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Vapor−Liquid Equilibrium for Benzene + 2-Methylpentane and Allyl Alcohol + 1-Propanol[†]

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The saturation pressures of 1-propanol at (311 to 353) K were measured by the ebulliometric method. The vapor−liquid equilibrium (VLE), simultaneous measurements of pressure, temperature, and composition of liquid and vapor phases (x, y, p, T), was measured by an ebulliometric method for the system benzene + 2-methylpentane at (313.14, 323.14, and 333.13) K and for the system allyl alcohol + 1-propanol at (313.15, 333.15, and 353.15) K. The experimental vapor pressures were correlated with the Antoine and association + equation of state (AEOS) equations, and VLE was correlated with equations representing the activity coefficient and with the AEOS equation of state.

Introduction

This work is part of an ongoing investigation of phase equilibria for systems of industrial interest sponsored by Project 805 of the Design Institute for Physical Property Data (DIPPR) of the American Institute of Chemical Engineers. In this paper, we report some of the experimental measurements that have been made under Project 805(E)/00. For the investigated mixtures, total pressure data have been reported in the literature only for the system benzene + 2-methylpentane by Funk et al.[1] The complete set of (x, y, p, T) vapor−liquid equilibrium (VLE) data have not been reported, and results cannot be predicted with sufficient accuracy either by using pure-component property data or using a semiempirical method (e.g., a method based on a group contribution concept such as ASOG[2] or UNIFAC[3]).

Experimental Section

Chemicals. Benzene (CA reg. no. 71-43-2) purchased from Sigma-Aldrich Chemie GmbH (HPLC standard >99.5 mol %, 99.69 mass % by GLC) was distilled at subambient pressure on a 25 theoretical plate column. The final purity was >99.9 mass %, and the water content was <0.04% (both by GLC). 2-Methylpentane (CA reg. no. 107-83-5) was purchased from Sigma-Aldrich Chemie GmbH (physicochemical standard >99.5 mol %, purity >99.82 mass %, and water content <0.07% by GLC). Allyl alcohol (CA reg. no. 107-18-6) was purchased from Fluka Chemie GmbH (physicochemical standard >99.5 mol %, purity >99.75 mass %, and water content <0.01% were found by GLC). 1-Propanol (CA reg. no. 71-23-8) was purchased from Fluka Chemie GmbH (physicochemical standard >99.8 mol %, purity >99.9 mass %, and water content <0.01% by GLC). The last three substances were used without further purification.

Analytical Procedure. For the determination of purity and for the analysis of samples equilibrated in the course of VLE measurements via the GLC method with the HP 5890 series II gas chromatograph equipped with an HP 3396 integrator, a thermal conductivity detector (TCD) and an HP−FFAP (poly(ethylene glycol)−TPA modified) 30 m × 0.53 mm × 0.01 μm film thickness column was used. An internal standard was used in the calibration procedure.

Vapor Pressure. Measurements of the pure-compound vapor pressure were performed in Swiętosławski's ebulliometer modified for the determination of VLE (x, y, p, T), as described earlier (Rogalski and Malanowski[4]).

The ebulliometer was connected to the pressure-stabilizing system, which consisted of a 0.6-m^3 buffer vessel coupled to a vacuum pump and a pressurized argon container. The pressure was manually adjusted using a system of valves and a pressurized rubber balloon until the boiling temperature of the sample in the ebulliometer had achieved the desired constant temperature within ±0.005 K. The equilibrium temperature was measured with a SYSTEMTEKNIK AB S1228 thermometer with a platinum resistance probe (resolution: 0.001 K). The temperature fluctuation during runs lasting several hours was within ±0.005 K. No systematic deviations in the temperature measurements were observed. The pressure was determined using a Texas Instruments 144-01 precision pressure gauge with a quartz Bourdon tube no. 8 type 2 (resolution: 0.3 Pa), enabling the pressure determination in the range of (1−137) kPa with a resolution of ±0.5 Pa.

The calibration of the thermometer was made with the ice point of water. The pressure meter was calibrated with vacuum to better than 10^{-2} Pa. In addition, the saturation vapor pressure as a function of temperature was measured for pure hexane and compared with literature data (Willingham et al.[5]). The results agree within the claimed $\delta P/\mathrm{Pa} = \pm 8$ and $\delta T/\mathrm{mK} = \pm 3$.

The estimated accuracy of the pressure measurement was ±10 Pa. The estimated accuracy of the temperature measurement was ±0.01 K. In the handling of vapor−liquid equilibria, the most crucial data are the saturation vapor pressure data of pure components. The vapor pressure data for benzene have been very widely discussed.[6] For the purpose of this paper, we have used the data of Forziati et al.[7] as the closest to our results. For 2-methylpentane, the data of Wilingham et al.[5] have been found to be the most suitable. The temperatures have been converted to the International Temperature Scale of 1990 ITS-90 according to method described by Preston-Thomas.[8] The data were fit with the Antoine equation, and the compari-

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[†] This will be part of a special print edition containing papers reporting experimental results from the various projects of the Design Institute for Physical Properties of the American Institute of Chemical Engineers.

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Table 1. Parameters of Vapor Pressure Equations for Hydrocarbons

	Antoine equation parameters			rmsd(p)/Pa	deviation from
	A	B	C	literature	literature
benzene[a]	6.027183	1208.767	52.664	0.8	3.2
2-methyl-pentane[b]	5.966299	1136.685	46.422	1.4	3.2

	AEOS Equation Parameters				
	T'_c/K	P'_c/bar	ω'	rmsd(p)/kPa	T range/K
benzene[c]	556.1	48.61	0.2451	1.5	287−334
2-methyl-pentane[c]	494.75	29.54	0.2929	1.6	285−334

[a] Reference 7. [b] Reference 5. [c] Reference 22.

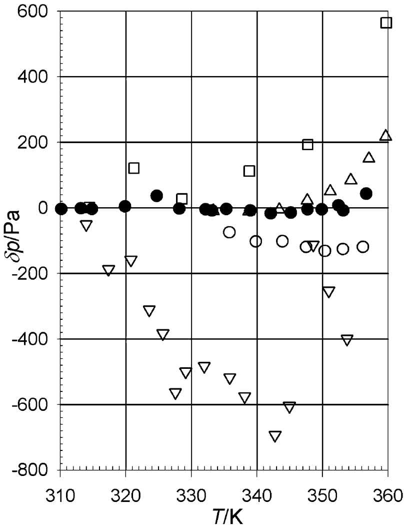

Figure 1. Vapor pressure of 1-propanol correlated with the Antoine equation. Deviations from experimental data: ●, this work; △, Ambrose and Sprake;[10] ▽, Kemme and Kreps;[11] □, Schmidt;[12] ○, Gierycz et al.[13]

Table 2. Vapor Pressure p as Function of the Temperature T of Alcohols

allyl alcohol				1-propanol			
T/K	p/kPa	T/K	p/kPa	T/K	p/kPa	T/K	p/kPa
311.42	6.954	341.54	31.723	310.17	5.876	339.01	26.907
315.81	8.869	344.27	35.822	313.15	6.983	342.11	31.121
319.97	11.079	346.97	40.304	314.84	7.693	345.18	35.819
326.70	15.672	351.37	48.613	319.89	10.176	347.71	40.123
331.84	20.194	353.15	52.334	324.71	13.142	349.93	44.262
334.20	22.603	353.59	53.299	328.14	15.748	352.44	49.359
337.96	26.943	355.70	58.108	332.18	19.313	353.17	50.949
				333.15	20.268	356.70	59.130
				335.34	22.559		

Table 3. Correlation of Alcohols' Vapor Pressures

compound:	allyl alcohol	1-propanol
T/K:	310−360	310−360
Parameters of Antoine Equation (T/K, p/kPa)		
A =	6.936209	7.219284
B =	1513.129	1629.492
C =	63.131	57.556
errors: rmsd(p)/Pa =	7.4	14.7
Parameters of AEOS Equation		
T'_c/K	577.132	478.990
P'_c/bar	63.425	48.416
ω'	0.2948	0.2875
$\Delta H°/(\mathrm{kJ \cdot mol^{-1}})$	−10.438	−22.539
$\Delta S°/(\mathrm{J \cdot mol^{-1}})$	−78.58	−90.63
$\Delta C_p{}^0/(\mathrm{J \cdot mol^{-1}})$	−251.7	−34.01
errors: rmsd(p)/Pa =	15.4	12.6
Enthalpy of Vaporization ($\Delta_{\mathrm{vap}}H°/\mathrm{kJ \cdot mol^{-1}}$) at T/K = 298.15		
calculated from our vapor pressure	46.41	47.75
calorimetric	47 ± 1[a]	47.3−47.5[a]
Daubert and Danner prediction	45.90[b]	47.75[b]

[a] Reference 24. [b] Reference 18.

Table 4. Experimental Results of Vapor−Liquid Equilibrium

x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa
T/K = 313.140			T/K = 323.137			T/K = 333.134		
Benzene (1) + 2-Methylpentane (2)								
0.0000	0.0000	50.650	0.0000	0.0000	72.200	0.0000	0.0000	100.400
0.1143	0.0867	49.389	0.1124	0.0911	70.448	0.1163	0.0861	98.167
0.2298	0.1580	47.676	0.2302	0.1558	68.153	0.2309	0.1578	95.014
0.3166	0.2137	46.293	0.3179	0.2054	66.175	0.3127	0.2046	92.276
0.4461	0.2835	44.110	0.4427	0.2752	63.203	0.4410	0.2703	88.330
0.5558	0.3396	41.932	0.5533	0.3411	60.112	0.5486	0.3398	83.984
0.6331	0.3925	40.112	0.6322	0.3951	57.605	0.6292	0.3929	80.684
0.7154	0.4627	37.907	0.7150	0.4629	54.417	0.7152	0.4653	76.350
0.7870	0.5401	35.318	0.7820	0.5399	51.023	0.7916	0.5392	72.075
0.8543	0.6133	33.025	0.8518	0.6233	47.765	0.8546	0.6144	67.362
0.8941	0.6913	31.087	0.8925	0.6938	45.216	0.8908	0.7050	63.997
0.9313	0.7844	28.731	0.9327	0.7899	41.952	0.9340	0.7939	59.779
0.9574	0.8596	27.140	0.9565	0.8597	39.907	0.9538	0.8539	57.408
1.0000	1.0000	24.350	1.0000	1.0000	36.150	1.0000	1.0000	52.170
T/K =313.15			T/K =333.15			T/K =353.15		
Allyl Alcohol (1) + 1-Propanol (2)								
0.0000	0.0000	6.983	0.0000	0.0000	20.268	0.0000	0.0000	50.951
0.0781	0.0882	7.057	0.0785	0.0851	20.393	0.0781	0.0827	51.133
0.1798	0.1988	7.148	0.1800	0.1943	20.576	0.1813	0.1885	51.361
0.2697	0.2917	7.211	0.2698	0.2861	20.716	0.2697	0.2790	51.516
0.3547	0.3802	7.292	0.3563	0.3730	20.854	0.3568	0.3666	51.739
0.4271	0.4510	7.348	0.4276	0.4444	20.953	0.4074	0.4360	51.845
0.4863	0.5090	7.401	0.4866	0.5023	21.052	0.4661	0.4896	51.953
0.4982	0.5235	7.407	0.5008	0.5164	21.063	0.4833	0.5120	51.999
0.5800	0.6020	7.470	0.5798	0.5940	21.181	0.5611	0.5847	52.088
0.6794	0.6970	7.532	0.6802	0.6902	21.276	0.6604	0.6849	52.233
0.7450	0.7570	7.569	0.7447	0.7538	21.327	0.7449	0.7483	52.269
0.7949	0.8072	7.584	0.7950	0.8019	21.365	0.7960	0.7951	52.296
0.9045	0.9095	7.632	0.9043	0.9073	21.454	0.9044	0.9042	52.322
1.0000	1.0000	7.672	1.0000	1.0000	21.510	1.0000	1.0000	52.336

son is given in Table 1. A discussion of the data for allyl alcohol was given earlier (Lubomska et al.[9]). These data were supplemented to cover a wider temperature range. The vapor pressure of 1-propanol has been determined in the course of this work because of discrepancies in the literature data.[10−13] Examples of the discrepancies are given in Figure 1. The estimated accuracy of the pressure measurement was ±10 Pa, and that of the temperature was ±10 mK. The results for both alcohols are given in Table 2. The vapor pressure data were correlated with the Antoine equation:

$$\log(p/\mathrm{kPa}) = A - \frac{B}{T/\mathrm{K} - \mathrm{C}} \tag{1}$$

The details were described earlier (Antosik et al.[14]). Both alcohols are associating compounds. To represent such mixtures properly, a special treatment is necessary. In previous work,[15] it has been found that the association + equation of state (AEOS) is the most suitable representation of phase equilibria in systems formed by associating or even chemically reacting compounds. In the AEOS model, the thermodynamic properties of an associated mixture are viewed as the result of chemical equilibrium between associated species and physical interactions between all, associated or inert, species in a mixture. Detailed equations have been given (Chylinski et al.[16]).

The correlation results are summarized in Table 3. The root-mean-square deviations of pressure (rmsd(p)/Pa) were calculated by

$$\mathrm{rmsd}(p/\mathrm{Pa}) = \sqrt{\frac{\sum_{i=1}^{n}(p_i^{\mathrm{exptl}} - p_i^{\mathrm{calcd}})^2}{n}} \tag{2}$$

Table 5. Correlation of Vapor−Liquid Equilibrium

Benzene (1) + 2-Methylpentane (2)

equation	parameters				rmsd(y)	rmsd(p)/Pa
	1	2	3	4		
	T/K = 313.14					
Redlich−Kister	0.566097				0.0214	389.6
	0.568363	0.108714			0.0230	113.7
	0.569499	0.109214	−0.010202		0.0228	112.2
	0.568310	0.118738	−0.006428	−0.033797	0.0227	108.1
WILSON	−2789.53	−4839.19			0.0234	131.2
UNIQUAC*	3368.48	−1488.15			0.0233	126.0
	T/K = 323.137					
Redlich−Kister	0.518517				0.0295	492.4
	0.520741	0.098894			0.0312	138.1
	0.521221	0.099050	−0.004225		0.0312	137.7
	0.520801	0.102661	−0.002834	−0.012685	0.0311	136.8
WILSON	−2546.52	−4675.95			0.0315	154.0
UNIQUAC*	3423.44	−1653.74			0.0314	149.5
	T/K = 333.134					
Redlich−Kister	0.481305				0.0404	753.4
	0.483482	0.109557			0.0420	196.1
	0.482938	0.109373	0.004392		0.0421	195.6
	0.480175	0.137503	0.013180	−0.096128	0.0415	115.5
WILSON	−1758.87	−5518.02			0.0424	221.0
UNIQUAC*	2470.51	−949.54			0.0423	212.8
	T/K = from 310 to 355					
AEOS		eq 5			0.0104	18.7

*q_1= 2.4; q_2= 4.164; r_1= 3.1878; r_2= 4.7265

Allyl Alcohol (1) + 1-Propanol (2)

equation	parameters				rmsd(y)	rmsd(p)/Pa
	1	2	3	4		
	T/K = 313.15					
Redlich−Kister	0.000000				0.0023	46.0
	0.032382	0.015024			0.0012	5.2
	0.033159	0.015456	−0.006839		0.0013	5.0
	0.033065	0.029722	−0.006292	−0.046049	0.0021	2.8
WILSON	4989.52	−6409.08			0.0012	5.5
UNIQUAC[a]	−3063.02	3720.42			0.0012	5.5
AEOS	1.9577×10^{-5}	−0.0083			0.0013	11.4
	T/K = 333.15					
Redlich−Kister	0.000000				0.0017	56.7
	0.013889	0.007473			0.0009	9.1
	0.015089	0.007985	−0.010404		0.0009	6.8
	0.015094	0.010884	0.010443	−0.009323	0.0010	6.3
WILSON	4739.92	−5690.91			0.0010	9.9
UNIQUAC[a]	−2727.78	3167.30			0.0010	9.8
AEOS	1.2306×10^{-5}	−0.0104			0.0009	36.1
	T/K = 353.15					
Redlich−Kister	0.000000				0.0119	46.1
	−0.003468	0.007391			0.0114	19.9
	−0.002353	0.007811	−0.009692		0.0114	14.1
	−0.002243	0.011764	−0.010080	−0.012720	0.0112	11.6
WILSON	5876.30	−7054.96			0.0115	22.5
UNIQUAC[a]	291.13	−291.13			0.0119	31.6
AEOS	0.6286×10^{-5}	−0.0273			0.0064	454.8
	T/K = from 310 to 355					
AEOS	eq 3	eq 4			0.0038	271.8

[a] $q_1 = 2.916$; $q_2 = 3.128$; $r_1 = 3.0198$; $r_2 = 3.2499$.

where n is the number of experimental points, p_i^{exptl} is the pressure measured at point number i, and p_i^{calcd} is the pressure calculated from eq 2 at point i. A comparison of correlation results with literature data for 1-propanol is given in Figure 1.

Vapor−Liquid Equilibrium. Vapor−liquid equilibrium measurements were carried out for both systems under isothermal conditions by means of the ebulliometric method described elsewhere.[4] The pure compound was introduced into the ebulliometer and heated until the boiling point was reached at the adjusted pressure. The readouts of pressure and temperature were taken at the equilibrium stage. The specified temperature was measured with an accuracy of ± 0.01 K. The pressure was measured with an accuracy of ± 10 Pa. Samples of boiling liquid and vapor condensate were collected for analysis. Next, a precise amount of the second component was added, and the steady state was reached at the desired temperature. The measure of the steady state was the stability of temperature within ±0.003 K for about 5 min. In general, the time between introducing

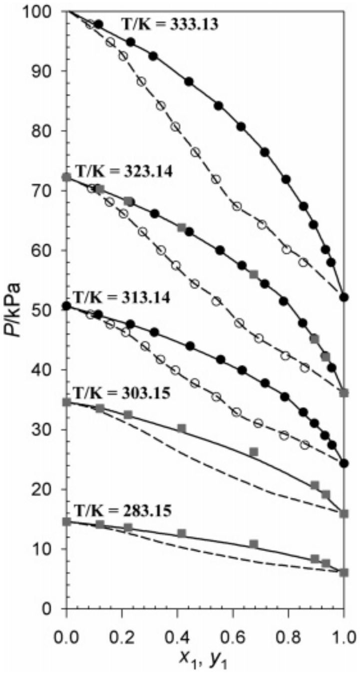

Figure 2. VLE for propylene benzene (1)+ 2-methylpentane (2): ●, this work; ■, Funk et al.[1] Lines represent the correlation with the AEOS. Solid symbols represent experimental bubble points, and hollow symbols represent experimental dew points.

the samples was about 30 min. The whole procedure was repeated until the concentration of the second component exceeded 50%. The sample composition was determined by using gas chromatography. For each system, the calibration procedure was used.

Vapor−liquid measurements were carried out under isothermal conditions. The estimated accuracy of the pressure measurement was ±10 Pa, and that of temperature was ±10 mK. The sample composition was determined by the GLC method, with an uncertainty of 0.1 mol % for the liquid phase and 0.5 mol % for the vapor phase. The results obtained are given in Table 4. The consistency check was made for each isotherm with the method proposed by Eubank et al.[17] (test 1). The auxiliary data were taken from Daubert and Danner.[18] The obtained differences between calculated and experimental liquid-phase compositions do not exceed 0.016, which is still reasonable taking into account the fact that $P^*(y)$ in this process is a higher-order polynomial.

The P, T, x, y data were reduced to activity coefficients. The equations of Redlich−Kister, with one to four adjustable parameters, Wilson, and UNIQUAC were used as activity coefficients models. The exact form of these equations is given in Malanowski and Anderko.[19]

The necessary fugacity coefficients (ϕ_i) of component i in the vapor phase were calculated from

$$\phi_i = \exp\left[\frac{(\nu_i^{\mathrm{L}} - \beta_i)(P - P_i^0) - P_i^0(1 - y_i)^2(\beta_i + \beta_2)/2}{RT}\right] \quad (3)$$

where virial coefficients β_i as functions of T were calculated from DIPPR data and equation[18]

$$p/\mathrm{Pa} = \exp\left(A + \frac{B}{T} + C \ln T + D\, T^{\mathrm{E}}\right) \quad (4)$$

A, B, C, D, and E are recommended parameters.

Second virial coefficients β_i as functions of T were calculated from the Daubert and Danner[18] data.

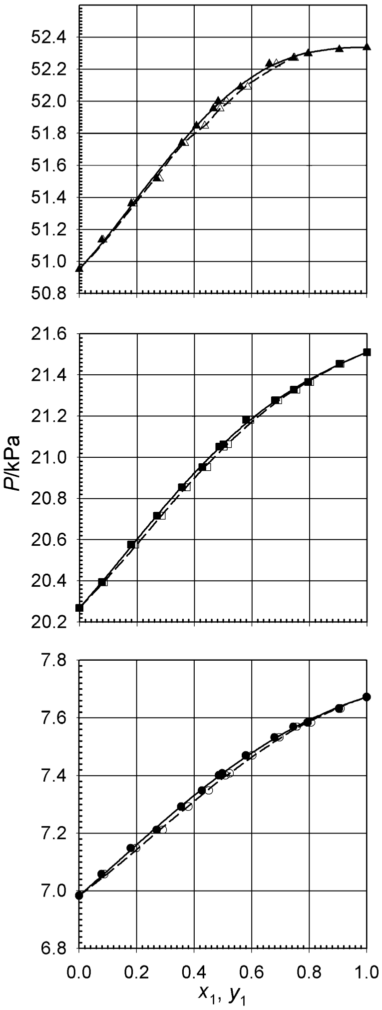

Figure 3. VLE for allyl alcohol (1) + 1-propanol (2): ●, 313.15 K; ■ 333.15 K; ▲, 353.15 K. Lines represent a prediction with the AEOS. Solid symbols represent experimental bubble points, and hollow symbols represent experimental dew points.

The results obtained are summarized in Table 5.

The mixture benzene + 2-methylpentane consists of two inert compounds, but allyl alcohol + 1-propanol consists of two associating compounds. It was concluded that the association with the equation of state (AEOS) is suitable for both systems. The use of the AEOS equation leads to the split of the compressibility factor into two parts

$$z = \frac{pV}{RT} = z^{(\mathrm{ph})} + z^{(\mathrm{ch})} - 1 \quad (5)$$

where $z^{(\mathrm{ph})}$ and $z^{(\mathrm{ch})}$ are the physical and chemical contributions to the compressibility factor, respectively.

The $z^{(\mathrm{ph})}$ contribution is equivalent to the equation of state for nonreacting monomeric species. In this work, it was calculated from the cubic equation of state of Yu et al.[20]

$$z^{(\mathrm{ph})} = \frac{v}{v - b} - \frac{a(T)v}{RT[v(v + c) + b(3v + c)]} \quad (6)$$

where $a(T)$, b, and c are generalized functions of the critical temperature T_{c}, critical pressure P_{c}, and acentric factor ω of a pure component, respectively.

The $z^{(\mathrm{ch})}$ contribution is equal to the reciprocal mean association number (K) and depends on the association model applied. The continuous linear association Mecke−

Kempter model is most suitable for representing the allyl alcohol + 1-propanol mixture at subambient pressure.[21] The following equation for the chemical term (eq 5) shows that the self- as well as cross-association was used,

$$z^{(\mathrm{ch})} = \sum_{i=1} \left(\frac{2x_{A_i}}{\left(1 + \sqrt{1 + 4RT\left(\sum_{j=1}^{2} K_{ij} x_{A_j}\right)/V}\right)} \right) \qquad (7)$$

where K_{ij} is either the self-association constant (for $i = j$) or the cross-association constant (for $i \neq j$).

The parameters of the AEOS obtained for pure-component data were used without modification for mixture calculations. For allyl alcohol and 1-propanol, data from Table 3 were used, and for benzene and 2-methylpentane, previously published parameters[22] were used. The detailed procedure was given by Antosik et al.[23]

The temperature dependence of the association constant K_{ij} can be expressed by assuming that $H°$ and $S°$ of association are linearly dependent on temperature (with appropriate values of C_p given in Table 4):

$$\ln K_{ij} = \frac{-\Delta H^{\mathrm{o}}(T_{\mathrm{o}}) + \Delta C_p^{\mathrm{o}} T_{\mathrm{o}}}{RT} + \frac{1}{R}[\Delta S^{\mathrm{o}}(T_{\mathrm{o}}) - \Delta C_p^{\mathrm{o}} - \Delta C_p^{\mathrm{o}} \ln T_{\mathrm{o}}] + \frac{\Delta C_p^{\mathrm{o}}}{R} \ln T \qquad (8)$$

The binary parameters a, b, and c of the Yu et al.[19] equation ($z^{(\mathrm{ph})}$ term) were calculated using classical mixing rules:

$$a = \sum_{i=1}^{2} \sum_{i=1}^{2} x_i x_j (1 - \theta_{ij}) \sqrt{a_i a_j} \qquad (9)$$

$$b = \sum_{i=1}^{2} x_i b_i \qquad (10)$$

$$c = \sum_{i=1}^{2} x_i c_i \qquad (11)$$

These mixing rules contain only one binary adjustable parameter θ_{12}. The mixture consists of two polar compounds, and better results were obtained with the cross-association constant K_{12} calculated from binary data. These mixing rules contain only one binary adjustable parameter θ_{12}. The allyl alcohol + 1-propanol system consists of two polar compounds. The cross-association constant K_{12} of eq 8 was calculated for this system from binary VLE data. The correlation results are summarized in Table 4. The temperature dependence of parameters K_{12} and θ_{12} has been calculated for the temperature range (310 to 355) K by linear regression from isothermal VLE data reported in this paper:

$$K_{12} = 1.23 \times 10^{-4} - 3.32 \times 10^{-7} T \qquad (12)$$

$$\theta_{12} = 0.1429 - 4.75 \times 10^{-4} T \qquad (13)$$

For the benzene + 2-methylpentane mixture, the following relation for θ_{12} has been found by the reduction of data reported in Table 4.

$$\theta_{12} = 0.02025 - 3.546 \times 10^{-5} T \qquad (14)$$

The rmsd values for p and y_1 obtained with these equations are given in Table 5.

The results of calculations by AEOS with eqs 12−14 used for K_{12} and θ_{12} are given in Table 5 and in Figures 2 and 3 and are satisfactory. A comparison of the correlation results for single isotherms with those predicted for the same isotherms using eqs 12−14 leads to the conclusion that the correlated results are similar to those predicted with the temperature-dependent K_{12} and θ_{12} parameters. A reasonable prediction of Funk et al.[1] data has been obtained (Figure 2).

The θ_{12} and K_{12} parameters are of similar or better accuracy than those correlated with equations for activity coefficients at one temperature only.

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