Registry No. K_2SO_4, 7778-80-5; acetone, 67-64-1; ethanol, 64-17-5; methanol, 67-56-1.

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Received for review June 5, 1989. Accepted November 9, 1989.

Isobaric Vapor–Liquid Equilibrium of Methyl Butanoate with Ethanol and 1-Propanol Binary Systems

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Binary T–p–c–y vapor–liquid equilibria (VLE) at 101.32 kPa are reported for methyl butanoate + ethanol or 1-propanol. The experimental VLE data of both systems were verified and found to be thermodynamically consistent. The azeotropic coordinates (mole fraction of the ester and temperature) are 0.091 and 350.97 K, for methyl butanoate + ethanol, and 0.409 and 366.77 K, for methyl butanoate + 1-propanol. The data were then compared with those obtained by using the UNIFAC and ASOG models.

Introduction

In continuation of our vapor–liquid equilibrium (VLE) studies on ester + alkanol binary mixtures (*1–4*), we present here VLE measurements at 101.32 kPa for methyl butanoate + ethanol or + 1-propanol.

Another aim of this paper is to compare the experimental data with those predicted with the ASOG model (OH/COO, Kojima and Tochigi (*5*)) and the different values for the ester group from the classical UNIFAC model (COH/COO, Fredenslund et al. (*6*); OH/COOC, Skjold-Jorgensen et al. (*7*); CCOH/COOC, Fredenslund et al. (*8*)).

Experimental Section

Materials. The compounds used in the present study were from Fluka AG. The physical properties of the alkanols used in this work were described earlier (*4*). "Purum" grade methyl butanoate of commercial purity greater than 99 mol % was degassed ultrasonically and stored in the dark for several days over a molecular sieve, type 4A from Fluka. The physical properties determined experimentally after this treatment were as follows: density, $\rho(298.15\ \text{K}) = 892.37\ \text{kg·m}^{-3}$; refractive index, $n_D(298.15\ \text{K}) = 1.3851$; normal boiling point, $T_b = 375.3$ K. These can be compared with the following literature values (*9*): 892.9 kg·m^{-3}, 1.3847, and 375.90 K, respectively.

Apparatus and Procedure. The experimental equipment and method of operation were as described previously (*1, 4*). Pressure was maintained constant to within 0.02 kPa, and the equilibrium temperature was measured in a digital thermometer (Comark, Model 6800), giving a reading of ±0.01 K and whose mean error was estimated to be 0.01% of the reading. The compositions of the coexisting phases were determined from the densities of liquid samples removed from the equilibrium still. The density vs ester mole fraction x_1 curves, $\rho(x_1)$, were established previously for each system (see ref 10). The accuracy of the mole fraction is 0.001 for the liquid phase and 0.002 for the vapor phase.

Experimental Results and Treatment of Data

Pure Compounds. The experimental vapor pressure of the pure liquids vs temperature T were correlated with use of the Antoine equation

$$\log (p^\circ_i/\text{kPa}) = A - B/[(T/\text{K}) - C] \qquad (1)$$

The constants A and B were determined for various values of C, by applying Marquardt's algorithm (*11*) for nonlinear functions (method 1), retaining the value of C that minimized the standard deviation $s(p^\circ_i) = [\sum(p_{i,\text{exp}} - p_{i,\text{cal}})^2/N]^{1/2}$, where N is the number of experimental points. Nonlinear simplex regression, as modified by Nelder and Mead (*12*) (method 2), was also used to obtain the constants A, B, and C. The results of both methods, along with the $s(p_i)$ values are set out in Table II.

Mixtures. The isobaric vapor–liquid equilibrium data at 101.32 kPa for methyl butanoate (1) + ethanol (2) or 1-propanol are presented in Table III. The activity coefficients γ_i of the components in the liquid phase, calculated from the experimental p–T–x–y data, are shown in Figure 1. Vapor-phase nonideality was accounted in terms of the second virial coefficients B_{ij} estimated by the method of Tsonopoulos (*15*) and the liquid molar volumes v_i^L estimated with the Spencer and Danner (*16*) form of the Rackett equation. The quality of the experimental data was verified by means of several consistency tests published in the literature. The data for the two systems studied satisfied Herington's test (*17*). However, the same did

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Table I. Experimental Vapor Pressures $p°_i$ of Pure Liquids as a Function of Temperature T

T/K	$p°_i$/kPa	T/K	$p°_i$/kPa
	Methyl Butanoate		
349.87	43.72	374.53	99.63
349.91	43.76	374.80	100.54
352.43	47.92	375.03	101.20
355.31	53.01	375.30	102.06
357.88	57.98	375.93	104.02
360.03	62.35	376.36	105.39
361.87	66.29	377.04	107.67
364.12	71.47	377.78	110.11
364.90	73.35	378.26	111.84
365.18	74.06	378.77	113.46
366.53	77.39	379.41	115.66
367.21	79.07	379.90	117.30
368.03	81.23	380.42	119.12
368.69	82.97	381.01	121.16
369.70	85.69	381.47	122.92
370.52	87.94	382.06	125.07
371.26	90.03	382.62	127.10
371.80	91.54	382.98	128.46
372.42	93.28	383.21	129.32
372.89	94.69	383.63	130.90
373.41	96.20	383.95	132.24
373.84	97.51	384.84	135.66
374.12	98.39		
	Ethanol		
342.03	69.03	351.45	101.51
343.04	72.02	351.64	102.31
343.94	74.83	352.15	104.36
344.96	78.03	352.50	105.84
345.86	80.99	352.81	107.12
346.52	83.22	353.32	109.31
347.12	85.30	353.62	110.60
347.65	87.17	354.30	113.56
348.36	89.75	355.07	117.03
348.49	90.21	355.93	120.96
348.96	91.91	356.60	124.10
349.61	94.33	357.03	126.19
350.46	97.62	357.59	128.90
351.22	100.61	357.91	130.50
	1-Propanol		
360.05	68.61	370.59	103.60
361.34	72.29	371.31	106.51
362.38	75.40	371.74	108.22
363.38	78.44	372.17	109.95
364.28	81.29	372.94	113.24
365.14	84.03	373.51	115.65
365.92	86.66	374.03	117.92
366.75	89.54	374.60	120.42
367.72	92.96	375.17	122.90
368.17	94.57	375.79	125.76
368.93	97.32	376.13	127.35
369.40	99.09	376.49	128.99
369.75	100.38	376.99	131.38
370.07	101.60	377.39	133.30
370.13	101.84		

Table II. Comparison between the Antoine Coefficients Obtained in This Work and Those Found in the Literature and the Standard Deviations $s(p°_i)$

compound	ref	A	B	C	$s(p°_i)$/ kPa
methyl butanoate	method 1	6.3036	1381.64	53.60	0.04
	method 2	6.2808	1368.26	55.01	0.04
	13	6.10644	1271.06	65.94	
ethanol	method 1	7.1130	1513.02	55.15	0.02
	method 2	7.0675	1486.91	57.64	0.02
	14	7.16879	1552.601	50.731	
1-propanol	method 1	6.8698	1434.94	74.98	0.04
	method 2	6.9611	1490.41	69.22	0.03
	14	6.87613	1441.705	74.291	

not hold true for the test developed by Van Ness et al. (*18*) as modified by Fredenslund et al. (*19*). This latter test requires that

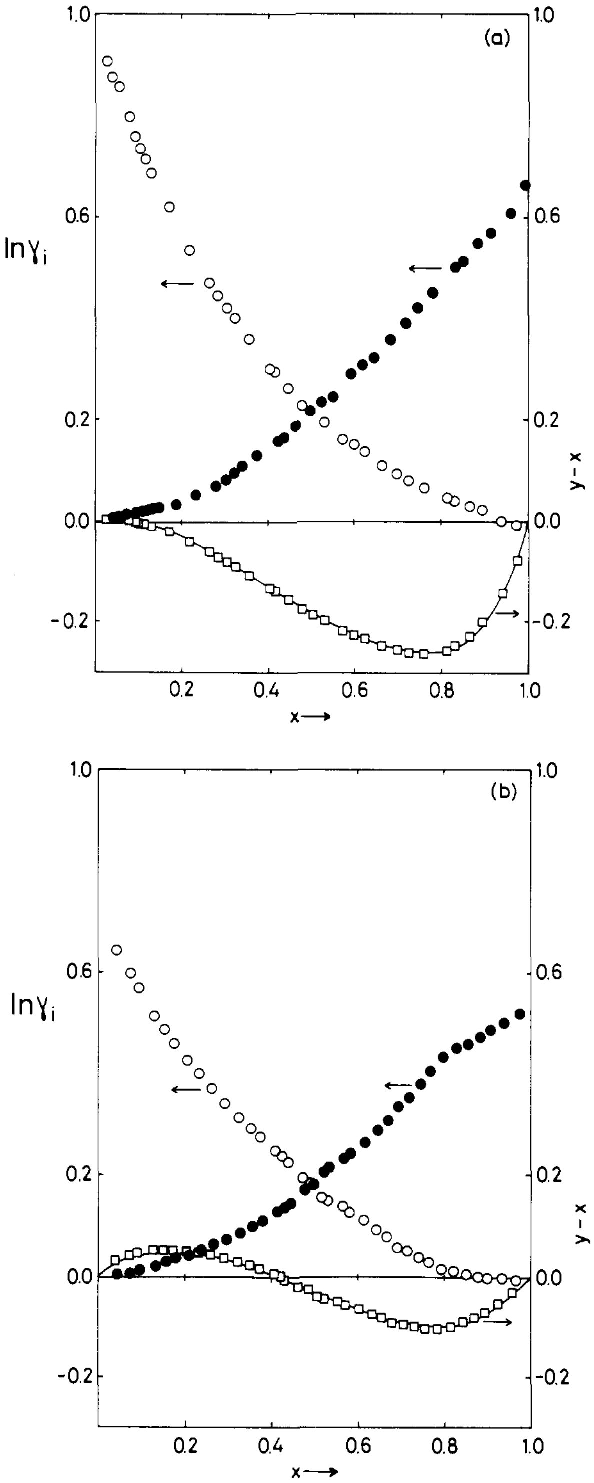

Figure 1. Experimental $y_1 - x_1$ data and calculated activity coefficients γ_i at 101.32 kPa for the binary systems (a) methyl butanoate (1) + ethanol (2) and (b) methyl butanoate (1) + 1-propanol (2). Points: ○, ln γ_1, ●, ln γ_2; □, $y_1 - x_1$. The curves are calculated by using eq 2.

the deviation between experimental and calculated values for the mole fraction of the vapor phase, y_1, should be less than 0.01. The overall deviations we found are 0.02 for methyl butanoate + ethanol and 0.012 for methyl butanoate + 1-propanol.

An additional version of the test of Van Ness et al. (*18*) was employed in the present study, using the subroutine for calculating virial coefficients based on the empirical expressions of Tsonopoulos (*15*) instead of the procedure of Hayden and O'Connell. The values of k_{ij} for the mixtures were optimized in

Table III. Experimental Vapor–Liquid Equilibrium Data at 101.32 kPa: Temperature T, Liquid Mole Fraction x_1, and Vapor Mole Fraction y_1

T/K	x_1	y_1	T/K	x_1	y_1
Methyl Butanoate (1) + Ethanol (2)					
351.46	0.0000	0.0000	353.05	0.4457	0.2906
351.15	0.0268	0.0313	353.35	0.4775	0.3035
351.10	0.0391	0.0442	353.65	0.5036	0.3192
351.00	0.0557	0.0615	354.15	0.5304	0.3355
350.98	0.0780	0.0813	354.65	0.5721	0.3556
350.97	0.0912	0.0914	355.15	0.5986	0.3742
350.98	0.1033	0.1010	355.75	0.6246	0.3932
350.99	0.1158	0.1110	356.65	0.6635	0.4182
351.05	0.1293	0.1207	357.45	0.6984	0.4449
351.25	0.1696	0.1490	358.15	0.7261	0.4671
351.45	0.2163	0.1756	359.25	0.7606	0.4998
351.75	0.2629	0.2019	361.25	0.8133	0.5592
351.77	0.2831	0.2126	362.15	0.8318	0.5852
351.83	0.3039	0.2227	363.85	0.8654	0.6351
351.90	0.3231	0.2328	365.60	0.8946	0.6898
352.15	0.3552	0.2475	369.35	0.9408	0.7941
352.65	0.4032	0.2695	372.45	0.9744	0.8956
352.75	0.4171	0.2776	375.30	1.0000	1.0000
Methyl Butanoate (1) + 1-Propanol (2)					
370.10	0.0000	0.0000	366.90	0.5160	0.4737
369.35	0.0419	0.0673	366.97	0.5310	0.4845
368.90	0.0730	0.1105	367.10	0.5638	0.5108
368.60	0.0918	0.1339	367.20	0.5800	0.5208
368.20	0.1278	0.1743	367.40	0.6128	0.5460
367.90	0.1514	0.1992	367.70	0.6428	0.5665
367.70	0.1742	0.2214	367.90	0.6656	0.5826
367.50	0.2043	0.2500	368.10	0.6898	0.5920
367.30	0.2327	0.2757	368.50	0.7144	0.6185
367.15	0.2615	0.2992	368.85	0.7410	0.6406
367.05	0.2913	0.3227	369.15	0.7638	0.6600
366.95	0.3234	0.3475	369.70	0.7934	0.6878
366.85	0.3516	0.3689	370.25	0.8229	0.7224
366.80	0.3745	0.3855	371.00	0.8527	0.7605
366.77	0.4087	0.4090	371.60	0.8779	0.7943
366.78	0.4244	0.4207	372.25	0.9019	0.8284
366.79	0.4401	0.4305	373.05	0.9336	0.8787
366.80	0.4714	0.4481	374.05	0.9665	0.9339
366.83	0.4949	0.4662	375.30	1.0000	1.0000

order to minimize the overall mean deviation in the mole fractions of the vapor phase, which was less than 0.01 for both mixtures, 0.008 for methyl butanoate + ethanol, and 0.009 for methyl butanoate + 1-propanol. Optimized k_{ij} values were around 0.05 for both mixtures, which agrees with the value recommended by Tsonopoulos (*15*) for binary mixtures in which one of the components is an alkanol.

The experimental y_1–x_1 data (Table III) were correlated with an equation of the form

$$y_1 - x_1 = x_1 x_2 \sum A_i [x_1/(x_1 + k x_2)]^i \qquad (2)$$

$$i = 0, 1, 2, \ldots$$

where the coefficients A_i were determined by a least-squares method and k was optimized to the best standard deviation, $s(y_1 - x_1)$, value. The parameters in eq 2 are $A_0 = 0.189$, $A_1 = -3.363$, $A_2 = 4.075$, $A_3 = -4.011$, $k = 1.60$, with $s(y_1 - x_1) = 0.001$, for methyl butanoate + ethanol and $A_0 = 0.796$, $A_1 = -2.382$, $A_2 = 3.071$, $A_3 = -2.542$, $k = 0.58$, with $s(y_1 - x_1) = 0.002$, for methyl butanoate + 1-propanol. Figure 1 presents the $y_1 - x_1$ and ln γ_i curves for the two systems.

The azeotropic coordinates are $x_1 = 0.091$, $T = 350.97$ K in the methyl butanoate + ethanol system and $x_1 = 0.409$, $T = 366.77$ K in the methyl butanoate + 1-propanol system. These values are in good agreement with those put forward by Horsley (*20*).

Comparison with ASOG and UNIFAC Predictions. The ASOG and UNIFAC theoretical methods were applied to the two systems using different interaction groups. So, the predictions made for the vapor mole fraction, y_1, were evaluated by the mean deviation, $\delta(y_i) = \sum |y_{i,\mathrm{exp}} - y_{i,\mathrm{cal}}|/N$. The results obtained in each case were, with the ASOG method and the pair COO/OH (*5*), $\bar{\delta}(y_1) = 0.016$ for methyl butanoate + ethanol and $\bar{\delta}(y_1) = 0.011$ for methyl butanoate + 1-propanol and with the UNIFAC method and the pairs COO/COH (*6*), COOC/OH (*7*), and COOC/CCOH (*8*), the mean deviations were, respectively, $\bar{\delta} = 0.010$, 0.012, and 0.019 for methyl butanoate + ethanol, and $\bar{\delta} = 0.014$, 0.014, and 0.008 for methyl butanoate + 1-propanol.

Conclusions

Vapor–liquid equilibrium data at 101.32 kPa for methyl butanoate + ethanol or 1-propanol binary systems and for the pure components were determined. The data indicate that the systems differed significantly from ideality, particularly in the region richest in 1-alkanol, mainly due to the presence of association effects. The data obtained were tested for thermodynamic consistency and found to be consistent.

The ASOG and UNIFAC methods produced generally good predictions of isobaric data, though with substantial differences in the estimates of the azeotropes formed in the systems considered. The ASOG model's predictions of vapor-phase composition had estimation errors of less than 6%, whereas the error achieved for the methyl butanoate + ethanol system with the UNIFAC model, taking the functional groups COOC/CCOH as the interaction pair, was around 10%. Conversely, this same interaction pair yielded the best estimates for the other system, methyl butanoate + 1-propanol.

Glossary

A, B, C	constants of the Antoine equation
A_i	parameter in eq 2
B_{ij}	second molar virial coefficients, cm^3 mol^{-1}
k	parameter in eq 2
p°_i	vapor pressure of pure component i, kPa
s	standard deviation
T	temperature, K
T_b	normal boiling point, K
x	liquid-phase mole fraction
y	vapor-phase mole fraction

Greek Letters

γ_i	activity coefficient of component i
ρ	liquid density, kg·m^{-3}
$\bar{\delta}$	mean deviation

Registry No. Methyl butanoate, 623-42-7; ethanol, 64-17-5; 1-propanol, 71-23-8.

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Received for review March 14, 1989. Revised August 28, 1989. Accepted January 30, 1990. We are grateful for the financial support of the Canarias Government to this work as part of the Research Project (52/86).

Infinite-Dilution Partition and Activity Coefficients for Alkanes and Bromo- and Chloroalkanes in Squalene–Dinonyl Phthalate Mixtures at 30 °C

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Using gas–liquid chromatography, we obtained infinite-dilution partition and activity coefficients at 30.0 °C for *n*-hexane, *n*-heptane, 3-methylpentane, 2,4-dimethylpentane, and bromo- and chloroalkanes in pure squalene, in pure dinonyl phthalate, and in three mixtures thereof. Where appropriate, the results are contrasted with those from previous studies. The values of the partition coefficients were tested for their agreement with the Purnell–Andrade equation and with an equation derived by Laub, Martire, and Purnell on the basis of conventional models of solution. From fits of the data to the latter equation, solute–sovent and solvent–solvent interaction parameters were calculated.

Introduction

For a variety of gas–liquid chromatographic (GLC) systems in which a volatile solute component (A) is distributed between a binary nonvolatile solvent mixture (X + Y) and the gas phase, Purnell and de Andrade (*1*) find that the linear relation

$$K^0_{R(M)} = \varphi_X K^0_{R(X)} + \varphi_Y K^0_{R(Y)} \tag{1}$$

is obeyed within experimental error. $K^0_{R(X)}$ and $K^0_{R(Y)}$ are the infinite-dilution solute partition coefficients in pure solvents X and Y, respectively. $K^0_{R(M)}$ is the infinite-dilution solute partition coefficient in a mixture where the volume fractions of X and Y are φ_X and φ_Y, respectively. On the other hand, Laub, Martire, and Purnell (*2*) derive the expression

$$\ln K^0_{R(M)} = \varphi_X \ln K^0_{R(X)} + \varphi_Y \ln K^0_{R(Y)} + (V_X/V_Y)\chi_{Y(X)}\varphi_X\varphi_Y \tag{2}$$

where V represents molar volumes and $\chi_{Y(X)}$ is the Flory-type interaction parameter characterizing X–Y interactions. Throughout this paper, the letters B, C, and D will refer to the solvents squalane (SQA), dinonyl phthalate (DNP), and squalene (SQE), respectively. The letter A will refer to the solute.

Although the model (*2*) on which eq 2 is based requires $\chi_{Y(X)}$ to be independent of the nature of the solute, experimental evidence (*2*, *10*, *11*) shows that $\chi_{Y(X)}$ depends on solute–solvent interaction. For a given $K^0_{R(X)}/K^0_{R(Y)}$ ratio, eq 2 predicts curvature in K^0_R versus φ_X plots that can deviate negatively (for $\chi_{Y(X)} \leq 0$) or positively (for $\chi_{Y(X)} > 0$) from linearity, with near linearity possible if the value of $\chi_{X(Y)}$ (whether positive or negative) is close to zero (*2*). While eq 1 has been used in the window diagram method (*3–5*) for optimizing chromatographic separations, there is no doubt now (*2*, *6–11*) that, in general, it is an approximate description of the true physical situation.

Table I. Properties of the Pure Components at 30.00 °C

	V/ (cm^3 mol^{-1})	P^0_A/ mmHg	$-B_{AA}$/ (cm^3 mol^{-1})
solutes			
hexane	132.53	187.10	1808
heptane	148.39	58.38	2717
3-methylpentane	131.52	232.91	1768
2,4-dimethylpentane	150.92	122.75	2390
tetrachloromethane	97.70	143.00	1451
trichloromethane	80.86	238.77	1142
dichloromethane	64.99	529.97	803
1,2-dichloropropane	98.88	63.24	2544
1,2-dichloroethane	79.91	99.81	1650
1,2-dibromoethane	87.05	15.26	
1-bromobutane	109.02	52.71	
solvents			
squalene (D)	484.37		
dinonyl phthalate (C)	434.82		

In our previous study (*11*), we obtained infinite-dilution partition and activity coefficients at 30.0 °C from GLC for *n*-pentane and six haloalkane solutes in squalane (SQA)–dinonyl phthalate (DNP) solvent mixtures. In this paper, we report values of infinite-dilution partition and activity coefficients at 30.0 °C from GLC for *n*-hexane, *n*-heptane, 3-methylpentane, 2,4-dimethylpentane, and chloro- and bromoalkanes in squalene (SQE)–dinonyl phthalate (DNP) solvent mixtures. The results are tested for their agreement with eqs 1 and 2 and are analyzed in the light of the treatment given in ref 2 to obtain solute–solvent and solvent–solvent interaction parameters.

Experimental Section

Squalene (SQE) and di-*n*-nonyl phthalate (DNP) were used as received from Phase Separations Ltd. (U.K.). High-purity solutes were also used as received from standard suppliers. The stationary liquids were deposited on Chromosorb W (60/80 mesh, acid-washed and silanized with dimethylchlorosilane) solid support from solutions in methylene chloride. The methylene chloride was removed by rotary evaporation. Traces of methylene chloride were removed from the coated supports by placing them in a vacuum dessicator for several days. The free-flowing powders were then packed in copper columns of 1-m length and 0.25-in. o.d. The weight percent of the liquid phase employed was in the neighborhood of 10% and was

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