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Volumetric properties of binary liquid mixtures of ketones with chloroalkanes at different temperatures and atmospheric pressure

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ABSTRACT

In this work, densities data of binary liquid mixtures of ketones (2-butanone, 2-heptanone and cyclohexanone) with chloroalkanes (1,2-dichloroethane and 1,1,2,2-tetracloroethane) as a function of composition, under atmospheric pressure and at different temperatures from 288.15 to 313.15 K have been used to calculate excess molar volume. The partial volumetric properties at an infinite dilution were calculated using Redlich–Kister polynomial. We have also considered another approach, which is more convenient and accurate by calculating the partial volumetric properties at an infinite dilution through apparent molar volume.

1. Introduction

The present work is focused on the study of binary mixtures of ketones (2-butanone, 2-heptanone and cyclohexanone) with 1,2-dichloroethane (DCE) and 1,1,2,2-tetrachloroethane (TCE) over the entire composition range and at different temperatures. Therefore, interesting results may be obtained regarding molecular interactions between unlike molecule in these binary mixtures.

In the present paper, we report the densities, ρ, of pure ketones, DCE, TCE at different temperatures from 288.15 K to 313.15 K. These measurements were performed in order to complement the data on VLE and excess molar properties [1–6] of mixtures containing 1,2-dichloroethane or 1,1,2,2-tetrachloroethane. Excess molar volumes, V^E, partial molar volumes and excess partial molar volumes, at an infinite dilution, $\bar{V}_i^{\infty}$ and $\bar{V}_i^{E,\infty}$, respectively, were calculated [7]. The excess molar volumetric properties, of a liquid mixture depends on the size and shape of the molecules and on the specific interactions, like hydrogen bonding or dipole–dipole and dipole-induced dipole interactions. Carbon atoms of chloroalkane compounds are known to act as proton donors in hydrogen bonds in mixtures with oxygenated solvents. Mixtures of ketone + chloroalkanes are of particular interest from the point of view.

A survey of the literature indicates that volumetric properties for (cyclohexanone + DCE or TCE) mixtures have been studied by other authors [8] at (288.15, 298.15 and 308.15) K. Earlier studies on excess volume were performed for (2-butanone + TCE or DCE) mixtures at (303.15 and 313.15) K [9,10]. Volumetric properties of 2-butanone + DCE have been also studied [11] at (293.15 and 303.15) K.

2. Experimental

All the chemicals used in the present study were not submitted any purification. DCE and cyclohexanone with mass fraction purity greater than 0.99 were obtained from Reild-De-Haëi. TCE, 2-butanone and 2-heptanone (puriss greater than 0.98) provided by Fluka. Table 1 presents a comparison between the measured and literature values of density at 298.15 K.

Density measurements of pure liquids and mixtures were performed at atmospheric pressure from 288.15 to 313.15 K by means of vibrating-tube densimeter (Anton Paar, DMA5000) with an estimating uncertainty of $\pm 5.10^{-6}$ g/cm^3. The thermoregulation of the whole is assured by a HAAKE G thermostat. The accuracy of the temperature was 0.01 K. The principle of the measurement is the determination of the oscillation period τ of the U-tube.

The following relation was used to evaluate ρ values from period τ of the U-tube

$$\rho = A \times \tau^2 - B \quad (1)$$

The constants A and B were determined by calibration at 293.15 K and at atmospheric pressure, using dry air and double distilled degassed water. All the binary mixtures were prepared

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Table 1
Comparison of measured values of density with those in the literature at 298.15 K and atmospheric pressure.

Component	ρ (g/cm^{-3})	
	Experimental	Literature
2-Butanone	0.799828	0.79998[a] 0.79989[b]
2-Heptanone	0.811198	0.81133[c] 0.8111[d]
Cyclohexanone	0.942243	0.94276[j] 0.94201[e]
1,2-Dichloroethane	1.245495	1.24558[f] 1.24548[j] 1.24567[g]
1,1,2,2-Tetrachloroethane	1.585865	1.58693[h] 1.58918[j] 1.58683[i]

[a] Ref. [12].
[b] Ref. [13].
[c] Ref. [14].
[d] Ref. [15].
[e] Ref. [16].
[f] Ref. [17].
[g] Ref. [18].
[h] Ref. [6].
[i] Ref. [19].
[j] Ref. [8].

by weight using a Mettler PE balance with a precision of $\pm 10^{-4}$ g. The uncertainty in the V^E calculation is less than $\pm 10^{-4}$ cm^3 mol^{-1}.

3. Results and discussion

The excess molar volume V^E is defined by

$$V^E = V^r - V^{id} \quad (2)$$

In which V^r and V^{id} stand for real molar volume and ideal molar volume respectively.

V^E can be expressed by the following equation

$$V^E = \frac{x_1M_1 + x_2M_2}{\rho_m} - \left(\frac{x_1M_1}{\rho_1} + \frac{x_2M_2}{\rho_2}\right) \quad (3)$$

In which M_1, M_2 and ρ_1, ρ_2 denote the molar masses and densities of the pure components, respectively, and ρ_m is the density of liquid solution, x_1 and x_2 are the mole fractions of components 1 (ketones) and 2 (chloroalkanes), respectively.

The experimental results were fitted with Redlich–Kister equation [20]

$$V^E = x_1(1-x_1)\sum_{i=1}^{p} A_i(2x_1-1)^{i-1} \quad (4)$$

The experimental densities, ρ_i, for the pure components at different temperatures and at atmospheric pressure, are listed in Table 2.

The experimental values of V^E are presented in Tables 3–8 which contained the mole fractions and the excess molar volumes for the binary mixtures at different temperatures.

The experimental values of V^E shown in Tables 3–8 are positives for the binaries (2-heptanone or cyclohexanone) with DCE and negatives with TCE. However for (2-butanone + DCE or TCE) the V^E values are negatives over the whole composition range and at all the investigate temperature.

Table 2
Experimental densities, ρ_i, for the pure components at different temperatures and at atmospheric pressure.

	ρ (g/cm^3)		
	2-Butanone	2-Heptanone	Cyclohexanone
288.15 K	0.810262	0.819786	0.951178
293.15 K	0.805058	0.815497	0.946713
303.15 K	0.794565	0.806887	0.937767
308.15 K	0.789273	0.802562	0.933285
313.15 K	0.783946	0.798222	0.928795

	ρ (g/cm^3)	
	1,2-Dichloroethane	1,1,2,2-Tetrachloroethane
288.15 K	1.259993	1.601447
293.15 K	1.252768	1.593654
303.15 K	1.238183	1.578067
308.15 K	1.230839	1.570266
313.15 K	1.223459	1.562451

Table 3
Excess molar volumes, V^E, at different temperatures of binary mixture butan-2-one (1) + DCE (2).

x_1	V^E (cm^3 mol^{-1})	x_1	V^E (cm^3 mol^{-1})	x_1	V^E (cm^3 mol^{-1})
	288.15 K		*288.15 K*		
0.0503	−0.0104	0.4003	−0.0314	0.6999	−0.0575
0.1006	−0.0170	0.4500	−0.0349	0.7497	−0.0609
0.1496	−0.0211	0.4998	−0.0402	0.7995	−0.0587
0.2005	−0.0235	0.5489	−0.0441	0.8499	−0.0537
0.2498	−0.0253	0.5997	−0.0479	0.8999	−0.0439
0.3003	−0.0268	0.6496	−0.0540	0.9498	−0.0260
0.3497	−0.0288				
	293.15 K		*293.15 K*		
0.0503	−0.0108	0.4003	−0.0366	0.6999	−0.0630
0.1006	−0.0180	0.4500	−0.0404	0.7497	−0.0659
0.1496	−0.0228	0.4998	−0.0459	0.7995	−0.0626
0.2005	−0.0260	0.5489	−0.0490	0.8499	−0.0570
0.2498	−0.0284	0.5997	−0.0537	0.8999	−0.0463
0.3003	−0.0307	0.6496	−0.0597	0.9498	−0.0273
0.3497	−0.0334				
	298.15 K		*298.15 K*		
0.0503	−0.0119	0.4003	−0.0429	0.6999	−0.0690
0.1006	−0.0201	0.4500	−0.0470	0.7497	−0.0711
0.1496	−0.0258	0.4998	−0.0527	0.7995	−0.0674
0.2005	−0.0298	0.5489	−0.0568	0.8499	−0.0608
0.2498	−0.0331	0.5997	−0.0605	0.8999	−0.0490
0.3003	−0.0360	0.6496	−0.0662	0.9498	−0.0287
0.3497	−0.0392				
	303.15 K		*303.15 K*		
0.0503	−0.0134	0.4003	−0.0500	0.6999	−0.0749
0.1006	−0.0228	0.4500	−0.0543	0.7497	−0.0768
0.1496	−0.0296	0.4998	−0.0597	0.7995	−0.0723
0.2005	−0.0347	0.5489	−0.0640	0.8499	−0.0624
0.2498	−0.0387	0.5997	−0.0678	0.8999	−0.0521
0.3003	−0.0421	0.6496	−0.0727	0.9498	−0.0304
0.3497	−0.0460				
	308.15 K		*308.15 K*		
0.0503	−0.0147	0.4003	−0.0584	0.6999	−0.0801
0.1006	−0.0254	0.4500	−0.0621	0.7497	−0.0828
0.1496	−0.0339	0.4998	−0.0673	0.7995	−0.0775
0.2005	−0.0395	0.5489	−0.0718	0.8499	−0.0693
0.2498	−0.0448	0.5997	−0.0753	0.8999	−0.0550
0.3003	−0.0497	0.6496	−0.0799	0.9498	−0.0320
0.3497	−0.0532				
	313.15 K		*313.15 K*		
0.0503	−0.0162	0.4003	−0.0658	0.6999	−0.0869
0.1006	−0.0288	0.4500	−0.0697	0.7497	−0.0887
0.1496	−0.0376	0.4998	−0.0758	0.7995	−0.0828
0.2005	−0.0442	0.5489	−0.0796	0.8499	−0.0736
0.2498	−0.0503	0.5997	−0.083	0.8999	−0.0580
0.3003	−0.0549	0.6496	−0.0873	0.9498	−0.0337
0.3497	−0.0600				