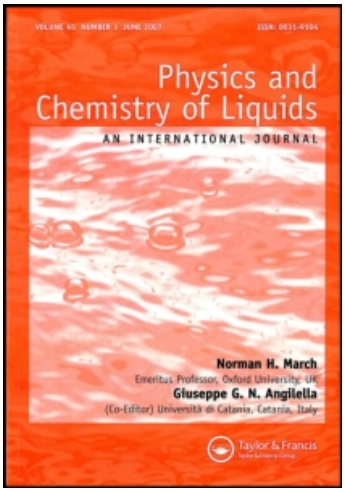

Physics and Chemistry of Liquids
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713646857

Excess molar volume measurements of ternary mixtures [2-propanol+ethyl acetate+n-hexane] and their binary constituents at 298.15, 308.15 and 313.15 K

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To cite this Article Mohsen-Nia, M. and Modarress, H.(2005) 'Excess molar volume measurements of ternary mixtures [2-propanol+ethyl acetate+n-hexane] and their binary constituents at 298.15, 308.15 and 313.15 K', Physics and Chemistry of Liquids, 43: 6, 535 — 541
To link to this Article: DOI: 10.1080/00319100500216522
URL: http://dx.doi.org/10.1080/00319100500216522

Physics and Chemistry of Liquids
Vol. 43, No. 6, December 2005, 535–541

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Excess molar volume measurements of ternary mixtures [2-propanol + ethyl acetate + n-hexane] and their binary constituents at 298.15, 308.15 and 313.15 K

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(*Received 10 May 2005*)

The excess molar volume of the ternary mixture [2-propanol + ethyl acetate + n-hexane], and its binary constituents; [2-propanol + ethyl acetate], [2-propanol + n-hexane] and [ethyl acetate + n-hexane] were evaluated by the mixtures density measurements over the whole concentration range at three temperatures 298.15, 308.15 and 313.15 K. The excess molar volumes data were fitted to the Redlich–Kister (RK) type equation and the parameters of this equation have been calculated and presented for the studied mixtures.

Keywords: Excess molar volume; Density; 2-Propanol; Ethyl acetate; n-Hexane

1. Introduction

The binary mixtures of organic polar–polar and polar–non-polar solvents are important for the different industrial purposes such as solvent extraction of aromatic hydrocarbons from alkanes [1–3], crystallization and extraction of pure organic and mineral salts from aqueous mixtures [4,5] and solvent cleaning processes [6]. Therefore, experimental and theoretical studies of thermodynamic behavior of mixed solvents have considerable current interest in the different steps of chemical engineering processes.

The ternary mixture of [2-propanol (1) + ethyl acetate (2) + n-hexane (3)] containing two highly polar (1, 2) and the non-polar (3) solvents can be considered as a suitable ternary mixture for various industrial applications. Therefore, it is worthwhile to study the non-ideal behavior of this ternary mixture and its binary constituents in terms of their molar excess volume change (V^{E}) upon mixing.

In this work, the molar excess volumes of the ternary mixture [2-propanol (1) + ethyl acetate (2) + n-hexane (3)] and its binary mixtures constituents were evaluated

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Physics and Chemistry of Liquids
ISSN 0031-9104 print: ISSN 1029-0451 online © 2005 Taylor & Francis
DOI: 10.1080/00319100500216522

Table 1. Measured densities of the pure components at different temperatures and atmospheric pressure.

Components	T (K)	ρ (g cm^{-3})
2-Propanol	298.15	0.7809
	298.15	0.7813[a]
	298.15	0.7813[b]
	308.15	0.7735
	313.15	0.7693
	313.15	0.7683[c]
Ethyl acetate	298.15	0.8949
	298.15	0.8947[c]
	308.15	0.8830
	313.15	0.8770
n-Hexane	298.15	0.6555
	298.15	0.6548[b]
	308.15	0.6459
	313.15	0.6412

(a, b, c), Experimental data references: [a][8], [b][9], [c][10].

Table 2. Experimental densities ρ (g cm^{-3}), and excess molar volume V^E (cm^3 mol^{-1}) for the mixture [2-propanol (1) + ethyl acetate (2) + n-hexane (3)] at 298.15 K and atmospheric pressure.

x_1	x_2	ρ	V^E	x_1	x_2	ρ	V^E
0.0224	0.9450	0.8817	0.0963	0.7582	0.2418	0.8104	0.3505
0.0415	0.3631	0.7271	0.7782	0.8686	0.1314	0.7970	0.2301
0.0537	0.0369	0.6650	0.2862	0.9636	0.0364	0.7853	0.0781
0.1081	0.0759	0.6759	0.4757	0.0372	0.0000	0.6575	0.1522
0.1788	0.7171	0.8414	0.4761	0.1351	0.0000	0.6639	0.3935
0.1947	0.0927	0.6864	0.6176	0.2152	0.0000	0.6698	0.5441
0.2232	0.7504	0.8620	0.3723	0.3546	0.0000	0.6822	0.6272
0.2432	0.1556	0.7039	0.7694	0.4060	0.0000	0.6873	0.6417
0.3033	0.6018	0.8309	0.5599	0.5723	0.0000	0.7061	0.6302
0.3304	0.3882	0.7714	0.8756	0.6165	0.0000	0.7121	0.5711
0.3516	0.3579	0.7664	0.8935	0.7122	0.0000	0.7263	0.4301
0.4145	0.5391	0.8336	0.5831	0.8948	0.0000	0.7588	0.1202
0.4844	0.4187	0.8093	0.6310	0.9289	0.0000	0.7656	0.0803
0.4965	0.3094	0.7777	0.7381	0.0000	0.0987	0.6705	0.3512
0.5182	0.3614	0.7978	0.6625	0.0000	0.1581	0.6820	0.5206
0.5520	0.2475	0.7694	0.7074	0.0000	0.2246	0.6944	0.6741
0.6368	0.0583	0.7304	0.5704	0.0000	0.3465	0.7185	0.8423
0.6787	0.2543	0.7971	0.4456	0.0000	0.4906	0.7505	0.8601
0.7114	0.0992	0.7541	0.4702	0.0000	0.5977	0.7763	0.7601
0.7613	0.1419	0.7767	0.4570	0.0000	0.6444	0.7884	0.6896
0.8006	0.1785	0.7975	0.3711	0.0000	0.7507	0.8174	0.5151
0.8266	0.1235	0.7847	0.3194	0.0000	0.8015	0.8322	0.4043
0.9006	0.0355	0.7723	0.0557	0.0000	0.9502	0.8783	0.1073
0.0470	0.9530	0.8901	0.0648				
0.1635	0.8365	0.8775	0.2601				
0.2252	0.7748	0.8707	0.3455				
0.3192	0.6808	0.8601	0.4167				
0.4162	0.5838	0.8498	0.4651				
0.5682	0.4318	0.8325	0.4727				
0.6716	0.3284	0.8206	0.4275				

Table 3. Experimental densities ρ (g cm^{-3}), and excess molar volume V^E(cm^3 mol^{-1}) for the mixture [2-propanol (1) + ethyl acetate (2) + n-hexane (3)] at 308.15 K and atmospheric pressure.

x_1	x_2	ρ	V^E	x_1	x_2	ρ	V^E
0.0224	0.9450	0.8698	0.1186	0.7582	0.2418	0.8008	0.4199
0.0415	0.3631	0.7159	0.9485	0.8686	0.1314	0.7885	0.2701
0.0537	0.0369	0.6550	0.3507	0.9636	0.0364	0.7775	0.0804
0.1081	0.0759	0.6658	0.5750	0.0372	0.0000	0.6478	0.1821
0.1788	0.7171	0.8297	0.5788	0.1351	0.0000	0.6538	0.5211
0.1947	0.0927	0.6762	0.7450	0.2152	0.0000	0.6594	0.7401
0.2232	0.7504	0.8504	0.4552	0.3546	0.0000	0.6716	0.8602
0.2432	0.1556	0.6943	0.9331	0.4060	0.0000	0.6768	0.8711
0.3033	0.6018	0.8192	0.6834	0.5723	0.0000	0.6957	0.8550
0.3304	0.3882	0.7602	1.0611	0.6165	0.0000	0.7018	0.7902
0.3516	0.3579	0.7552	1.0956	0.7122	0.0000	0.7161	0.6311
0.4145	0.5391	0.8225	0.7089	0.8948	0.0000	0.7495	0.2402
0.4844	0.4187	0.7985	0.7720	0.9289	0.0000	0.7568	0.1501
0.4965	0.3094	0.7670	0.9070	0.0000	0.0987	0.6613	0.5011
0.5182	0.3614	0.7872	0.8043	0.0000	0.1581	0.6713	0.7555
0.5520	0.2475	0.7590	0.8676	0.0000	0.2246	0.6830	0.9300
0.6368	0.0583	0.7208	0.6990	0.0000	0.3465	0.7066	1.0868
0.6787	0.2543	0.7874	0.5434	0.0000	0.4906	0.7383	1.0915
0.7114	0.0992	0.7451	0.5742	0.0000	0.5977	0.7667	0.9750
0.7613	0.1419	0.7674	0.5581	0.0000	0.6444	0.7758	0.8950
0.8006	0.1785	0.7884	0.4575	0.0000	0.7507	0.8044	0.7101
0.8266	0.1235	0.7759	0.3868	0.0000	0.8015	0.8196	0.5655
0.9006	0.0355	0.7643	0.0716	0.0000	0.9502	0.8659	0.1602
0.0470	0.9530	0.8775	0.1010				
0.1635	0.8365	0.8654	0.2930				
0.2252	0.7748	0.8589	0.3900				
0.3192	0.6808	0.8487	0.4901				
0.4162	0.5838	0.8384	0.5411				
0.5682	0.4318	0.8219	0.5502				
0.6716	0.3284	0.8101	0.5044				

by mixture density measurements over the whole concentration range at three temperatures 298.15, 308.15, and 313.15 K. The obtained V^E for the studied binary and ternary mixtures were correlated by a Redlich–Kister [7] type equation. The parameters of the correlated equations were evaluated and presented (see tables 1–6 and figures 1 and 2).

2. Experimental

The chemicals n-hexane, 2-propanol and ethyl acetate (purities >99%), were supplied by Aldrich. Therefore, all chemicals were used without further purification.

Pure and mixtures densities, ρ were measured with a 25 cm^3 pycnometer. The pycnometer was calibrated with double-distilled water.

The mixtures were prepared by mass using an analytical balance with a precision of ± 0.01 mg. The reproducibility of density measurements was estimated as ± 0.0005 g cm^{-3}.

In density measurements, the temperature of the samples was controlled by using a water bath equipped with a thermostat of accuracy of ± 0.1 K.

Table 4. Experimental densities ρ (g cm^3), and excess molar volume V^E(cm^3 mol^{-1}) for the mixture [2-propanol (1) + ethyl acetate (2) + n-hexane (3)] at 313.15 K and atmospheric pressure.

x_1	x_2	ρ	V^E	x_1	x_2	ρ	V^E
0.0224	0.9450	0.8638	0.1302	0.7582	0.2418	0.7962	0.4780
0.0415	0.3631	0.7105	1.0116	0.8686	0.1314	0.7840	0.3012
0.0537	0.0369	0.6502	0.3696	0.9636	0.0364	0.7733	0.1031
0.1081	0.0759	0.6608	0.6282	0.0372	0.0000	0.6428	0.2497
0.1788	0.7171	0.8238	0.6271	0.1351	0.0000	0.6483	0.6400
0.1947	0.0927	0.6711	0.8157	0.2152	0.0000	0.6542	0.8615
0.2232	0.7504	0.8446	0.4830	0.3546	0.0000	0.6664	0.9900
0.2432	0.1556	0.6882	1.0089	0.4060	0.0000	0.6715	1.0167
0.3033	0.6018	0.8135	0.7305	0.5723	0.0000	0.6904	1.0126
0.3304	0.3882	0.7546	1.1452	0.6165	0.0000	0.6964	0.9557
0.3516	0.3579	0.7497	1.1728	0.7122	0.0000	0.7107	0.8011
0.4145	0.5391	0.8168	0.7680	0.8948	0.0000	0.7446	0.3501
0.4844	0.4187	0.7931	0.8200	0.9289	0.0000	0.7523	0.2284
0.4965	0.3094	0.7617	0.9651	0.0000	0.0987	0.6559	0.6301
0.5182	0.3614	0.7818	0.8638	0.0000	0.1581	0.6659	0.8470
0.5520	0.2475	0.7538	0.9252	0.0000	0.2246	0.6776	1.0511
0.6368	0.0583	0.7159	0.7526	0.0000	0.3465	0.7009	1.2852
0.6787	0.2543	0.7823	0.5874	0.0000	0.4906	0.7319	1.3151
0.7114	0.0992	0.7403	0.6096	0.0000	0.5977	0.7575	1.2014
0.7613	0.1419	0.7625	0.6013	0.0000	0.6444	0.7693	1.1401
0.8006	0.1785	0.7836	0.4856	0.0000	0.7507	0.7798	0.9255
0.8266	0.1235	0.7712	0.4125	0.0000	0.8015	0.8145	0.7602
0.9006	0.0355	0.7599	0.0783	0.0000	0.9502	0.8604	0.2267
0.0470	0.9530	0.8601	0.1141				
0.1635	0.8365	0.8537	0.3501				
0.2252	0.7748	0.8539	0.4296				
0.3192	0.6808	0.8439	0.5174				
0.4162	0.5838	0.8335	0.5901				
0.5682	0.4318	0.8172	0.5974				
0.6716	0.3284	0.8058	0.5575				

Table 5. The coefficients A_p of equation (2) in (cm^3 mol^{-1}) and the standard deviations σ, for the binary mixtures at the different temperatures.

T (K)	A_0	A_1	A_2	A_3	σ
2-Propanol (1) + ethyl acetate (2)					
298.15	1.9536	−0.2251	−0.1256	0.7481	0.005
308.15	2.2727	0.0492	0.0015	−0.0349	0.020
313.15	2.4212	0.0714	0.3674	0.1256	0.011
2-Propanol (1) + n-hexane (3)					
298.15	2.5573	0.5921	−0.0464	−1.4126	0.003
308.15	1.9293	−1.2487	−1.4365	−0.8446	0.020
313.15	4.0853	0.3175	1.1831	−1.8857	0.013
Ethyl acetate (2) + n-hexane (3)					
298.15	3.3964	−1.2314	−0.3975	0.3916	0.012
308.15	4.2851	−1.3833	0.7946	−0.4424	0.037
313.15	5.1751	−0.9264	1.0856	−0.6359	0.020

3. Results and discussion

The density of the studied pure compounds at different temperatures and atmospheric pressure were measured. The measured densities are shown in table 1. In this table, the obtained data are compared with the available density data in the literature

Table 6. Coefficients B ($cm^3\,mol^{-1}$) of equation (3) and the corresponding standard deviation σ, for the ternary mixtures of [2-propanol (1) + ethyl acetate (2) + n-hexane (3)] at the different temperatures.

T (K)	B_0	B_1	B_2	σ
298.15	−0.50795	2.02883	1.21135	0.040
308.15	2.80456	14.3485	4.24504	0.063
313.15	−6.4861	−1.20157	9.64494	0.113

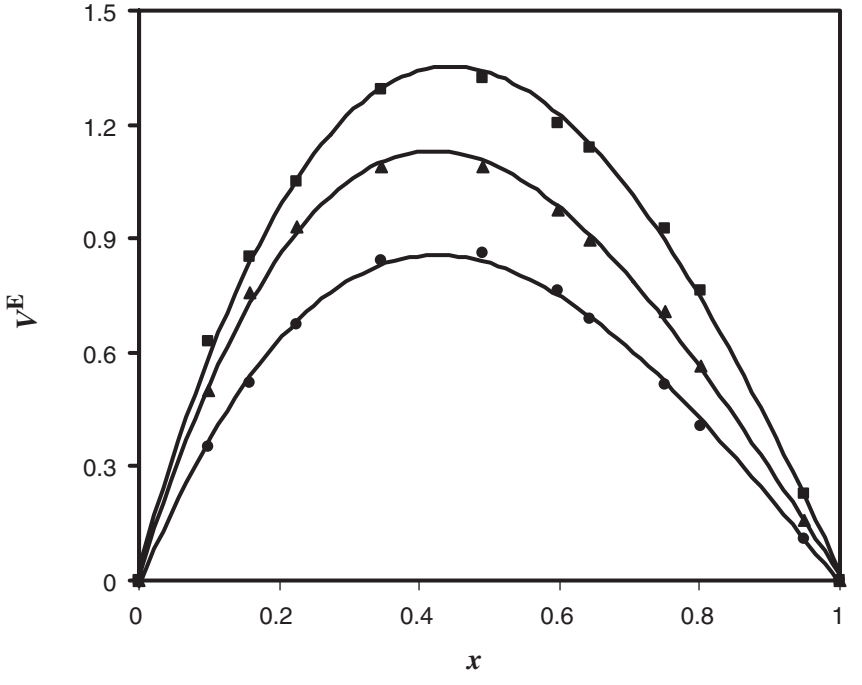

Figure 1. Calculated excess volume V^E by Redlich–Kister equation (lines), and the experimental data of V^E (points) for the binary mixtures: [ethyl acetate (2) + n-hexane (3)] *vs.* mole fraction of ethyl acetate (2) at 298.15 K (●), 308.15 K (▲) and at 313.15 K (■) and atmospheric pressure.

[8–10]. These comparisons indicated good consistency between these results and those presented in the literature.

The densities ρ of the ternary mixture [2-propanol (1) + ethyl acetate (2) + n-hexane (3)] and its binary constituents at three temperatures; 298.15, 308.15 and 313.15 K are reported in tables 2–4.

The molar excess volume, V^E, for the binary mixtures have been calculated from experimental data, according to the following expressions [8]:

$$V^E = \frac{\sum_{i=1}^{n} x_i M_i}{\rho} - \sum_{i=1}^{n} x_i \frac{M_i}{\rho_i} \tag{1}$$

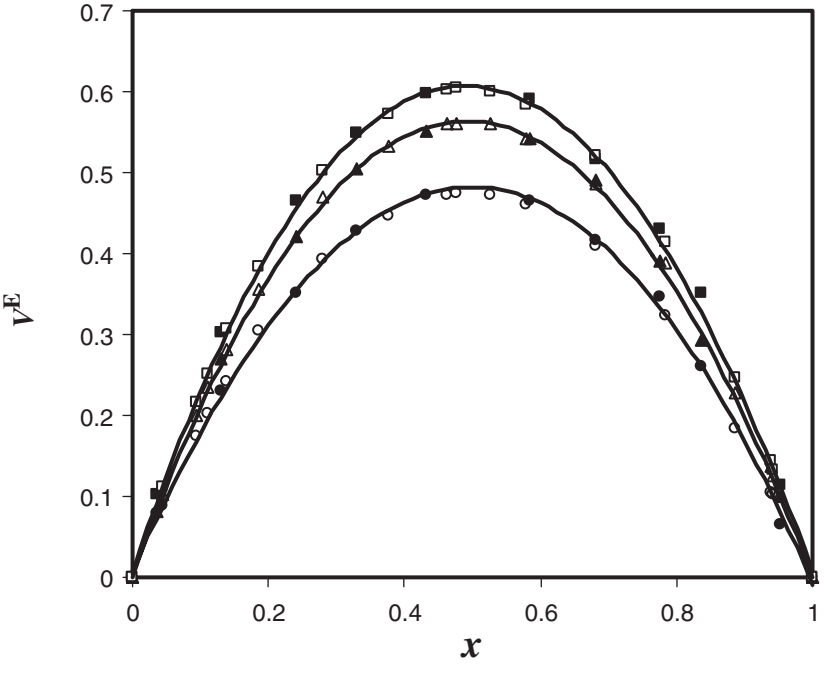

Figure 2. The comparison between the measured excess volume V^E by this work (black points) and by Oswal and Putta [12] (white points), for the binary mixtures: [2-propanol (1) + ethyl acetate (2)] *vs.* mole fraction of ethyl acetate (2) at 298.15 K (●), 308.15 K (▲) and at 313.15 K (■) and atmospheric pressure. Lines refer to the calculated excess volume V^E by Redlich–Kister equation.

where ρ and ρ_i are the density of the mixture and pure components respectively and n represents the number of components in the mixture. M_i and x_i are the molecular weight and the mole fraction of the component i respectively. Each set of molar excess volumes V^E for the binary mixtures was fitted to the Redlich–Kister type equation [7]:

$$V_{ij}^E = x_i x_j \sum_{p=0}^{n} A_p (x_I - x_j)^p \tag{2}$$

where x denotes the mole fraction and the parameters A_p were obtained by the suitable optimization method using the experimental data. The subscripts i and j indicate the components i and j in the binary mixture and according to the numbers allocated to the compounds used in this study, the values of i and j are respectively (1, 2), (1, 3), (2, 3) for the binary mixtures: [2-propanol (1) + ethyl acetate (2)], [(2-propanol (1) + n-hexane (3)] and [ethyl acetate (2) + n-hexane (3)].

For the ternary mixture [2-propanol (1) + ethyl acetate (2) + n-hexane (3)], the molar excess volumes V^E can be evaluated from their respective values (V_{ij}^E) of the binary mixtures via the following equations [7]:

$$V^E = V_{12}^E + V_{23}^E + V_{13}^E + x_1 x_2 x_3 [B_0 + B_1(x_1 - x_2) + B_2(x_2 - x_3)]. \tag{3}$$

The values of molar excess volumes V^E, for the binary mixtures have been calculated from experimental data, by equations (1). The results are also shown in tables 2–4.

The coefficients of Redlich–Kister type equations, A and B for molar excess volumes, along with the calculated standard deviations σ for fitting the experimental data with the applied equations, for the studied binary and ternary mixtures are reported in tables 5 and 6, respectively. The standard deviation σ is presented by the following equation:

$$\sigma = \left[\sum_{i=1}^{N} \frac{(V^E_{\text{exp.}} - V^E_{\text{calc.}})^2}{N - q} \right] \tag{4}$$

where, N and q are respectively number of experimental data and required parameters for fitting the experimental molar excess volumes data with the applied equations.

Considering the standard deviation σ, as reported in these tables, indicates acceptable correlation of the experimental data with the applied Redich–Kister type equations.

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