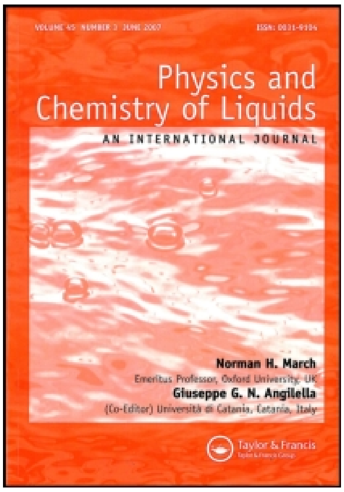

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BOILING TEMPERATURE MEASUREMENTS ON THE BINARY MIXTURES OF *n*-HEXANE WITH SOME ALIPHATIC ALCOHOLS

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Boiling temperatures at 95 kPa, over the entire composition range are measured for the eight binary systems formed by *n*-Hexane with: Methanol, Ethanol, *n*-Propanol, *iso*-Propanol, *n*-Butanol, *iso*-Butanol, *sec*-Butanol and *tert*-Butanol – using a Swietoslawski type ebulliometer. The composition *versus* temperature measurements are well represented by Wilson model.

Keywords: Boiling temperatures; *n*-Hexane; Aliphatic alcohols

INTRODUCTION

This investigation on the boiling temperature measurements 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, alcohols and chlorohydrocarbons [1–6]. The measurements have been carried out at 95 kPa. *n*-hexane (1) + methanol(2) system has been studied isothermally at 318.15 K by Ferguson [7] and isobarically at 101.3 kPa by Raal *et al.* [8] and at 99 kPa by Vilim [9]. Ethanol(1) + *n*-hexane(2) system has been investigated isothetmally – at 101.3 kPa by Kudrysteva and Suserev [10] and Sinor and Weber [11]. *n*-Hexane(1) + *n*-propanol(2) system has been investigated isothermally at 318.15 K by Brown *et al.* [12] and at 338.15 K by Strubl *et al.* [13] while Prabhu and van Wimkel [14] studied the same system isobarically at 101.3 kPa. *n*-Hexane(1) + *iso*-propanol system has been studied isobarically: at 101.3 kPa by Rotter and Knickle [15] and Govindaswamy *et al.* [16] and at 91.2 kPa by Vijaya Raghavan *et al.*, [17]. Hexane(1) + *n*-butanol(2) system has been studied isobarically at 101.3 kPa by Govindaswamy *et al.* [18]. *n*-Hexane(1) + *sec*-butanol(2) system has been studied isothermally at 333.15 K by Hanson and van Winkle [19]

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while *n*-hexane(1) + *tert*-butanol(2) system has been studied isobarically at 101.3 kPa by Govindaswamy *et al.* [20]. Comparisons of the present work with the available literature data have been carried out.

EXPERIMENTAL SECTION

A Swietoslawski type ebulliometer, very similar to the one described by Hala *et al.* [21] is used for this experimental investigation. The experimental procedure and the details of the method adopted for the measurements are as described in Vijaya Kumar *et al.*, [1]. All the AR grade chemicals used in this study are further purified according to the easiest possible of the methods described in Riddick *et al.* [22]. The purity of the chemicals is ascertained by measuring their density and refractive index, which compare favorably with the literature values as shown in Table I.

RESULTS AND DISCUSSION

The experimental liquid phase composition (X_1) *versus* temperature (T) data, summarized in Table II, are fitted to the Wilson model. The optimum Wilson parameters are obtained by minimizing the objective function defined as

$$\mathrm{Phi} = [(\mathrm{P_{cal}}/\mathrm{P_{expt}}) - 1]^2 \tag{1}$$

where $\mathrm{P_{cal}}$ and $\mathrm{P_{expt}}$ stand for the calculated and experimental total pressures. The Nelder–Mead optimization technique discussed and described in detail in Kuester and Mize [23] is used. Vapor pressures needed in the computations are calculated from the Antoine constants collected from Ried *et al.* [24] and noted in Table III, for ready reference. The Antoine equation, with the constants noted in Table III, represents the literature vapor pressure data as well as the present measurements with an average absolute deviation of 0.5%, for the nine pure liquids involved in the present study. The molar volumes of the pure liquids calculated from the density

TABLE I Comparison of the density (D) and refractive-index(n) of the pure substances used in this study with literature data from Riddick *et al.*, [22] at 298.15 K

Substance	$D/(\mathrm{kg/m^{-3}})$		n	
	This work	*Literature*	*This work*	*Literature*
n-Hexane	654.8	654.84	1.3723	1.37226
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	805.75	1.3974	1.39741
Isobutanol	797.8	797.80	1.3939	1.39389
sec-Butanol	802.4	802.41	1.3953	1.39530
tert-Butanol	781.2	781.20	1.3852	1.38520

TABLE II The boiling temperature measurements

x_1	T/K	x_1	T/K	x_1	T/K	x_1	T/K
Methanol(1) + *n*-Hexane(2)		*n*-Hexane(1) + Ethanol(2)		*n*-Hexane(1) + n-Propanol(2)		*n*-Hexane(1) + *iso*-Propanol(2)	
0.0000	339.85	0.0000	349.75	0.0000	368.55	0.0000	353.65
0.1001	321.45	0.1002	335.15	0.1004	360.25	0.1003	343.25
0.2002	321.25	0.2003	331.65	0.2005	355.35	0.2004	338.05
0.3003	321.15	0.3004	330.45	0.3006	351.95	0.3005	335.35
0.4004	321.15	0.4005	329.95	0.4007	349.25	0.4006	333.95
0.5005	321.15	0.5006	329.75	0.5008	347.45	0.5007	333.15
0.6006	321.15	0.6007	350.85	0.6009	345.75	0.6008	332.75
0.7007	321.25	0.7008	329.65	0.7010	344.15	0.7009	332.55
0.8008	321.45	0.8009	329.75	0.8011	342.65	0.8010	332.55
0.9009	322.75	0.9010	330.35	0.9012	341.15	0.9011	332.75
1.0000	335.95	1.0000	339.85	1.0000	339.85	1.0000	339.85
n-Hexane(1) + *n*-Butanol(2)		*n*-Hexane(1) + *iso*-Butanol(2)		*n*-Hexane(1) + *sec*-Butanol(2)		*n*-Hexane(1) + *tert*-Butanol(2)	
0.0000	389.15	0.0000	379.25	0.0000	370.95	0.0000	354.05
0.1501	360.75	0.1502	354.35	0.1503	345.95	0.1504	347.55
0.3002	349.45	0.3004	346.05	0.3004	341.15	0.3005	343.35
0.4503	344.15	0.4503	342.45	0.4505	339.55	0.4506	340.75
0.6004	341.55	0.6006	340.85	0.6006	338.55	0.6007	339.15
0.7505	340.15	0.7507	339.75	0.7507	338.25	0.7508	338.35
0.9006	339.55	0.9008	339.25	0.9000	338.05	0.9009	338.35
1.0000	339.75	1.0000	339.75	1.0000	339.75	1.0000	339.75

TABLE III Antoine constants $\mathrm{Ln}(P/\mathrm{kPa}) = \mathrm{A} - \mathrm{B}/[(T/\mathrm{K}) + \mathrm{C}]$

Substance	*A*	*B*	*C*
n-Hexane	13.8214	2697.55	−48.78
Methanol	16.5723	3626.59	−34.29
Ethanol	16.8970	3803.98	−41.68
n-Propanol	15.5287	3166.38	−80.15
iso-Propanol	16.6777	3640.20	−53.54
n-Butanol	15.2008	3137.02	−94.43
iso-Butanol	14.8560	2874.73	−100.30
sec-Butanol	15.1950	3026.03	−86.65
tert-Butanol	14.8396	2658.29	−95.90

measurements of this study (recorded in Table I) are used as the input in obtaining the optimum Wilson parameters. The results of the representation of the phase equilibrium data by Wilson model, summarized in Table IV, indicate that the data and the representation are quite good. An attempt has been made to compare the values of the vapor phase composition of the more volatile component (Y_1) from the Wilson parameters for the system presented in Table IV, with the experimental data from the literature under the same conditions. The results of such extensive comparisons, summarized in Table V, show good agreement with some sets of data while in a few exceptional cases there is considerable disagreement as evident from the table. The same pattern is observed when multiple sets of the observations on the same systems available in the literature are compared with each other. The data and the representation presented in the article are expected to be useful for engineering design purposes.

TABLE IV Representation of the measurements by Wilson model

System	*[($\lambda_{12}-\lambda_{11}$)/R]*/K	*[($\lambda_{12}-\lambda_{22}$)/R]*/K	*Standard Deviation in T*/K
Methanol(1) + *n*-Hexane(2)	1124.3	699.5	0.02
n-Hexane(1)–Ethanol(2)	520.2	770.4	0.03
n-Hexane(1) + *n*-Propanol(2)	304.6	0.0	0.10
n-Hexane(1) + *iso*-Propanol(2)	245.1	1002.6	0.05
n-Hexane(1) + *n*-Butanol(2)	128.0	890.6	0.06
n-Hexane(1) + *iso*-Butanol(2)	243.0	611.5	0.08
n-Hexane(1) + *sec*-Butanol(2)	456.7	475.9	0.05
n-Hexane(1) + *tert*-Butanol(2)	27.9	412.1	0.08

TABLE V Summary of the comparison with literature data

Literature source	*Condition*	*% Av. Abs. Dev. in Y_1*
	Methanol(1)-*n*-Hexane(2)	
Ferguson [7]	318.15 K	0.02
Raal *et al.* [8]	101.3 kPa	0.01
Vilim [9]	99.0 kPa	0.07
	n-Hexane(1)+Ethanol(2)	
Kudryavsteva [10]	101.3 kPa	0.01
Sinor *et al.* [11]	101.3 kPa	0.05
	n-Hexane(1)+n-Propanol(2)	
Brown *et al.* [12]	318.15 K	0.04
Strubl *et al.* [13]	338.15 K	0.06
Prabhu and van Winkle [14]	101.3 kPa	0.09
	n-Hexane(1)+*iso*-Propanol(2)	
Rotter and Knicle [15]	101.3 kPa	0.02
Govindaswamy *et al.* [16]	101.3 kPa	0.01
Vijaya Raghavan *et al.* [17]	91.2 kPa	0.02
	n-Hexane(1)+n-Butanol(2)	
Govindaswamy *et al.* [18]	101.3 kPa	0.01
	n-Hexane(1)+*sec*-Butanol(2)	
Hanson and van Winkle [19]	333.15 K	0.04
	n-Hexane(1)+tert-Butanol(2)	
Govindaswamy *et al.* [20]	101.3 kPa	0.04

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