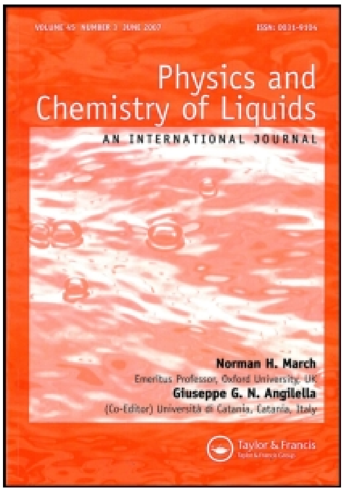

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Phase equilibria in the binary mixtures formed by ethylbenzene with some aliphatic alcohols at 95.8 kPa

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Phase equilibria are determined over the entire composition range, through measurements on the bubble points of the binary mixtures of ethylbenzene with methanol, ethanol, *n*-propanol, *iso*-propanol, *n*-butanol, *iso*-butanol, *sec*-butanol and *tert*-butanol. A Swietoslawski-type ebulliometer is used for the measurements. The liquid phase composition *versus* temperature measurements, found to be well represented by the Wilson model, are used to establish the phase equilibria.

Keywords: Phase equilibria; Bubble points; Ethylbenzene; Aliphatic alcohols

1. Introduction

This investigation on the phase equilibria of the binary mixtures noted in the abstract is in continuation of our recent studies on the phase equilibria of the binary mixtures containing hydrocarbons and alcohols [1–4]. The measurements have been carried out at 95.8 kPa. Ellis and Spurr [5] investigated the phase equilibria of ethanol + ethylbenzene mixtures at 101.3 kPa, while Ellis and Razavipour [6] studied the behaviour of the *n*-butanol + ethylbenzene mixtures at 101.3 kPa. We could not obtain the phase equilibrium data on the other mixtures chosen for the present study in the open literature.

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2. Experimental section

2.1 *Method*

A Swietoslawski type ebulliometer, similar to the one described by Hala *et al.* [7], is used in this experimental investigation. Connecting the ebulliometer to a good vacuum system, through a mercury manometer in line, facilitated the creation and maintainance of the chosen pressure within ±0.1 kPa. The equilibrium temperatures are measured to an accuracy of ±0.1 K, by means of a platinum resistance thermometer, carefully calibrated by a point-to-point comparison with a Standard Platinum Resistance Thermometer, certified by the National Bureau of Standards and Technology, Boulder (USA). The liquid mixtures for the studies are prepared gravimetrically, making use of electronic balance precise to ±0.0001 g and stirred well before being placed in the ebulliometer. The heating rate is adjusted to yield the desired condensate drop rate of 30 drops per minute, following the suggestion of Hala *et al.* [7]. The equilibrium temperatures, measured after the steady condensate drop rate and constancy of temperature are maintained for at least 30 min, have been reported.

2.2 *Materials*

Synthetic grade ethylbenzene (E. Merck, Mumbai, India) is fractionally distilled twice, after prior drying over silica gel for two days. Spectroscopic grade methanol (SDC Fine Chemicals, Boisar, India) is fractionally distilled twice after drying over silica gel. Anhydrous ethanol (Aldrich Chemical Co., Gillingham, England) is dried over silica gel and fractionally distilled twice. AR grade *n*-propanol (SD's Fine-Chem. Ltd., Poicha, India) is dried over sodium and fractionally distilled twice. GR grade *iso*-propanol (Loba Chemie, Mumbai, India) is dried over calcium chloride followed by barium oxide and fractionally distilled twice. Laboratory reagent grade *n*-butanol (Qualigenes Fine Chemicals, Mumbai, India) is refluxed over the freshly ignited calcium oxide for 4 h. The decanted alcohol is fractionally distilled twice. GR grade *iso*-butanol (Loba Chemie, Mumbai, India) is dried over the freshly ignited potassium, followed by calcium hydroxide for 4 h each. The alcohol is then fractionally distilled twice. Extrapure AR grade *sec*-Butanol (SISCO Research Laboratories, Mumbai, India) is dried over calcium hydroxide and fractionally

Table 1. Comparison of the density (D) and refractive index (n) of the pure substances used in this study with the literature data of Riddick *et al.* at 298.15 K.

Substance	$D/(\mathrm{kg\,m^{-3}})$		n	
	This work	Literature	This work	Literature
Ethylbenzene	862.5	862.53	1.4932	1.49320
Methanol	786.4	786.37	1.3265	1.32652
Ethanol	784.9	784.93	1.3594	1.35941
n-Propanol	799.6	799.60	1.3837	1.38370
iso-Propanol	781.3	781.26	1.3752	1.37520
n-Butanol	805.7	805.73	1.3974	1.39741
iso-Butanol	797.8	797.80	1.3939	1.39389
sec-Butanol	802.4	802.41	1.3953	1.39530
tert-Butanol	781.2	781.20	1.3877	1.38770

Table 2. Boiling temperatures of select binary ethylbenzene + alcohol mixtures at 95.8 kPa.

x_1	T/K	y_1	x_1	T/K	y_1	x_1	T/K	y_1	x_1	T/K	y_1
Methanol(1) + Ethylbenzene(2)			Ethanol(1) + Ethylbenzene(2)			*n*-Propanol(1) + Ethylbenzene(2)			*iso*-Propanol(1) + Ethylbenzene(2)		
0.0000	407.35	0.0000	0.0000	407.35	0.0000	0.0000	407.35	0.0000	0.0000	407.35	0.0000
0.1007	356.95	0.8160	0.0820	373.15	0.5730	0.1123	385.25	0.5254	0.0951	379.55	0.5996
0.1886	347.55	0.8794	0.1080	369.05	0.6303	0.2144	378.35	0.6490	0.2009	368.65	0.7454
0.2946	342.75	0.9064	0.2600	358.55	0.7759	0.3015	375.15	0.7027	0.3001	363.75	0.8040
0.3965	340.45	0.9188	0.4010	355.15	0.8314	0.3958	373.15	0.7405	0.3904	360.85	0.8454
0.5019	339.35	0.9266	0.5100	353.75	0.8623	0.4901	371.65	0.7689	0.5103	358.55	0.8633
0.6939	338.75	0.9364	0.6160	352.75	0.8893	0.5936	370.55	0.7960	0.6156	357.05	0.8820
0.8012	338.25	0.9430	0.7100	352.05	0.9132	0.7125	369.65	0.8285	0.6901	356.35	0.8943
0.8972	337.85	0.9544	0.8200	351.15	0.9429	0.8037	369.25	0.8601	0.8001	355.35	0.9147
0.9870	337.45	0.9885	0.9010	350.55	0.9669	0.9001	368.75	0.9090	0.9103	354.55	0.9461
1.0000	336.25	1.0000	1.0000	350.05	1.0000	1.0000	368.95	1.0000	1.0000	354.05	1.0000
n-Butanol(1) + Ethylbenzene(2)			*iso*-Butanol(1) + Ethylbenzene(2)			*sec*-Butanol(1) + Ethylbenzene(2)			*tert*-Butanol(1) + Ethylbenzene(2)		
0.0000	407.35	0.0000	0.0000	407.35	0.0000	0.0000	407.35	0.0000	0.0000	407.35	0.0000
0.1003	397.45	0.3103	0.0950	395.65	0.3461	0.0990	392.85	0.4063	0.0998	385.15	0.5263
0.1990	393.05	0.4444	0.1980	388.85	0.5149	0.1990	384.45	0.5827	0.1951	374.95	0.6898
0.2999	390.45	0.5252	0.4087	382.55	0.6766	0.4102	375.45	0.7532	0.3001	368.35	0.7786
0.4111	388.85	0.5870	0.5001	380.95	0.7184	0.5991	371.45	0.8276	0.4041	364.05	0.8304
0.5001	388.05	0.6278	0.5976	379.85	0.7555	0.7012	370.35	0.8551	0.4992	361.25	0.8629
0.6001	387.55	0.6713	0.7001	379.15	0.7918	0.8070	369.85	0.8788	0.6069	359.05	0.8906
0.6999	387.25	0.7184	0.8051	378.75	0.8333	0.8889	369.55	0.8971	0.6998	357.55	0.9106
0.8006	387.15	0.7774	0.8998	378.65	0.8860	0.9565	369.75	0.9231	0.8021	356.25	0.9319
0.9006	387.85	0.8614	0.9500	378.95	0.9301	0.9784	369.95	0.9444	0.9010	355.15	0.9567
1.0000	389.35	1.0000	1.0000	379.55	1.0000	1.0000	371.05	1.0000	1.0000	354.15	1.0000

Table 3. Antoine constants for the equation in $(P/\text{kPa}) = A - B/[(T/\text{K}) + C]$.

Substance	A	B	C
Ethylbenzene	14.0064	3269.47	−59.95
Methanol	16.5723	3626.59	−34.29
Ethanol	16.8945	3803.98	−41.08
n-Propanol	15.5287	3166.28	−80.15
iso-Propanol	16.6755	3640.20	−53.54
n-Butanol	15.1986	3137.20	−94.43
iso-Butanol	14.8538	2874.72	−100.30
sec-Butanol	15.1928	3026.03	−86.65
tert-Butanol	14.8374	2658.29	−95.50

distilled twice. LR grade *tert*-Butanol (SD's Fine Chemie, Boisar, India) is washed with a saturated solution of potassium carbonate and refluxed with 10% sodium hydroxide solution and distilled. The product is subsequently dried over potassium carbonate and fractionally distilled twice.

All the fractional distillations are carried out using a packed column of length equivalent to 30 theoretical plates. The middle fractions of the second distillations are collected in amber-colored bottles for use in the experiments. The final distillations of the substances are carried out only a few hours before the commencement of the phase equilibrium experiments and enough care is taken to prevent any absorption of moisture, oxidation, etc., during the intervening period. The purity of the chemicals used is ascertained by measuring their density and refractive index, which compare favourably with the literature values of Riddick *et al.* [8], as shown in table 1.

3. Results and discussion

The experimental liquid-phase composition (x_1) *versus* temperature (T) data, summarized in table 2, are fitted to the Wilson [9] model. The optimum Wilson parameters are obtained by minimizing the objective function defined as

$$\varphi = \sum [(P_{\text{cal}}/P_{\text{expt}}) - 1]^2 \tag{1}$$

where, P_{cal} and P_{expt} stand for the calculated and the experimental total pressures. The Nelder–Mead optimization technique described by Kuester and Mize [10] is used. Table 2 also gives the vapor-phase compositions (y_1) computed from the model. Vapor pressures needed in the computations are calculated from the Antoine constants noted in table 3. The Antoine equation, with the constants noted in table 3, represents the literature vapor pressure data as well as the present measurements on pure liquids with an average absolute deviation of 0.5%. The molar volumes of the pure liquids, calculated from the density measurements of this study (recorded in table 1) are used as the input in obtaining the optimum Wilson parameters. The results of the representation of the phase equilibrium data by the Wilson [9] model, summarized in table 4, indicate that the data and

Table 4. Representation of the measurements by Wilson model.

System	$[(\lambda_{12}-\lambda_{11})/R]$/K	$[(\lambda_{12}-\lambda_{22})/R]$/K	Std. Dev. in T/K
Methanol(1) + Ethylbenzene(2)	291.54	627.22	0.07
Ethanol(1) + Ethylbenzene (2)	308.87	420.22	0.03
n-Propanol(1) + Ethylbenzene(2)	240.85	350.03	0.06
iso-Propanol(1) + Ethylbenzene(2)	132.58	465.78	0.05
n-Butanol(1) + Ethylbenzene(2)	219.48	270.07	0.06
iso-Butanol(1) + Ethylbenzene(2)	580.10	484.03	0.06
sec-Butanol(1) + Ethylbenzene(2)	−75.44	1052.37	0.06
tert-Butanol(1) + Ethylbenzene(2)	−27.29	482.38	0.03

the representation are quite good. The Wilson parameters presented in table 4 for the ethanol (1) + ethylbenzene (2) system have been used to calculate the vapor-phase compositions at 101.3 kPa of the investigations of Ellis and Spurr [5], while the parameters of the *n*-butanol (1) + ethylbenzene (2) system have been used to calculate the vapor-phase compositions at the conditions of the study of Ellis and Razavipour [6]. The agreement is reasonable with average absolute deviations of 0.037 and 0.026 units, respectively. The data and the representation presented in the article are expected to be useful for engineering design purposes.

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