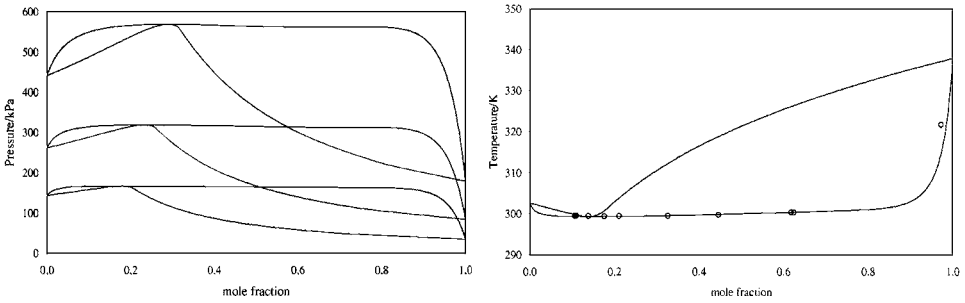
Once the value of the binary parameter Θ in EoSC is known, the corresponding phase diagram of the system can be determined via EoSC. It is also possible to calculate auxiliary thermodynamic functions such as excess Gibbs energy of mixing and activity coefficients of the components. These thermodynamic quantities are related to Θ via equations for chemical potentials yielded by EoSC (see Goral *et al.*[1,4]). These relations can be also used in the opposite direction e.g., if value of any of the thermodynamic functions at some concentration is known then the value of Θ for the corresponding mixture can be determined and after then VLE can

TABLE 1. Methanol–1-pentene

Components	References
Methanol; CH_4O; [67-56-1] 1-Pentene; C_5H_{10}; [109-67-1]	[17]S. K. Ogorodnikov, V. B. Kogan, M. S. Nemtsov, Zh. Prikl. Khim. (Leningrad) **33**, 2685 (1960).

Reference vapor-liquid equilibrium data

T/K = 313.15, predicted			T/K = 333.15, predicted			T/K = 353.15, predicted			P/kPa = 101.32, Reference 17		
P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	T/K	x_1	$y_{1,calc}$
143.85	0.00	0.0000	261.49	0.00	0.0000	441.17	0.00	0.0000	299.55	0.106	0.1350
163.85	0.05	0.1399	304.96	0.05	0.1593	523.10	0.05	0.1695	299.58	0.109	0.1356
166.48	0.10	0.1640	314.41	0.10	0.1976	549.80	0.10	0.2241	299.47	0.138	0.1398
167.11	0.15	0.1750	317.62	0.15	0.2159	561.11	0.15	0.2521	299.45	0.176	0.1439
167.15	0.20	0.1817	318.69	0.20	0.2271	566.20	0.20	0.2695	299.47	0.211	0.1471
166.93	0.25	0.1865	318.80	0.25	0.2348	568.24	0.25	0.2817	299.54	0.326	0.1548
166.57	0.30	0.1903	318.40	0.30	0.2407	568.59	0.30	0.2907	299.78	0.446	0.1617
166.12	0.35	0.1933	317.72	0.35	0.2452	567.96	0.35	0.2977	300.35	0.618	0.1703
165.62	0.40	0.1959	316.88	0.40	0.2489	566.75	0.40	0.3031	300.33	0.624	0.1705
165.10	0.45	0.1980	315.98	0.45	0.2518	565.27	0.45	0.3073	321.68	0.972	0.3897
164.59	0.50	0.1998	315.10	0.50	0.2541	563.75	0.50	0.3105			
164.12	0.55	0.2012	314.33	0.55	0.2557	562.39	0.55	0.3128			
163.75	0.60	0.2021	313.75	0.60	0.2568	561.41	0.60	0.3141			
163.49	0.65	0.2027	313.45	0.65	0.2573	560.99	0.65	0.3146			
163.38	0.70	0.2030	313.45	0.70	0.2573	561.24	0.70	0.3143			
163.34	0.75	0.2030	313.59	0.75	0.2571	561.90	0.75	0.3138			
163.00	0.80	0.2036	313.17	0.80	0.2576	561.79	0.80	0.3138			
161.21	0.85	0.2065	309.92	0.85	0.2610	556.90	0.85	0.3173			
154.17	0.90	0.2176	296.66	0.90	0.2746	534.71	0.90	0.3324			
128.88	0.95	0.2649	249.82	0.95	0.3310	455.06	0.95	0.3946			
35.09	1.00	1.0000	83.94	1.00	1.0000	179.28	1.00	1.0000			
	q_0=0.600			q_0=0.574			q_0=0.539		q_1=0.602 q_0=0.611	σ_1=0.44 σ_0=1.28	



be calculated with EoSC. It enables us to use the physically meaningful quantity for the VLE prediction instead of the empirical parameter Θ.

In this work the prediction of VLE is based on excess chemical potential of the hydrocarbon at an equimolar mixture with alkanol. This quantity ($\mu^E_{0.5}$) divided by gas constant (R) and temperature (T) is denoted here by q

$$q = \mu^E_{0.5}/RT. \tag{2}$$

The advantage of using q is that it is not confined to the equation used for the correlation of the VLE data provided that the equation is able to correlate adequately the data. Therefore the proposed values of q can be checked by investigators, which use another correlating equations.

Figures 1 and 2 show comparison between values of q in the corresponding binary mixtures, which are formed by pairs of the corresponding unsaturated and saturated hydrocarbons (for example cyclohexene and cyclohexane) with the same alcohol at the same temperature.

The values of q for alkenes and alkynes in mixtures with alkanols were obtained from correlation of VLE data with EoSC. The corresponding values for saturated hydrocarbons were calculated with method of VLE prediction for mixtures of alkanols with saturated hydrocarbons described in Part 1 (Goral *et al.*[1]) and Part 2 (Goral *et al.*[2]) of this series.

Each point in Figs. 1 and 2 corresponds to experimental data set, which passed previous stages of verification. Shift of q from the approximating line equal to 0.01 corresponds to shift of the calculated equimolar vapor pressure equal to approximately 1%. With a few exceptions the points are well approximated with straight lines shown in the figures. Therefore it is assumed that the deviations result mainly from errors of the data.

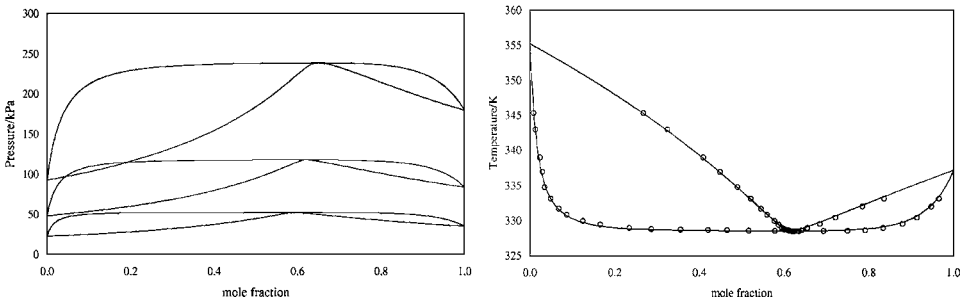
The equations of the lines in Figs. 1 and 2 are as follows:

TABLE 2. Methanol–cyclohexene

Components	**References**
Methanol; CH_4O; [67-56-1] Cyclohexene; C_6H_{10}; [110-83-8]	[8]J. Juza, V. Svoboda, R. Holub, and J. Pick, Collect. Czech. Chem. Commun. **42**, 1453 (1977).

Reference vapor-liquid equilibrium data

T/K = 313.15, predicted			T/K = 333.15, predicted			T/K = 353.15, predicted			P/kPa = 98.66, Reference 8		
P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	T/K	x_1	y_1
22.62	0.00	0.0000	48.11	0.00	0.0000	92.67	0.00	0.0000	345.29	0.0083	0.2677
46.84	0.05	0.5255	99.18	0.05	0.5219	185.96	0.05	0.5058	342.95	0.0130	0.3247
50.11	0.10	0.5604	109.33	0.10	0.5714	211.98	0.10	0.5721	338.99	0.0238	0.4093
51.23	0.15	0.5726	113.25	0.15	0.5896	223.27	0.15	0.5980	336.94	0.0292	0.4488
51.73	0.20	0.5784	115.12	0.20	0.5988	229.13	0.20	0.6116	334.77	0.0347	0.4901
51.96	0.25	0.5815	116.12	0.25	0.6041	232.49	0.25	0.6200	333.12	0.0488	0.5215
52.08	0.30	0.5833	116.69	0.30	0.6075	234.54	0.30	0.6256	331.68	0.0680	0.5454
52.14	0.35	0.5843	117.02	0.35	0.6099	235.86	0.35	0.6297	330.82	0.0868	0.5604
52.17	0.40	0.5850	117.23	0.40	0.6116	236.75	0.40	0.6330	329.93	0.1248	0.5774
52.19	0.45	0.5855	117.37	0.45	0.6131	237.38	0.45	0.6358	329.40	0.1658	0.5868
52.20	0.50	0.5860	117.48	0.50	0.6146	237.86	0.50	0.6386	328.96	0.2344	0.5950
52.21	0.55	0.5868	117.56	0.55	0.6164	238.23	0.55	0.6416	328.78	0.2859	0.5992
52.22	0.60	0.5882	117.61	0.60	0.6187	238.50	0.60	0.6452	328.70	0.3557	0.6022
52.20	0.65	0.5905	117.60	0.65	0.6221	238.61	0.65	0.6499	328.67	0.4205	0.6064
52.13	0.70	0.5944	117.46	0.70	0.6272	238.44	0.70	0.6564	328.62	0.4656	0.6098
51.94	0.75	0.6010	117.07	0.75	0.6352	237.76	0.75	0.6658	328.54	0.5166	0.6127
51.51	0.80	0.6126	116.16	0.80	0.6482	236.09	0.80	0.6803	328.51	0.5782	0.6163
50.58	0.85	0.6333	114.22	0.85	0.6703	232.50	0.85	0.7036	328.50	0.6350	0.6188
48.61	0.90	0.6731	110.20	0.90	0.7107	225.15	0.90	0.7440	328.50	0.6934	0.6238
44.40	0.95	0.7591	101.81	0.95	0.7927	210.23	0.95	0.8215	328.51	0.7497	0.6318
35.09	1.00	1.0000	83.96	1.00	1.0000	179.44	1.00	1.0000	328.59	0.7916	0.6414
									328.93	0.8342	0.6554
									329.51	0.8804	0.6847
									330.42	0.9137	0.7216
									331.99	0.9476	0.7849
									333.11	0.9656	0.8364
	q_0 =0.640			q_0 =0.614			q_0 =0.582		q_1 =0.622 q_0 =0.622	σ_1 =0.56 σ_0 =0.59	



$$q_{\text{alkene}} = 1.04 \cdot q_{\text{alkane}} - 0.048, \tag{3}$$

$$q_{\text{alkyne}} = 0.91 \cdot q_{\text{alkane}} - 0.059. \tag{4}$$

One can be surprised that q_{alkene} and q_{alkyne} in Eqs. (3) and (4) behave differently in respect to q_{alkane} but other properties such as critical temperatures or free volumes in the series: alkane, alkene and alkyne also do not change monotously.

Equations (3) and (4) were used for VLE prediction in this paper. The prediction for a given mixture consists of the following steps:

(1) Calculation of q_{alkane} with the method of prediction described in Part 1[1] and Part 2[2]. For example, if a mixture of 2-methyl–2-butene is considered then the corresponding q_{alkane} is calculated for mixture of 2-methylbutane with the same alkanol at the same temperature;
(2) Calculation of q_{alkene} or q_{alkyne} in the considered mixture with Eq. (3) or Eq. (4);
(3) Calculation of Θ for the considered mixture from the corresponding value of q; and
(4) Calculation of VLE with EoSC using the determined value of Θ.

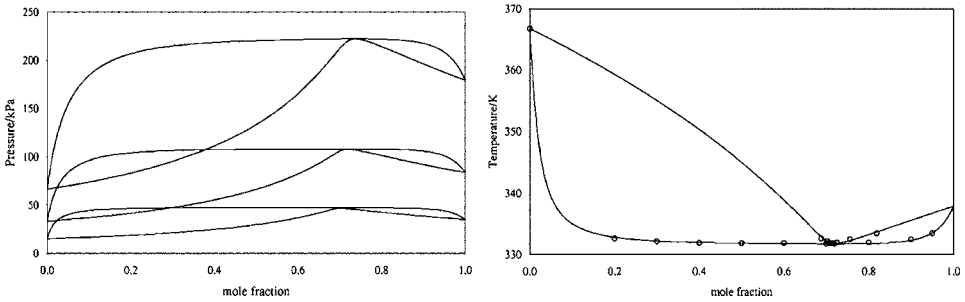
For all the investigated mixtures both the prediction and correlation were done with the same parameters of self-association as those used in previous parts.[1–3] K_{ij} was calculated with Eqs (1a)–(1c). In the case of the correlation $\Theta_{i,j}$ was adjusted to each data set individually, in the case of the prediction $\Theta_{i,j}$ was calculated from the scheme described

TABLE 3. Methanol–1-heptene

Components	References
Methanol; CH_4O; [67-56-1] 1-Heptene; C_7H_{14}; [592-76-7]	[5]L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. **49**, 1844 (1975).

Reference vapor-liquid equilibrium data

T/K = 313.15, predicted			T/K = 333.15, predicted			T/K = 353.15, predicted			P/kPa = 101.32, Reference 5		
P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	T/K	x_1	y_1
14.94	0.00	0.0000	33.26	0.00	0.0000	66.52	0.00	0.0000	366.75	0.00	0.000
40.35	0.05	0.6354	83.95	0.05	0.6079	154.24	0.05	0.5696	332.60	0.20	0.688
44.50	0.10	0.6726	96.33	0.10	0.6623	184.35	0.10	0.6440	332.15	0.30	0.702
46.01	0.15	0.6854	101.50	0.15	0.6825	198.76	0.15	0.6734	331.90	0.40	0.706
46.70	0.20	0.6915	104.15	0.20	0.6928	206.80	0.20	0.6892	331.85	0.50	0.710
47.04	0.25	0.6947	105.63	0.25	0.6989	211.71	0.25	0.6991	331.85	0.60	0.714
47.21	0.30	0.6964	106.52	0.30	0.7029	214.88	0.30	0.7058	331.75	0.70	0.719
47.28	0.35	0.6973	107.07	0.35	0.7056	217.02	0.35	0.7108	331.95	0.80	0.725
47.31	0.40	0.6976	107.42	0.40	0.7075	218.53	0.40	0.7147	332.45	0.90	0.756
47.30	0.45	0.6976	107.65	0.45	0.7090	219.62	0.45	0.7180	333.45	0.95	0.819
47.29	0.50	0.6973	107.80	0.50	0.7102	220.44	0.50	0.7209			
47.27	0.55	0.6968	107.91	0.55	0.7113	221.07	0.55	0.7236			
47.25	0.60	0.6961	107.99	0.60	0.7124	221.57	0.60	0.7265			
47.24	0.65	0.6954	108.04	0.65	0.7136	221.95	0.65	0.7296			
47.24	0.70	0.6949	108.08	0.70	0.7153	222.19	0.70	0.7333			
47.24	0.75	0.6948	108.06	0.75	0.7178	222.25	0.75	0.7382			
47.21	0.80	0.6961	107.92	0.80	0.7223	221.94	0.80	0.7453			
47.06	0.85	0.7012	107.43	0.85	0.7311	220.82	0.85	0.7572			
46.44	0.90	0.7171	105.87	0.90	0.7511	217.61	0.90	0.7800			
44.13	0.95	0.7686	100.93	0.95	0.8042	208.37	0.95	0.8329			
35.09	1.00	1.0000	83.96	1.00	1.0000	179.44	1.00	1.0000			
									q_1 =0.598		σ_1 =0.45
	q_0 =0.637			q_0 =0.600			q_0 =0.557		q_0 =0.603		σ_0 =1.26



above. The resulting standard deviation of pressure (σ) was calculated with Eq. (5)

$$\sigma = \left[\sum_{k=1}^{N-n} (P_{\text{exper.}} - P_{\text{calc.}})_k^2/(N-n-m)\right]^{0.5}, \tag{5}$$

where $P_{\text{exper.}}$ is experimental pressure, $P_{\text{calc.}}$ is the calculated pressure, N is total number of the experimental points in the data set, n is the number of data points for pure substances, and m is the 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 this respect that the vapor pressure and vapor composition were adjusted to liquid composition and temperature via EoSC. Hence accuracy of the VLE description for both types of data is characterized by σ calculated with Eq. (5).

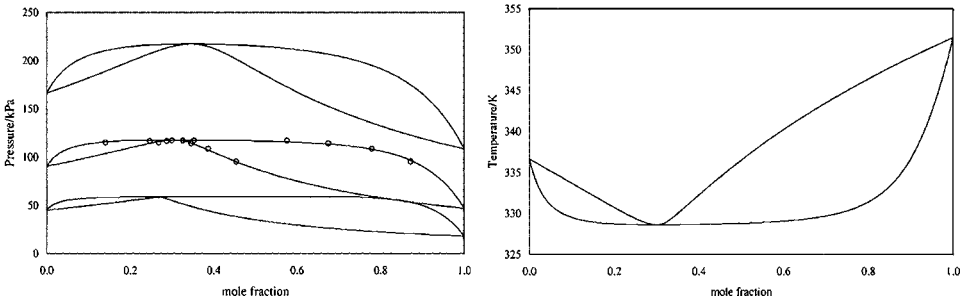
In case of the correlation σ depends mainly on scattering of the VLE data, whereas in the case of the prediction σ is additionally increased by systematic error of the data and error of the prediction. Thus the error of the prediction cannot be estimated from the corresponding σ alone. One should rather consider the difference between the standard deviations of the prediction and the correlation. The two values of σ corresponding to the prediction and the correlation are given below each data set. In order to compare accuracy for data sets measured at various conditions each σ was divided by average pressure in the data set ($\bar{P}$). The mean value of $\sigma/\bar{P}$ for the recommended VLE data is 0.80% in the case of prediction and 0.54% for the correlation. The small difference between these two values indicates excellent accuracy of the prediction as well as the absence of significant systematic errors in the recommended data.

TABLE 4. Ethanol–1-hexene

Components	**References**
Ethanol; C_2H_6O; [64-17-5] 1-Hexene; C_6H_{12}; [592-41-6]	[16]G. W. Lindberg and D. Tassios, J. Chem. Eng. Data **16**, 52 (1971).

Reference vapor-liquid equilibrium data

T/K = 313.15, predicted			T/K = 333.15, Reference 16			T/K = 353.15, predicted			P/kPa = 101.32, predicted		
P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	T/K	x_1	y_1
45.06	0.00	0.0000	115.11	0.141	0.268	166.32	0.00	0.0000	336.63	0.00	0.0000
55.37	0.05	0.2076	116.42	0.247	0.287	193.45	0.05	0.1665	331.01	0.05	0.1900
57.48	0.10	0.2483	117.11	0.353	0.300	205.19	0.10	0.2347	329.51	0.10	0.2447
58.16	0.15	0.2645	117.04	0.576	0.326	211.16	0.15	0.2732	328.95	0.15	0.2697
58.39	0.20	0.2725	114.07	0.675	0.346	214.40	0.20	0.2989	328.72	0.20	0.2841
58.45	0.25	0.2766	108.48	0.779	0.387	216.14	0.25	0.3180	328.62	0.25	0.2936
58.46	0.30	0.2785	95.42	0.872	0.454	216.98	0.30	0.3334	328.60	0.30	0.3003
58.45	0.35	0.2791				217.19	0.35	0.3467	328.62	0.35	0.3055
58.46	0.40	0.2787				216.93	0.40	0.3587	328.66	0.40	0.3098
58.50	0.45	0.2778				216.24	0.45	0.3702	328.72	0.45	0.3136
58.58	0.50	0.2765				215.12	0.50	0.3817	328.80	0.50	0.3174
58.68	0.55	0.2752				213.54	0.55	0.3938	328.91	0.55	0.3215
58.79	0.60	0.2739				211.37	0.60	0.4071	329.07	0.60	0.3264
58.86	0.65	0.2733				208.44	0.65	0.4224	329.31	0.65	0.3329
58.78	0.70	0.2739				204.47	0.70	0.4408	329.69	0.70	0.3423
58.39	0.75	0.2768				199.06	0.75	0.4640	330.32	0.75	0.3568
57.32	0.80	0.2842				191.53	0.80	0.4951	331.41	0.80	0.3808
54.89	0.85	0.3007				180.89	0.85	0.5394	333.31	0.85	0.4232
49.79	0.90	0.3383				165.52	0.90	0.6084	336.67	0.90	0.5041
39.35	0.95	0.4406				142.80	0.95	0.7302	342.48	0.95	0.6677
18.00	1.00	1.0000				108.34	1.00	1.0000	351.45	1.00	1.0000
			q_1=0.537		σ_1=0.95						
q_0=0.626			q_0=0.539		σ_0=0.99	q_0=0.454			q_0=0.509		



4. Description of Tables Containing the Recommended Data

Each system is presented on a separate page, which includes a table of VLE data, the corresponding figures, and auxiliary information.

For the presented systems, 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. These artificial data sets are specified as "predicted." The value of q used for the prediction is denoted as q_0 and given below each artificial data set.

Each experimental data is acompanied by a q value and standard deviation of pressure resulting from the correlation of the data with EoSC. They are denoted by q_1 and σ_1, respectively. For comparison values of q_0 and σ_0 resulting from the prediction are also given. In Tables 8, 10, and 17 one can notice that $\sigma_1 > \sigma_0$. It occurs when the sum of squares in Eq. (5) has a similar value both for correlation and prediction. In such a case the denominator of Eq. (5), which is lower for the correlation, can produce this effect.

It was found that during the correlation of the isobaric data the temperature dependence of the binary parameter, Θ, in EoSC can be ignored, which reduces the number of adjustable parameters. As a consequence isobaric data sets were correlated in a way similar to isothermal data using Θ independent of temperature. In this case q_0 and q_1 given below the isobaric data set correspond to temperature at equimolar concentration of the data set.

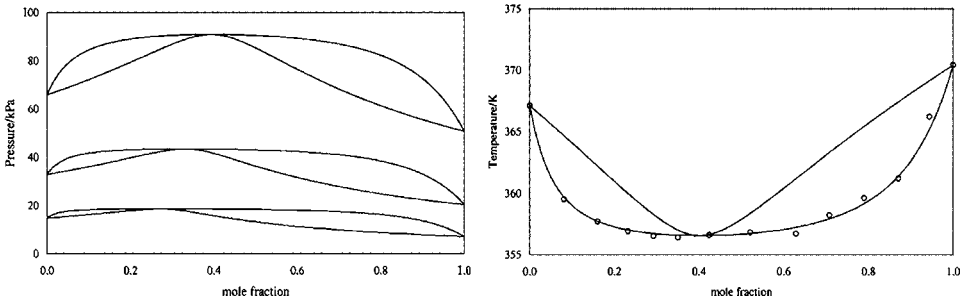
If experimental vapor concentration y is not reported for the selected data set then the experimental data are appended with the calculated values of y. These values are not shown in the figures to differentiate them from the

TABLE 5. 1-Propanol–1-heptene

Components	References
1-Propanol; C_3H_8O; [71-23-8] 1-Heptene; C_7H_{14}; [592-76-7]	[18]I. B. Pukinskii, G. G. Chernik, G. O. Chistyakova, and N. A. Smirnova, Khim. Termodin. Rastvorov (Leningrad) **5**, 157 (1982).

Reference vapor-liquid equilibrium data

T/K = 313.15, predicted			T/K = 333.15, predicted			T/K = 353.15, predicted			P/kPa = 101.3, Reference 18		
P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	T/K	x_1	$y_{1,calc}$
14.75	0.00	0.0000	32.89	0.00	0.0000	65.84	0.00	0.0000	367.1	0.000	0.0000
17.62	0.05	0.1875	39.53	0.05	0.1949	78.88	0.05	0.1936	359.5	0.081	0.2424
18.23	0.10	0.2283	41.63	0.10	0.2524	84.47	0.10	0.2671	357.7	0.160	0.3144
18.46	0.15	0.2477	42.55	0.15	0.2816	87.36	0.15	0.3074	356.9	0.232	0.3493
18.56	0.20	0.2598	43.01	0.20	0.3002	89.00	0.20	0.3339	356.5	0.292	0.3701
18.59	0.25	0.2688	43.25	0.25	0.3139	89.96	0.25	0.3535	356.4	0.350	0.3872
18.59	0.30	0.2763	43.35	0.30	0.3250	90.52	0.30	0.3693	356.6	0.424	0.4076
18.56	0.35	0.2830	43.36	0.35	0.3347	90.80	0.35	0.3830	356.8	0.521	0.4339
18.51	0.40	0.2893	43.30	0.40	0.3438	90.87	0.40	0.3954	356.7	0.629	0.4665
18.44	0.45	0.2957	43.16	0.45	0.3527	90.76	0.45	0.4073	358.2	0.708	0.5026
18.33	0.50	0.3024	42.96	0.50	0.3618	90.48	0.50	0.4193	359.6	0.790	0.5540
18.19	0.55	0.3097	42.66	0.55	0.3716	90.00	0.55	0.4319	361.2	0.871	0.6359
18.01	0.60	0.3182	42.26	0.60	0.3827	89.30	0.60	0.4457	366.2	0.944	0.7824
17.76	0.65	0.3283	41.71	0.65	0.3956	88.30	0.65	0.4614	370.4	1.000	1.0000
17.41	0.70	0.3410	40.96	0.70	0.4115	86.91	0.70	0.4802			
16.93	0.75	0.3579	39.91	0.75	0.4320	84.97	0.75	0.5037			
16.23	0.80	0.3818	38.43	0.80	0.4601	82.24	0.80	0.5346			
15.20	0.85	0.4185	36.27	0.85	0.5013	78.32	0.85	0.5783			
13.63	0.90	0.4813	33.06	0.90	0.5679	72.58	0.90	0.6449			
11.15	0.95	0.6100	28.13	0.95	0.6924	63.96	0.95	0.7595			
7.11	1.00	1.0000	20.34	1.00	1.0000	50.67	1.00	1.0000			
	q_0=0.549			q_0=0.506			q_0=0.457		q_1=0.442 q_0=0.445	σ_1=0.96 σ_0=1.19	



experimental points. The only points shown in the figures correspond to experimental values. The approximating lines result from correlation with EoSC. For the artificial data sets only the predicted curves are shown.

5. Conclusions

The whole collection of data sets for the 18 systems given in the paper (Tables 1–18) is internally consistent, because separate data sets for various mixtures are approximated very well with the same equation, Eq. (3) or Eq. (4). This statement is supported by good agreement of q_1 and q_0 given below each experimental data set. The values of q_1 and q_0 describe the experimental data with similar accuracy as is shown by values of the corresponding standard deviations σ_1 and σ_0. The good accuracy of the prediction demonstrated on the experimental data allows us to believe in good accuracy of the predicted data used to fill the experimental gaps in the tables.

TABLE 6. 2-Propanol–1-hexene

Components

2-Propanol; C_3H_8O; [67-63-0]
1-Hexene; C_6H_{12}; [592-41-6]

References

[20]J. Wisniak and E. Gabai, J. Chem. Eng. Data **41**, 143 (1996).

Reference vapor-liquid equilibrium data

T/K = 313.15, predicted			*T*/K = 333.15, predicted			*T*/K = 353.15, predicted			*P*/kPa = 101.3, Reference 20		
P/kPa	x_1	y_1	*P*/kPa	x_1	y_1	*P*/kPa	x_1	y_1	*T*/K	x_1	$y_{1,calc}$
45.00	0.00	0.0000	90.54	0.00	0.0000	166.15	0.00	0.0000	336.65	0.000	0.0000
49.16	0.05	0.1140	99.65	0.05	0.1232	183.20	0.05	0.1256	332.49	0.127	0.1838
50.06	0.10	0.1476	102.74	0.10	0.1716	191.16	0.10	0.1876	332.44	0.161	0.1989
50.29	0.15	0.1648	103.95	0.15	0.1987	195.19	0.15	0.2256	331.58	0.202	0.2112
50.27	0.20	0.1759	104.36	0.20	0.2168	197.20	0.20	0.2523	331.77	0.224	0.2178
50.15	0.25	0.1843	104.35	0.25	0.2304	198.06	0.25	0.2727	332.38	0.248	0.2254
49.94	0.30	0.1914	104.10	0.30	0.2417	198.18	0.30	0.2895	332.51	0.254	0.2272
49.67	0.35	0.1978	103.64	0.35	0.2517	197.77	0.35	0.3042	332.53	0.343	0.2465
49.33	0.40	0.2041	103.02	0.40	0.2612	196.92	0.40	0.3179	332.56	0.347	0.2474
48.90	0.45	0.2106	102.20	0.45	0.2706	195.65	0.45	0.3312	332.76	0.406	0.2595
48.35	0.50	0.2177	101.15	0.50	0.2805	193.94	0.50	0.3447	333.28	0.494	0.2790
47.67	0.55	0.2257	99.82	0.55	0.2914	191.70	0.55	0.3591	333.96	0.555	0.2953
46.78	0.60	0.2351	98.12	0.60	0.3040	188.82	0.60	0.3750	334.41	0.590	0.3061
45.63	0.65	0.2467	95.93	0.65	0.3189	185.10	0.65	0.3935	335.00	0.639	0.3232
44.13	0.70	0.2616	93.08	0.70	0.3376	180.28	0.70	0.4158	335.71	0.690	0.3451
42.13	0.75	0.2815	89.32	0.75	0.3618	173.98	0.75	0.4438	337.09	0.739	0.3743
39.45	0.80	0.3096	84.32	0.80	0.3950	165.67	0.80	0.4808	338.32	0.791	0.4135
35.82	0.85	0.3522	77.60	0.85	0.4434	154.62	0.85	0.5325	339.71	0.818	0.4425
30.84	0.90	0.4240	68.48	0.90	0.5206	139.77	0.90	0.6101	343.92	0.895	0.5639
23.92	0.95	0.5686	55.97	0.95	0.6620	119.65	0.95	0.7400	344.39	0.908	0.5922
14.21	1.00	1.0000	38.63	1.00	1.0000	92.12	1.00	1.0000	345.70	0.923	0.6330
									350.95	0.976	0.8450
									355.51	1.000	1.0000
									q_1=0.465		σ_1=1.10
q_0=0.518			q_0=0.471			q_0=0.416			q_0=0.466		σ_0=1.22

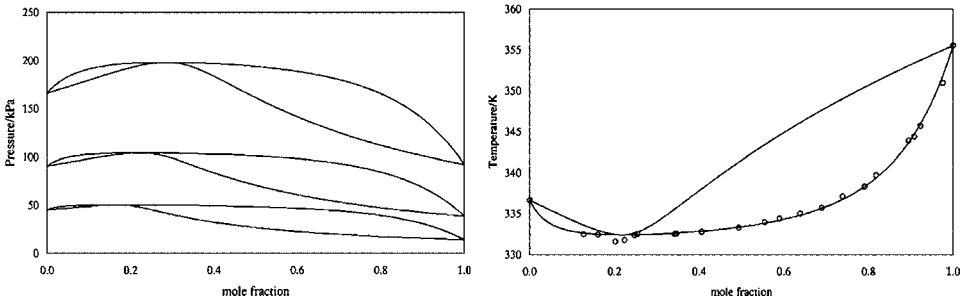


TABLE 7. 1-Butanol–3-ethylcyclopentene

Components

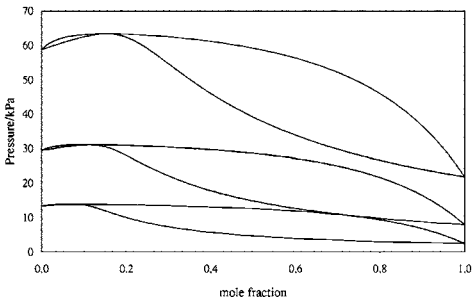
1-Butanol; $C_4H_{10}O$; [71-36-3]
3-Ethylcyclopentene; C_7H_{12}; [694-35-9]

References

[12]L. Kudryavtseva, H. Kirss, and G. Kuranov, Thermochim. Acta **157**, 113 (1990).

Reference vapor-liquid equilibrium data

T/K = 313.15, predicted			T/K = 333.15, predicted			T/K = 353.15, predicted			P/kPa = 79.99, Reference 12		
P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	T/K	x_1	$y_{1,calc}$
13.28	0.00	0.0000	29.43	0.00	0.0000	58.77	0.00	0.0000	363.01	0.000	0.0000
13.79	0.05	0.0655	30.90	0.05	0.0799	62.18	0.05	0.0901	360.75	0.073	0.1167
13.80	0.10	0.0825	31.12	0.10	0.1071	63.13	0.10	0.1286	360.61	0.100	0.1367
13.74	0.15	0.0920	31.08	0.15	0.1228	63.35	0.15	0.1521	360.29	0.140	0.1585
13.65	0.20	0.0990	30.93	0.20	0.1343	63.24	0.20	0.1695	360.23	0.207	0.1850
13.54	0.25	0.1051	30.72	0.25	0.1441	62.94	0.25	0.1839	360.63	0.300	0.2142
13.41	0.30	0.1107	30.44	0.30	0.1530	62.48	0.30	0.1969	360.72	0.354	0.2293
13.25	0.35	0.1163	30.11	0.35	0.1616	61.89	0.35	0.2094	361.49	0.475	0.2657
13.07	0.40	0.1221	29.70	0.40	0.1704	61.15	0.40	0.2218	362.96	0.570	0.3021
12.85	0.45	0.1282	29.22	0.45	0.1797	60.25	0.45	0.2347	363.61	0.608	0.3194
12.59	0.50	0.1349	28.65	0.50	0.1898	59.17	0.50	0.2486	365.16	0.669	0.3536
12.28	0.55	0.1426	27.97	0.55	0.2012	57.87	0.55	0.2640	371.40	0.834	0.5123
11.91	0.60	0.1516	27.15	0.60	0.2144	56.32	0.60	0.2815	384.22	1.000	1.0000
11.45	0.65	0.1625	26.15	0.65	0.2302	54.44	0.65	0.3021			
10.89	0.70	0.1764	24.94	0.70	0.2498	52.16	0.70	0.3271			
10.20	0.75	0.1947	23.46	0.75	0.2753	49.39	0.75	0.3586			
9.32	0.80	0.2206	21.61	0.80	0.3099	45.99	0.80	0.4002			
8.20	0.85	0.2602	19.31	0.85	0.3606	41.80	0.85	0.4583			
6.76	0.90	0.3283	16.40	0.90	0.4423	36.58	0.90	0.5457			
4.89	0.95	0.4740	12.70	0.95	0.5967	30.05	0.95	0.6937			
2.43	1.00	1.0000	7.93	1.00	1.0000	21.81	1.00	1.0000			
	q_0=0.495			q_0=0.456			q_0=0.415		q_1=0.399 q_0=0.393		σ_1=0.44 σ_0=0.51



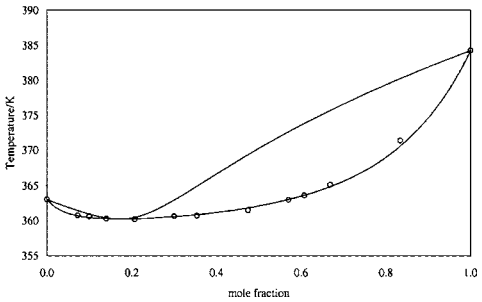


TABLE 8. 1-Butanol–1-butylcyclopentene

Components

1-Butanol; $C_4H_{10}O$; [71-36-3]
1-Butylcyclopentene; C_9H_{16}; [2423-01-0]

References

[10]H. Kirss and I. Vink, Eesti NSV Tead. Akad. Toim., Keem. Geol. **37**, 118 (1988).

Reference vapor-liquid equilibrium data

T/K = 333.15, predicted			T/K = 353.15, predicted			T/K = 373.15, predicted			P/kPa = 79.99, Reference 10		
P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	T/K	x_1	$y_{1,calc}$
3.12	0.00	0.0000	7.83	0.00	0.0000	17.33	0.00	0.0000	421.48	0.000	0.0000
5.79	0.05	0.4788	13.51	0.05	0.4407	27.89	0.05	0.4008	395.84	0.172	0.5934
6.70	0.10	0.5599	16.01	0.10	0.5407	33.59	0.10	0.5175	391.33	0.268	0.6597
7.20	0.15	0.5980	17.49	0.15	0.5892	37.26	0.15	0.5768	388.06	0.407	0.7161
7.53	0.20	0.6227	18.51	0.20	0.6203	39.90	0.20	0.6151	386.02	0.549	0.7600
7.78	0.25	0.6414	19.29	0.25	0.6435	41.95	0.25	0.6434	384.78	0.700	0.8077
7.99	0.30	0.6569	19.91	0.30	0.6624	43.63	0.30	0.6662	384.20	0.799	0.8465
8.15	0.35	0.6705	20.44	0.35	0.6788	45.05	0.35	0.6858	383.89	0.898	0.9016
8.30	0.40	0.6830	20.89	0.40	0.6938	46.29	0.40	0.7034	383.89	0.947	0.9408
8.42	0.45	0.6948	21.29	0.45	0.7079	47.38	0.45	0.7198	384.22	1.000	1.0000
8.52	0.50	0.7064	21.64	0.50	0.7216	48.37	0.50	0.7356			
8.62	0.55	0.7180	21.94	0.55	0.7353	49.25	0.55	0.7511			
8.69	0.60	0.7300	22.22	0.60	0.7493	50.06	0.60	0.7669			
8.76	0.65	0.7429	22.46	0.65	0.7641	50.78	0.65	0.7833			
8.81	0.70	0.7572	22.66	0.70	0.7803	51.43	0.70	0.8009			
8.84	0.75	0.7738	22.82	0.75	0.7986	51.99	0.75	0.8202			
8.85	0.80	0.7943	22.93	0.80	0.8201	52.45	0.80	0.8422			
8.82	0.85	0.8207	22.96	0.85	0.8467	52.78	0.85	0.8682			
8.73	0.90	0.8573	22.87	0.90	0.8812	52.92	0.90	0.9004			
8.53	0.95	0.9115	22.59	0.95	0.9289	52.75	0.95	0.9422			
8.14	1.00	1.0000	21.98	1.00	1.0000	52.09	1.00	1.0000			
									q_1=0.353		σ_1=0.10
	q_0=0.470			q_0=0.422			q_0=0.373		q_0=0.339		σ_0=1.08

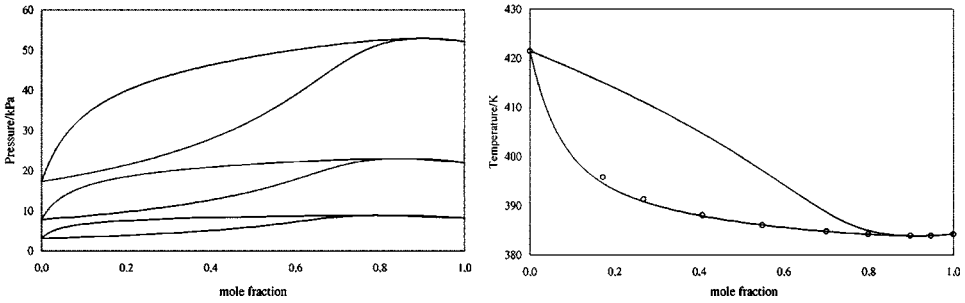


TABLE 9. 1-Butanol–1-octene

Components	References
1-Butanol; $C_4H_{10}O$; [71-36-3] 1-Octene; C_8H_{16}; [111-66-0]	[15]M. Kuus, L. Kudryavtseva, H. Kirss, and O. Eisen, Monatsh. Chem. **112**, 415 (1981).

Reference vapor-liquid equilibrium data

T/K = 333.15, predicted			T/K = 353.15, predicted			T/K = 373.15, predicted			P/kPa = 101.32, Reference 15		
P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	T/K	x_1	$y_{1,calc}$
12.44	0.00	0.0000	27.18	0.00	0.0000	53.70	0.00	0.0000	394.44	0.000	0.0000
14.81	0.05	0.1890	32.18	0.05	0.1867	62.91	0.05	0.1787	385.00	0.153	0.3205
15.57	0.10	0.2468	34.34	0.10	0.2594	67.86	0.10	0.2632	382.43	0.311	0.4192
15.92	0.15	0.2775	35.48	0.15	0.3005	70.84	0.15	0.3147	381.97	0.503	0.4988
16.11	0.20	0.2981	36.15	0.20	0.3287	72.77	0.20	0.3509	382.61	0.700	0.5902
16.21	0.25	0.3141	36.57	0.25	0.3505	74.07	0.25	0.3790	390.83	1.000	1.0000
16.26	0.30	0.3276	36.82	0.30	0.3686	74.96	0.30	0.4025			
16.27	0.35	0.3398	36.95	0.35	0.3848	75.54	0.35	0.4231			
16.24	0.40	0.3513	36.99	0.40	0.3999	75.90	0.40	0.4422			
16.19	0.45	0.3626	36.95	0.45	0.4146	76.05	0.45	0.4605			
16.10	0.50	0.3740	36.83	0.50	0.4293	76.02	0.50	0.4786			
15.98	0.55	0.3861	36.63	0.55	0.4447	75.80	0.55	0.4972			
15.82	0.60	0.3993	36.32	0.60	0.4613	75.38	0.60	0.5169			
15.60	0.65	0.4143	35.90	0.65	0.4798	74.73	0.65	0.5385			
15.32	0.70	0.4320	35.33	0.70	0.5013	73.79	0.70	0.5630			
14.93	0.75	0.4543	34.54	0.75	0.5275	72.47	0.75	0.5918			
14.39	0.80	0.4838	33.47	0.80	0.5609	70.64	0.80	0.6274			
13.62	0.85	0.5262	31.96	0.85	0.6063	68.10	0.85	0.6736			
12.49	0.90	0.5930	29.80	0.90	0.6733	64.52	0.90	0.7377			
10.77	0.95	0.7146	26.63	0.95	0.7836	59.37	0.95	0.8345			
8.05	1.00	1.0000	21.82	1.00	1.0000	51.79	1.00	1.0000			
									q_1=0.352		σ_1=0.55
	q_0=0.480			q_0=0.431			q_0=0.378		q_0=0.354		σ_0=0.56

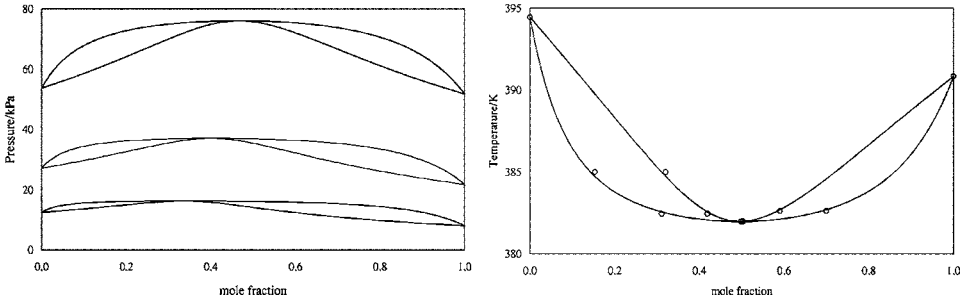


TABLE 10. 1-Butanol–trans-2-octene

Components	**References**
1-Butanol; $C_4H_{10}O$; [71-36-3]	[13]L. Kudryavtseva, M. Kuus, E. Piotrovskaya, and H. Kirss, Eesti NSV Tead. Akad.
trans-2-Octene; C_8H_{16}; [13389-42-9]	Toim. Keem. **34**, 186 (1985).

Reference vapor-liquid equilibrium data

T/K = 333.15, predicted			*T*/K = 353.15, predicted			*T*/K = 373.15, predicted			*P*/kPa = 101.3, Reference 13		
P/kPa	x_1	y_1	*P*/kPa	x_1	y_1	*P*/kPa	x_1	y_1	*T*/K	x_1	$y_{1,calc}$
10.61	0.00	0.0000	23.69	0.00	0.0000	47.63	0.00	0.0000	398.14	0.000	0.0000
13.07	0.05	0.2158	28.85	0.05	0.2089	57.09	0.05	0.1970	384.46	0.310	0.4482
13.87	0.10	0.2784	31.09	0.10	0.2866	62.19	0.10	0.2865	383.36	0.502	0.5281
14.26	0.15	0.3112	32.30	0.15	0.3298	65.31	0.15	0.3400	383.86	0.702	0.6197
14.47	0.20	0.3331	33.04	0.20	0.3592	67.37	0.20	0.3774	386.16	0.851	0.7333
14.60	0.25	0.3500	33.52	0.25	0.3817	68.80	0.25	0.4062	390.86	1.000	1.0000
14.68	0.30	0.3642	33.83	0.30	0.4005	69.81	0.30	0.4301			
14.71	0.35	0.3770	34.03	0.35	0.4172	70.53	0.35	0.4512			
14.72	0.40	0.3890	34.14	0.40	0.4327	71.02	0.40	0.4706			
14.70	0.45	0.4007	34.18	0.45	0.4478	71.32	0.45	0.4891			
14.65	0.50	0.4126	34.14	0.50	0.4629	71.44	0.50	0.5074			
14.57	0.55	0.4250	34.02	0.55	0.4785	71.40	0.55	0.5262			
14.45	0.60	0.4384	33.81	0.60	0.4953	71.17	0.60	0.5460			
14.29	0.65	0.4536	33.51	0.65	0.5139	70.73	0.65	0.5675			
14.08	0.70	0.4715	33.07	0.70	0.5353	70.04	0.70	0.5917			
13.77	0.75	0.4937	32.45	0.75	0.5612	69.03	0.75	0.6201			
13.34	0.80	0.5230	31.59	0.80	0.5939	67.57	0.80	0.6547			
12.72	0.85	0.5646	30.36	0.85	0.6380	65.50	0.85	0.6993			
11.79	0.90	0.6293	28.57	0.90	0.7021	62.53	0.90	0.7601			
10.36	0.95	0.7442	25.91	0.95	0.8053	58.20	0.95	0.8503			
8.06	1.00	1.0000	21.82	1.00	1.0000	51.75	1.00	1.0000			
	q_0=0.481			q_0=0.431			q_0=0.378		q_1=0.340 q_0=0.350		σ_1=1.15 σ_0=0.94

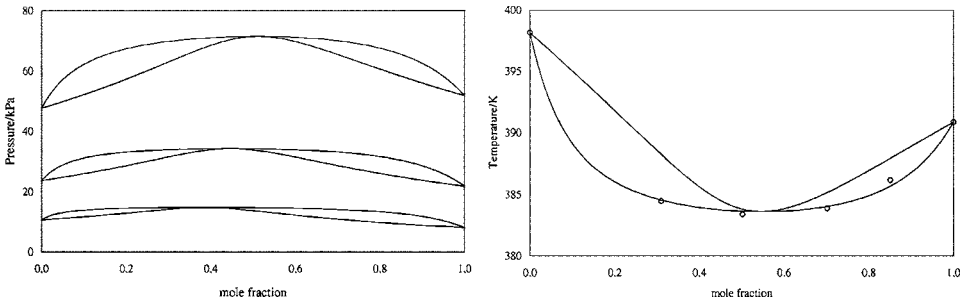


TABLE 11. 1-Butanol–cis-4-octene

Components	References
1-Butanol; $C_4H_{10}O$; [71-36-3] cis-4-Octene; C_8H_{16}; [7642-15-1]	[15]M. Kuus, L. Kudryavtseva, H. Kirss, and O. Eisen, Monatsh. Chem. **112**, 415 (1981).

Reference vapor-liquid equilibrium data

T/K = 333.15, predicted			T/K = 353.15, predicted			T/K = 373.15, predicted			P/kPa = 101.32, Reference 15		
P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	T/K	x_1	$y_{1,calc}$
12.02	0.00	0.0000	26.16	0.00	0.0000	51.69	0.00	0.0000	395.76	0.000	0.0000
14.41	0.05	0.1947	31.21	0.05	0.1928	60.99	0.05	0.1845	387.67	0.103	0.2713
15.19	0.10	0.2542	33.42	0.10	0.2676	66.05	0.10	0.2714	383.30	0.296	0.4226
15.56	0.15	0.2858	34.60	0.15	0.3099	69.13	0.15	0.3241	382.41	0.497	0.5074
15.75	0.20	0.3069	35.31	0.20	0.3387	71.14	0.20	0.3611	383.05	0.698	0.5996
15.86	0.25	0.3232	35.75	0.25	0.3608	72.52	0.25	0.3896	385.25	0.849	0.7156
15.92	0.30	0.3369	36.03	0.30	0.3792	73.46	0.30	0.4133	390.83	1.000	1.0000
15.93	0.35	0.3492	36.19	0.35	0.3955	74.11	0.35	0.4341			
15.92	0.40	0.3608	36.25	0.40	0.4106	74.51	0.40	0.4532			
15.87	0.45	0.3721	36.24	0.45	0.4253	74.72	0.45	0.4713			
15.80	0.50	0.3836	36.14	0.50	0.4400	74.75	0.50	0.4893			
15.69	0.55	0.3956	35.97	0.55	0.4552	74.60	0.55	0.5077			
15.54	0.60	0.4086	35.70	0.60	0.4716	74.26	0.60	0.5270			
15.34	0.65	0.4234	35.32	0.65	0.4897	73.69	0.65	0.5481			
15.08	0.70	0.4408	34.80	0.70	0.5108	72.85	0.70	0.5720			
14.72	0.75	0.4626	34.07	0.75	0.5363	71.65	0.75	0.6000			
14.21	0.80	0.4914	33.07	0.80	0.5688	69.97	0.80	0.6346			
13.49	0.85	0.5328	31.66	0.85	0.6131	67.59	0.85	0.6795			
12.41	0.90	0.5982	29.61	0.90	0.6784	64.19	0.90	0.7419			
10.74	0.95	0.7176	26.55	0.95	0.7865	59.23	0.95	0.8366			
8.05	1.00	1.0000	21.83	1.00	1.0000	51.79	1.00	1.0000			
									q_1 =0.349		σ_1 =0.56
	q_0 =0.480			q_0 =0.431			q_0 =0.378		q_0 =0.353		σ_0 =0.77

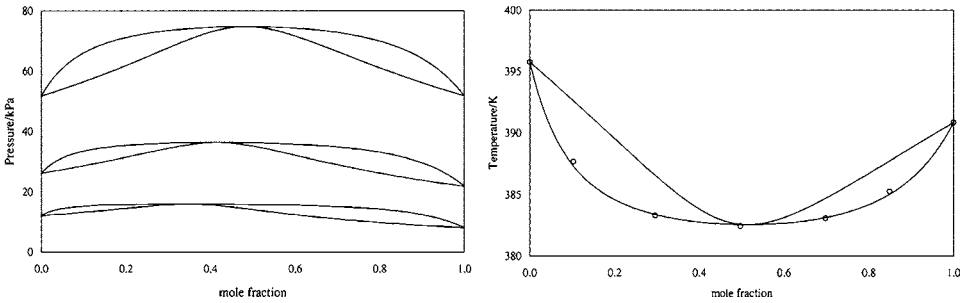


TABLE 12. 1-Butanol–trans-4-octene

Components	**References**
1-Butanol; $C_4H_{10}O$; [71-36-3]	[14]M. Kuus, R. H. Kamdron, and H. H. Kirss, Tr. Tallin. Politekhn. Inst. **509**, 37 (1981).
trans-4-Octene ; C_8H_{16}; [14850-23-8]	

Reference vapor-liquid equilibrium data

T/K = 333.15, predicted			*T*/K = 353.15, predicted			*T*/K = 373.15, predicted			*P*/kPa = 101.32, Reference 14		
P/kPa	x_1	y_1	*P*/kPa	x_1	y_1	*P*/kPa	x_1	y_1	*T*/K	x_1	y_1
11.88	0.00	0.0000	26.09	0.00	0.0000	51.80	0.00	0.0000	395.57	0.000	0.000
14.28	0.05	0.1966	31.15	0.05	0.1932	61.09	0.05	0.1841	387.72	0.102	0.278
15.05	0.10	0.2556	33.32	0.10	0.2670	66.06	0.10	0.2698	382.91	0.299	0.440
15.41	0.15	0.2867	34.48	0.15	0.3087	69.07	0.15	0.3217	382.17	0.499	0.518
15.61	0.20	0.3077	35.17	0.20	0.3371	71.03	0.20	0.3581	382.81	0.694	0.594
15.72	0.25	0.3239	35.60	0.25	0.3590	72.36	0.25	0.3864	384.91	0.849	0.702
15.77	0.30	0.3377	35.87	0.30	0.3774	73.28	0.30	0.4100	390.83	1.000	1.000
15.79	0.35	0.3500	36.02	0.35	0.3937	73.90	0.35	0.4308			
15.77	0.40	0.3616	36.08	0.40	0.4090	74.29	0.40	0.4500			
15.73	0.45	0.3731	36.06	0.45	0.4238	74.49	0.45	0.4684			
15.65	0.50	0.3847	35.97	0.50	0.4388	74.50	0.50	0.4867			
15.55	0.55	0.3969	35.79	0.55	0.4544	74.33	0.55	0.5055			
15.40	0.60	0.4102	35.51	0.60	0.4711	73.97	0.60	0.5254			
15.20	0.65	0.4254	35.12	0.65	0.4899	73.38	0.65	0.5472			
14.93	0.70	0.4433	34.59	0.70	0.5116	72.51	0.70	0.5718			
14.57	0.75	0.4657	33.85	0.75	0.5378	71.28	0.75	0.6008			
14.06	0.80	0.4955	32.83	0.80	0.5714	69.57	0.80	0.6364			
13.33	0.85	0.5380	31.41	0.85	0.6168	67.17	0.85	0.6824			
12.26	0.90	0.6046	29.37	0.90	0.6833	63.79	0.90	0.7458			
10.63	0.95	0.7246	26.37	0.95	0.7916	58.93	0.95	0.8406			
8.05	1.00	1.0000	21.83	1.00	1.0000	51.79	1.00	1.0000			
									q_1 =0.359		σ_1 =0.34
	q_0 =0.481			q_0 =0.431			q_0 =0.378		q_0 =0.353		σ_0 =0.74

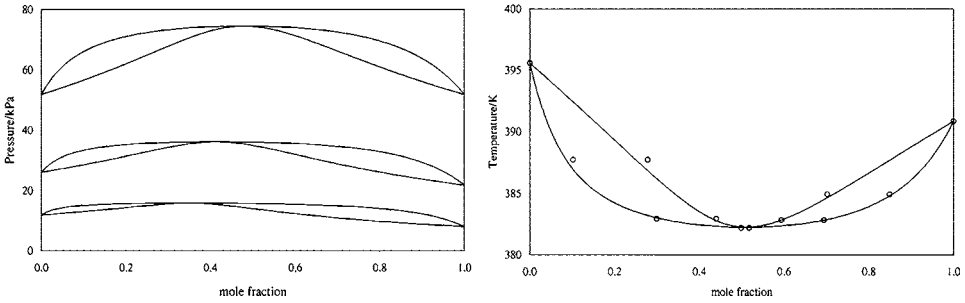


TABLE 13. 2-Butanol–1-hexene

Components

2-Butanol; $C_4H_{10}O$; [78-92-2]
1-Hexene; C_6H_{12}; [592-41-6]

References

[7]D. O. Hanson and M. Van Winkle, J. Chem. Eng. Data **12**, 319 (1967).

Reference vapor-liquid equilibrium data

T/K = 313.15, predicted			T/K = 333.15, Reference 7			T/K = 353.15, predicted			P/kPa = 101.32, predicted		
P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	T/K	x_1	y_1
45.06	0.00	0.0000	90.62	0.000	0.000	166.32	0.00	0.0000	336.63	0.00	0.0000
45.75	0.05	0.0484	91.67	0.062	0.058	168.78	0.05	0.0554	336.13	0.05	0.0538
45.55	0.10	0.0644	91.39	0.099	0.075	168.66	0.10	0.0869	336.21	0.10	0.0790
45.20	0.15	0.0732	91.38	0.103	0.076	167.53	0.15	0.1086	336.44	0.15	0.0950
44.81	0.20	0.0793	89.57	0.201	0.101	165.88	0.20	0.1254	336.75	0.20	0.1072
44.39	0.25	0.0842	87.13	0.304	0.121	163.89	0.25	0.1397	337.12	0.25	0.1175
43.92	0.30	0.0886	83.58	0.416	0.142	161.59	0.30	0.1526	337.54	0.30	0.1272
43.39	0.35	0.0928	79.37	0.518	0.161	158.97	0.35	0.1650	338.03	0.35	0.1368
42.79	0.40	0.0970	74.59	0.605	0.183	156.00	0.40	0.1774	338.60	0.40	0.1468
42.08	0.45	0.1015	63.65	0.747	0.239	152.62	0.45	0.1903	339.27	0.45	0.1577
41.25	0.50	0.1064	49.18	0.861	0.332	148.74	0.50	0.2042	340.08	0.50	0.1702
40.24	0.55	0.1120	36.57	0.930	0.476	144.26	0.55	0.2196	341.06	0.55	0.1848
39.02	0.60	0.1188	36.45	0.930	0.478	139.08	0.60	0.2373	342.26	0.60	0.2027
37.51	0.65	0.1272	18.15	1.000	1.000	133.04	0.65	0.2582	343.75	0.65	0.2251
35.61	0.70	0.1379				125.96	0.70	0.2837	345.62	0.70	0.2543
33.23	0.75	0.1525				117.63	0.75	0.3160	348.00	0.75	0.2937
30.20	0.80	0.1735				107.79	0.80	0.3588	351.03	0.80	0.3486
26.30	0.85	0.2065				96.11	0.85	0.4189	354.92	0.85	0.4282
21.27	0.90	0.2653				82.20	0.90	0.5102	359.86	0.90	0.5468
14.73	0.95	0.3994				65.55	0.95	0.6667	366.02	0.95	0.7270
6.15	1.00	1.0000				45.56	1.00	1.0000	373.43	1.00	1.0000
	q_0=0.495		q_1=0.418 q_0=0.427		σ_1=0.53 σ_0=0.90		q_0=0.361			q_0=0.359	

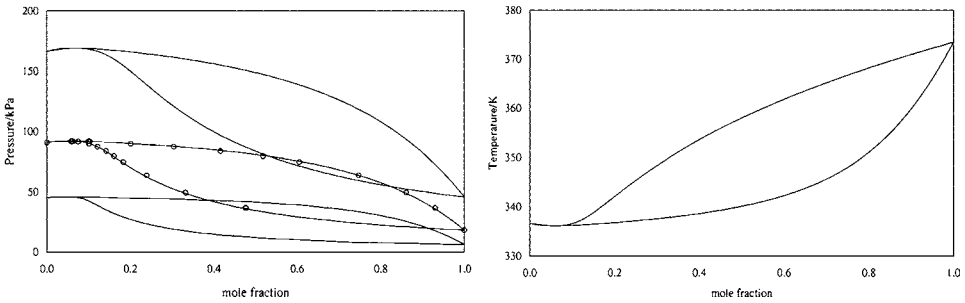


TABLE 14. 2-Methyl-2-propanol–2-methyl-2-butene

Components	**References**
2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0] 2-Methyl-2-butene; C_5H_{10}; [513-35-9]	[19]W. V. Wilding, N. F. Giles, and L. C. Wilson, J. Chem. Eng. Data **41**, 1239 (1996).

Reference vapor-liquid equilibrium data

T/K = 303.15, Ref. 1			T/K = 338.15, predicted			T/K = 373.15, Reference 19			P/kPa = 101.32, predicted		
P/kPa	x_1	$y_{1,calc}$	P/kPa	x_1	y_1	P/kPa	x_1	$y_{1,calc}$	T/K	x_1	y_1
74.888	0.0000	0.0000	231.14	0.00	0.0000	566.85	0.0000	0.0000	311.72	0.00	0.0000
75.085	0.0238	0.0189	231.19	0.05	0.0415	569.39	0.0292	0.0320	311.81	0.05	0.0330
74.787	0.0448	0.0273	228.98	0.10	0.0644	569.84	0.0494	0.0503	312.14	0.10	0.0462
73.866	0.0975	0.0385	226.00	0.15	0.0804	568.58	0.1034	0.0893	312.53	0.15	0.0549
71.448	0.2063	0.0505	222.58	0.20	0.0933	556.99	0.2156	0.1462	312.95	0.20	0.0621
68.309	0.3161	0.0603	218.75	0.25	0.1048	537.80	0.3253	0.1898	313.44	0.25	0.0688
64.528	0.4175	0.0702	214.49	0.30	0.1158	515.35	0.4093	0.2219	313.99	0.30	0.0756
64.600	0.4225	0.0708	209.71	0.35	0.1269	511.28	0.4399	0.2340	314.64	0.35	0.0829
60.328	0.5150	0.0822	204.34	0.40	0.1384	486.20	0.5109	0.2641	315.41	0.40	0.0912
59.809	0.5272	0.0840	198.28	0.45	0.1509	480.13	0.5447	0.2798	316.32	0.45	0.1007
53.265	0.6401	0.1049	191.42	0.50	0.1647	443.87	0.6268	0.3239	317.41	0.50	0.1120
53.129	0.6404	0.1050	183.68	0.55	0.1805	439.33	0.6515	0.3393	318.71	0.55	0.1259
46.048	0.7322	0.1328	174.91	0.60	0.1989	393.87	0.7259	0.3948	320.29	0.60	0.1433
36.447	0.8270	0.1864	164.99	0.65	0.2210	341.11	0.8206	0.4968	322.20	0.65	0.1658
24.115	0.9160	0.3129	153.79	0.70	0.2482	269.74	0.9163	0.6755	324.54	0.70	0.1957
16.037	0.9606	0.4878	141.13	0.75	0.2829	235.91	0.9560	0.7970	327.42	0.75	0.2366
12.619	0.9781	0.6297	126.86	0.80	0.3290	214.59	0.9795	0.8934	330.98	0.80	0.2945
7.723	1.0000	1.0000	110.78	0.85	0.3936	195.05	1.0000	1.0000	335.37	0.85	0.3789
			92.68	0.90	0.4913				340.80	0.90	0.5059
			72.34	0.95	0.6568				347.41	0.95	0.7007
			49.52	1.00	1.0000				355.24	1.00	1.0000

q_1 =0.423	σ_1 =0.64		q_1 =0.271	σ_1 =2.41			
q_0 =0.427	σ_0 =0.66	q_0 =0.338	q_0 =0.264	σ_0 =4.04	q_0 =0.362		

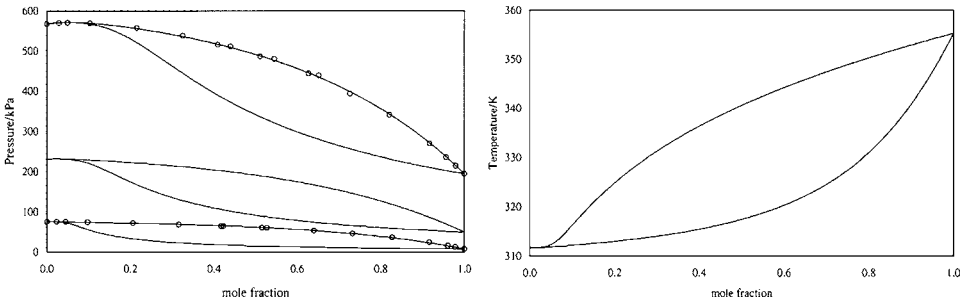


TABLE 15. Methanol–1-hexyne

Components

Methanol; CH_4O; [67-56-1]
1-Hexyne; C_6H_{10}; [693-02-7]

References

[6]M. Yu. Toome and L. S. Kudryavtseva, Tr. Tallin. Politekh. Inst. **509**, 27 (1981).

Reference vapor-liquid equilibrium data

T/K = 313.15, predicted			T/K = 333.15, predicted			T/K = 353.15, predicted			P/kPa = 101.3, Reference 6		
P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	T/K	x_1	$y_{1,\mathrm{calc}}$
33.75	0.00	0.0000	69.99	0.00	0.0000	131.79	0.00	0.0000	344.51	0.000	0.0000
47.79	0.05	0.3132	99.04	0.05	0.3121	184.52	0.05	0.3023	328.04	0.503	0.5164
51.53	0.10	0.3746	109.16	0.10	0.3889	207.61	0.10	0.3937	327.92	0.537	0.5238
53.23	0.15	0.4032	114.17	0.15	0.4259	220.24	0.15	0.4398	328.01	0.608	0.5414
54.20	0.20	0.4212	117.14	0.20	0.4491	228.08	0.20	0.4690	328.67	0.753	0.5922
54.81	0.25	0.4347	119.07	0.25	0.4660	233.36	0.25	0.4901	337.85	1.000	1.0000
55.24	0.30	0.4459	120.42	0.30	0.4797	237.10	0.30	0.5069			
55.53	0.35	0.4561	121.38	0.35	0.4917	239.84	0.35	0.5213			
55.72	0.40	0.4658	122.06	0.40	0.5029	241.87	0.40	0.5343			
55.82	0.45	0.4756	122.52	0.45	0.5138	243.33	0.45	0.5467			
55.83	0.50	0.4858	122.77	0.50	0.5249	244.32	0.50	0.5589			
55.74	0.55	0.4968	122.80	0.55	0.5366	244.85	0.55	0.5716			
55.55	0.60	0.5089	122.59	0.60	0.5493	244.89	0.60	0.5851			
55.21	0.65	0.5226	122.09	0.65	0.5636	244.37	0.65	0.6001			
54.69	0.70	0.5388	121.21	0.70	0.5803	243.14	0.70	0.6172			
53.91	0.75	0.5587	119.82	0.75	0.6005	240.96	0.75	0.6378			
52.76	0.80	0.5843	117.67	0.80	0.6263	237.41	0.80	0.6637			
51.03	0.85	0.6197	114.35	0.85	0.6616	231.73	0.85	0.6985			
48.29	0.90	0.6739	109.05	0.90	0.7144	222.55	0.90	0.7492			
43.67	0.95	0.7710	100.15	0.95	0.8049	207.10	0.95	0.8329			
35.10	1.00	1.0000	83.97	1.00	1.0000	179.47	1.00	1.0000			
									q_1 =0.505		σ_1 =0.21
	q_0 =0.525			q_0 =0.496			q_0 =0.461		q_0 =0.504		σ_0 =0.28

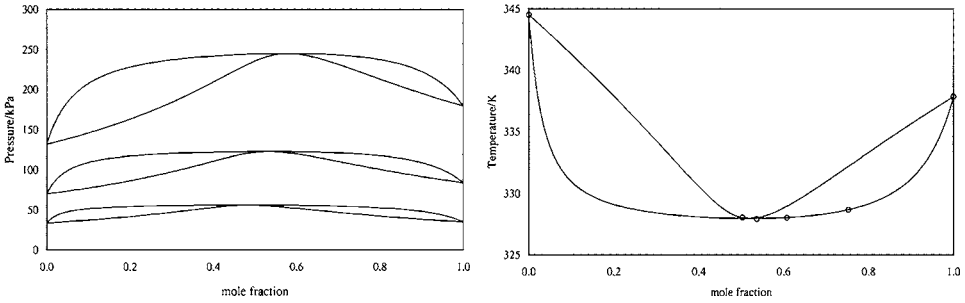


TABLE 16. 1-Propanol–1-octyne

Components	**References**
1-Propanol; C_3H_8O; [71-23-8] 1-Octyne; C_8H_{14}; [629-05-0]	[11]L. Kudryavtseva, M. Grinchak, E. Kiryanen, I. Balashova, and E. Siimer, Eesti NSV Tead. Akad. Toim., Keem. **38**, 34 (1989).

Reference vapor-liquid equilibrium data

T/K = 333.15, predicted			T/K = 353.15, predicted			T/K = 373.15, predicted			P/kPa = 101.32, Reference 11		
P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	T/K	x_1	$y_{1,calc}$
9.86	0.00	0.0000	22.27	0.00	0.0000	45.31	0.00	0.0000	399.39	0.0000	0.0000
15.25	0.05	0.3767	32.83	0.05	0.3466	63.79	0.05	0.3150	373.35	0.3491	0.6429
17.73	0.10	0.4791	38.70	0.10	0.4631	75.71	0.10	0.4420	372.13	0.4411	0.6793
19.17	0.15	0.5297	42.45	0.15	0.5242	84.05	0.15	0.5129	370.33	0.5854	0.7301
20.13	0.20	0.5617	45.08	0.20	0.5635	90.23	0.20	0.5598	369.29	0.7435	0.7926
20.82	0.25	0.5852	47.04	0.25	0.5923	95.04	0.25	0.5943	369.27	0.7937	0.8174
21.35	0.30	0.6040	48.58	0.30	0.6152	98.91	0.30	0.6218	368.96	0.8766	0.8686
21.78	0.35	0.6202	49.84	0.35	0.6347	102.13	0.35	0.6450	370.10	1.0000	1.0000
22.13	0.40	0.6349	50.89	0.40	0.6522	104.88	0.40	0.6655			
22.43	0.45	0.6488	51.79	0.45	0.6685	107.25	0.45	0.6844			
22.68	0.50	0.6625	52.56	0.50	0.6843	109.33	0.50	0.7024			
22.88	0.55	0.6763	53.22	0.55	0.7000	111.16	0.55	0.7201			
23.05	0.60	0.6907	53.79	0.60	0.7162	112.78	0.60	0.7380			
23.18	0.65	0.7063	54.26	0.65	0.7333	114.19	0.65	0.7566			
23.25	0.70	0.7236	54.62	0.70	0.7519	115.39	0.70	0.7764			
23.27	0.75	0.7436	54.86	0.75	0.7730	116.35	0.75	0.7981			
23.21	0.80	0.7678	54.94	0.80	0.7977	117.03	0.80	0.8229			
23.03	0.85	0.7986	54.79	0.85	0.8278	117.32	0.85	0.8521			
22.66	0.90	0.8403	54.30	0.90	0.8667	117.08	0.90	0.8880			
21.97	0.95	0.9012	53.27	0.95	0.9201	116.02	0.95	0.9348			
20.72	1.00	1.0000	51.32	1.00	1.0000	113.62	1.00	1.0000			
									q_1 =0.334		σ_1 =0.86
	q_0 =0.432			q_0 =0.384			q_0 =0.334		q_0 =0.339		σ_0 =0.93

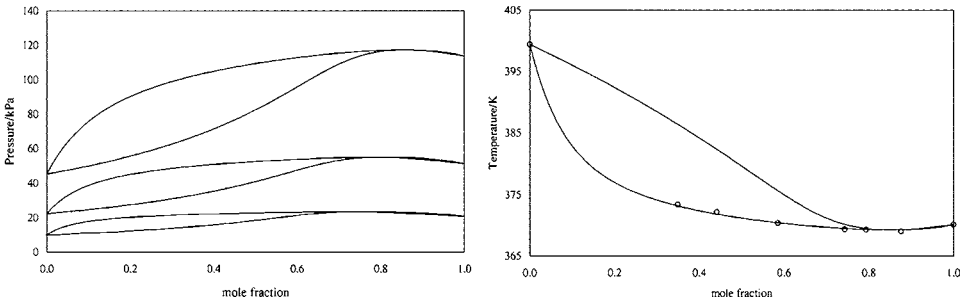


TABLE 17. 1-Propanol–1-nonyne

Components	References
1-Propanol; C_3H_8O; [71-23-8] 1-Nonyne; C_9H_{16}; [3452-09-3]	[21]E. Siimer, M. Grintchak, M. Kuus, and L. Kudryavtseva, Thermochim. Acta, **140**, 49 (1989).

Reference vapor-liquid equilibrium data

T/K = 333.15, predicted			T/K = 353.15, predicted			T/K = 373.15, predicted			P/kPa = 101.32, Reference 21		
P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	T/K	x_1	$y_{1,calc}$
5.03	0.00	0.0000	11.58	0.00	0.0000	23.68	0.00	0.0000	424.21	0.000	0.0000
10.68	0.05	0.5462	22.66	0.05	0.5071	43.01	0.05	0.4681	375.20	0.511	0.8220
13.37	0.10	0.6476	28.99	0.10	0.6266	55.77	0.10	0.6029	372.29	0.703	0.8683
14.97	0.15	0.6927	33.11	0.15	0.6821	64.86	0.15	0.6689	371.16	0.873	0.9225
16.05	0.20	0.7197	36.07	0.20	0.7157	71.74	0.20	0.7094	370.19	1.000	1.0000
16.86	0.25	0.7386	38.32	0.25	0.7391	77.20	0.25	0.7377			
17.49	0.30	0.7533	40.14	0.30	0.7571	81.70	0.30	0.7594			
18.02	0.35	0.7657	41.65	0.35	0.7720	85.53	0.35	0.7771			
18.47	0.40	0.7766	42.96	0.40	0.7850	88.87	0.40	0.7923			
18.87	0.45	0.7867	44.12	0.45	0.7968	91.86	0.45	0.8060			
19.23	0.50	0.7963	45.17	0.50	0.8079	94.58	0.50	0.8187			
19.55	0.55	0.8059	46.13	0.55	0.8187	97.09	0.55	0.8309			
19.84	0.60	0.8155	47.01	0.60	0.8296	99.43	0.60	0.8429			
20.11	0.65	0.8256	47.84	0.65	0.8408	101.64	0.65	0.8550			
20.36	0.70	0.8366	48.60	0.70	0.8526	103.73	0.70	0.8670			
20.59	0.75	0.8488	49.32	0.75	0.8657	105.72	0.75	0.8810			
20.78	0.80	0.8633	49.98	0.80	0.8806	107.61	0.80	0.8960			
20.94	0.85	0.8814	50.57	0.85	0.8984	109.39	0.85	0.9130			
21.03	0.90	0.9056	51.05	0.90	0.9212	111.02	0.90	0.9340			
20.99	0.95	0.9413	51.32	0.95	0.9525	112.39	0.95	0.9610			
20.66	1.00	1.0000	51.15	1.00	1.0000	113.24	1.00	1.0000			
									q_1 =0.323		σ_1 =0.96
	q_0 =0.433			q_0 =0.384			q_0 =0.333		q_0 =0.326		σ_0 =0.85

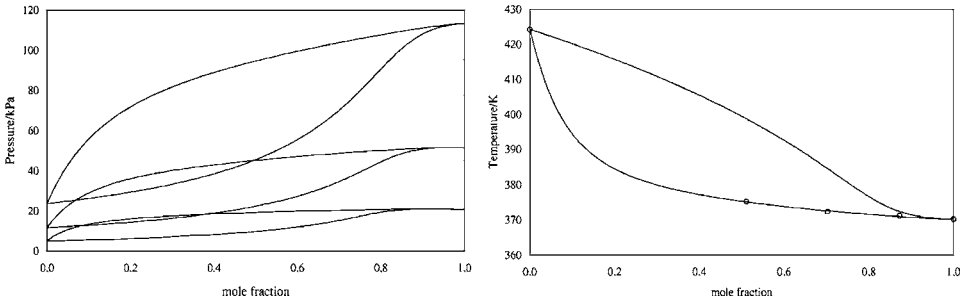
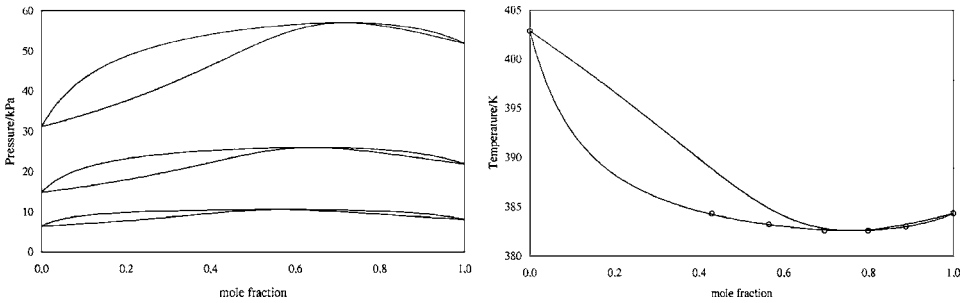


TABLE 18. 1-Butanol–2-octyne

Components	References
1-Butanol; $C_4H_{10}O$; [71-36-3] 2-Octyne; C_8H_{14}; [2809-67-8]	[9]H. Kirss, E. Siimer, and L. Kudryavtseva, Thermochim. Acta, **228**, 283 (1993).

Reference vapor-liquid equilibrium data

T/K = 333.15, predicted			T/K = 353.15, predicted			T/K = 373.15, predicted			P/kPa = 79.99, Reference 9		
P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	T/K	x_1	$y_{1,calc}$
6.37	0.00	0.0000	14.84	0.00	0.0000	31.13	0.00	0.0000	402.84	0.000	0.0000
8.21	0.05	0.2539	18.76	0.05	0.2407	38.50	0.05	0.2242	384.30	0.430	0.5921
9.04	0.10	0.3424	20.88	0.10	0.3407	43.12	0.10	0.3324	383.19	0.565	0.6559
9.52	0.15	0.3914	22.23	0.15	0.3990	46.32	0.15	0.3993	382.56	0.696	0.7216
9.84	0.20	0.4250	23.17	0.20	0.4397	48.68	0.20	0.4468	382.55	0.799	0.7849
10.07	0.25	0.4509	23.87	0.25	0.4712	50.50	0.25	0.4839	382.98	0.888	0.8577
10.23	0.30	0.4727	24.41	0.30	0.4974	51.96	0.30	0.5148	384.32	1.000	1.0000
10.36	0.35	0.4919	24.84	0.35	0.5205	53.15	0.35	0.5419			
10.45	0.40	0.5096	25.17	0.40	0.5417	54.13	0.40	0.5666			
10.52	0.45	0.5265	25.44	0.45	0.5619	54.94	0.45	0.5898			
10.56	0.50	0.5432	25.64	0.50	0.5816	55.61	0.50	0.6123			
10.58	0.55	0.5602	25.78	0.55	0.6015	56.15	0.55	0.6348			
10.58	0.60	0.5780	25.86	0.60	0.6222	56.56	0.60	0.6577			
10.55	0.65	0.5974	25.88	0.65	0.6442	56.84	0.65	0.6817			
10.48	0.70	0.6194	25.83	0.70	0.6685	56.98	0.70	0.7075			
10.37	0.75	0.6452	25.69	0.75	0.6961	56.94	0.75	0.7362			
10.20	0.80	0.6770	25.42	0.80	0.7288	56.71	0.80	0.7689			
9.95	0.85	0.7183	25.00	0.85	0.7692	56.20	0.85	0.8076			
9.56	0.90	0.7753	24.35	0.90	0.8216	55.34	0.90	0.8552			
8.98	0.95	0.8601	23.37	0.95	0.8935	53.96	0.95	0.9165			
8.09	1.00	1.0000	21.88	1.00	1.0000	51.85	1.00	1.0000			
									q_1 =0.287		σ_1 =0.20
	q_0 =0.413			q_0 =0.363			q_0 =0.315		q_0 =0.290		σ_0 =0.23



6. References

[1] M. Góral, P. Oracz, A. Skrzecz, A. Bok, and A. Mączynski, J. Phys. Chem. Ref. Data **31**, 701 (2002).
[2] M. Góral, P. Oracz, A. Skrzecz, A. Bok, and A. Mączynski, J. Phys. Chem. Ref. Data **32**, 1429 (2003).
[3] M. Góral, A. Skrzecz, A. Bok, A. Mączynski, and P. Oracz, J. Phys. Chem. Ref. Data **33**, 959 (2004).
[4] M. Góral, Fluid Phase Equilib. **118**, 27 (1996).
[5] L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. **49**, 1844 (1975).
[6] M. Yu. Toome and L. S. Kudryavtseva, Tr. Tallin. Politekh. Inst. 509, 27 (1981).
[7] D. O. Hanson and M. J. Van Winkle, J. Chem. Eng. Data **12**, 319 (1967).
[8] J. Juza, V. Svoboda, R. Holub, and J. Pick, Collect. Czech. Chem. Commun. **42**, 1453 (1977).
[9] H. Kirss, E. Siimer, and L. Kudryavtseva, Thermochim. Acta **228**, 283 (1993).
[10] H. Kirss and I. Vink, Eesti NSV Tead. Akad. Toim., Keem., Geol. 37, 118 (1988).
[11] L. Kudryavtseva, M. Grinchak, E. Kiryanen, I. Balashova, and E. Siimer, Eesti NSV Tead. Akad. Toim., Keem. 38, 34 (1989).
[12] L. Kudryavtseva, H. Kirss, and G. Kuranov, Thermochim. Acta **157**, 113 (1990).
[13] L. Kudryavtseva, M. Kuus, E. Piotrovskaya, and H. Kirss, Eesti NSV Tead. Akad. Toim. Keem. 34, 186 (1985).
[14] M. Kuus, R. H. Kamdron, and H. H. Kirss, Tr. Tallin. Politekhn. Inst. 509, 37 (1981).
[15] M. Kuus, L. Kudryavtseva, H. Kirss, and O. Eisen, Monatsh. Chem. 112, 415 (1981).
[16] G. W. Lindberg and D. J. Tassios, J. Chem. Eng. Data **16**, 52 (1971).
[17] S. K. Ogorodnikov, V. B. Kogan, and M. S. Nemtsov, Zh. Prikl. Khim. (Leningrad) 33, 2685 (1960).
[18] I. B. Pukinskii, G. G. Chernik, G. O. Chistyakova, and N. A. Smirnova, Khim. Termodin. Rastvorov (Leningrad) 5, 157 (1982).
[19] W. V. Wilding, N. F. Giles, and L. C. Wilson, J. Chem. Eng. Data **41**, 1239 (1996).
[20] J. Wisniak and E. Gabai, J. Chem. Eng. Data **41**, 143 (1996).
[21] E. Siimer, M. Grintchak, M. Kuus, and L. Kudryavtseva, Thermochim. Acta **140**, 49 (1989).