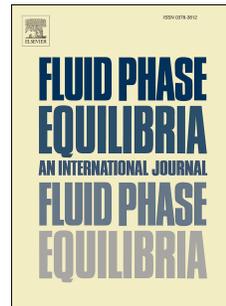# Accepted Manuscript

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High Pressure and High Temperature Volumetric Properties of (2-propanol + Di-isopropyl ether) System

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Abstract

New experimental density data are reported for binary mixtures of 2-propanol + di-isopropyl ether over the composition range (6 compositions; $0.15 \leq$ 2-propanol mole fraction $x \leq 0.85$), between 293.15 and 393.28 K, and for 23 pressures from 0.1 MPa up to 140 MPa. Measurements were performed by means of an Anton Paar vibrating tube densitometer, calibrated with an uncertainty of 7×10^{-4} g·cm^{-3}. A Tait like equation was used to fit the experimental density data, with low standard deviations. Excess volumes have been calculated from the experimental data and fitted by the Redlich–Kister equation. Moreover, the isothermal compressibility and the isobaric thermal expansivity have been derived from the Tait-like equation.

Keywords

2-Propanol, Di-isopropyl ether, Density, Excess Volume, Isobaric Thermal Expansivity, Isothermal Compressibility.

1. Introduction

Oxygenated compounds, such as ethers and alcohols, are used to improve the thermo-physical properties of new bio-fuels as environmentally friendly fluids. Future developments

of vehicles require essentially that engine is efficient and clean-burning, even in electrical hybrid vehicles. Present advanced bio-ethers (bio-ETBE, bio-MTBE, bio-TAME and bio-TAEE), are part of the present solution towards a low carbon transport fuels [1]. The branched alkyl ether di-isopropyl ether (DIPE), due to its exceptionally good octane enhancing properties when used as a gasoline blend stock, could also be considered as potential bio-ether. Concerning alcohols, besides the most popular bioethanol, the potential of biologically derived propanols (biopropanols) and butanols (biobutanols) are considered also as an alternative to bioethanol as a transportation fuel. It is due to their higher carbon number and therefore a higher energy density than ethanol [2], as well as they improve combustion and reduce emissions and the contaminant agents of automobile catalysts. Study of mixtures of DIPE with higher bio-alcohols could help to increase the knowledge of complex multicomponent biofuels. 2-propanol, which can be produced from biomass by microbial fermentation [3], has the potential of becoming fuel additive. Accurate PVT properties of the system 2-propanol + DIPE are required to develop and test equations of state, particularly at high pressure due to the requirements of the chemical industry.

This contribution continues the research on volumetric properties of binary mixtures of alcohols and ethers at high pressure carried out by our group [4-6]. In this work we report volumetric properties of (2-propanol + DIPE) over the complete composition range at the temperatures from 298.15 K to 393.29 K and at pressure up to 140MPa. The excess molar volumes were also calculated, as well as some derived thermodynamic properties such as isobaric thermal expansivity, α_p, and the isothermal compressibility, κ_T, for the given binary mixtures. Previous measurements of the system 2-propanol + DIPE have been performed at only 298.15 K and 0.1 MPa [7-12]. No literature references at high pressure for these mixtures have been found.

2. Experimental

2.1 Materials

Table 1 presents the purity and related data of 2-propanol and DIPE, which were obtained from Sigma-Aldrich. Storage over a molecular sieve and previous careful degassing of both liquids were the only operations performed before its use. Degasification of pure fluids was done at a first step, by means of an ultrasonic bath PSelecta, model Ultrasons-H, to prevent bubbles formation and consequently an air intake in the densitometer.

2.2. Measurement technique. Experimental procedure

Density has been measured with a vibrating-tube densitometer Anton Paar, model DMA HPM, previously described in reference [13]. For the pressure, the measurements were performed from 0.1 MPa up to 140 MPa, with 5 MPa intervals from 0.1 MPa to 65 MPa, and at every 10 MPa from 70 MPa to 140 MPa. For the temperatures, measurements were performed at (293.15, 298.15, 313.15, 333.15, 353.19, 373.24 and 393.28) K. The procedure described by Lagourette *et al.* [14], modified by Comuñas *et al.* [15] was used to calibrate the densitometer. Two reference fluids, water and vacuum, were used to calibrate the vibrating-tube densitometer. Vacuum and water were used within the interval $0.1 \leq p \leq 140$ MPa and $293.15 \leq T \leq 363.15$ K. At $p > 0.1$ MPa and $T \geq 373.15$ K, the reference pressure for water density is 1 MPa instead of 0.1 MPa [15]. For water, the equation of state (EoS) reported by Wagner and Pruss [16] was used.

The Pt 100 probe directly inserted into the densitometer leads to an expanded uncertainty in temperature of 0.03 K. The expanded uncertainty for the pressure is 0.04 MPa (pressure transducer WIKA CPH 6000). Then, the estimated expanded uncertainty ($k = 2$) in density was estimated, calculated following the EA-4/02 document [17]. This procedure involves the accuracy of the temperature, the pressure, the period of oscillation measurement for water, vacuum, the studied system, and the water density accuracy. The expanded uncertainty for density is estimated to be $7 \cdot 10^{-4}$ g·cm^{-3} (*i.e,* around 0.07 % for density close to water density). No measurements were made at $p = 0.1$ MPa and at 353.15 K, at 373.15 K and at 393.15 K because the boiling point of DIPE is 341.5 K.

Each mixture was prepared in glass vials sealed, to avoid evaporation. A Mettler Toledo balance model MS204S has been used for weighing, with uncertainty 0.0001 g, resolution of 10^{-4} g. The estimated uncertainty in the composition of the mixture is $4 \cdot 10^{-5}$ in mole fraction. Then, the excess molar volume accuracy is 0.004 cm^3·mol^{-1}.

3. Results and Discussion

3.1. Experimental density data

The results for densities of (2-propanol + di-isopropyl) at six 2-propanol molar ratio compositions (0.1503, 0.2979, 0.4228, 0.5000, 0.6737, 0.8483) are reported in Table 2 along the six isotherms from (298.15 to 393.28) K at pressures up to 140 MPa (23 isobars).

3.2. New Tait representation

A Tait-like equation was used to correlate the experimental data over the entire temperature and pressure ranges:

$$\rho(T,p) = \frac{\rho_0(T)}{1 - C\ln\left(\dfrac{B(T) + p}{B(T) + 0.1\ \text{MPa}}\right)} \tag{1}$$

where

$$\rho_0(T) = A_0 + A_1T + A_2T^2 + A_3T^3 \tag{2}$$

$$B(T) = B_0 + B_1T + B_2T^2 \tag{3}$$

The A_i, B_i and C parameters values were determined, for each mole fraction, by correlating the experimental densities values with respect to pressure and temperature. Table 3 gives the Tait-correlation parameters, as well as the AAD, MD, and standard deviation, σ, obtained with this correlation.

From close observation of Table 3, it can be observed that the values of all deviations parameters (AAD%, MD% and the standard deviation, σ) are equal or lower than the experimental uncertainty. As a consequence, interpolation of density at any T, p conditions by means of equations 1 to 3 is possible.

Figures 1(a) and (b) present the evolution of density as a function of temperature at $p = $ (1 and 140) MPa at different compositions of 2-propanol. This figure show that, when temperature increases, density decreases. Moreover, at low pressure, the variation of the density versus temperature is non-linear, as the temperature interval considered here is sufficiently large, which makes reliable the use of equation (1). Figures 1 (c) and (d) show the evolution of density as a function of pressure at $T = $ (298.15 and 393.28) K at different compositions of 2-propanol. Density increases when pressure increases, as shown. Again, the non-linear form the Tait-type equation makes it reliable to represent the behavior of the density versus pressure.

3.3. Excess Molar Volumes

The excess molar volumes were calculated over the complete temperature and pressure intervals according to the relation,

$$V^E = \sum_{i=1}^{n} x_i M_i \left[\left(\frac{1}{\rho}\right) - \left(\frac{1}{\rho_i}\right) \right] \tag{4}$$

being n the number of components; x_i the mole fraction of component i in the mixture while M_i is its molar mass; ρ and ρ_i are the experimental densities of the mixture and pure component i, respectively. As they are needed in equation (4), density data for pure 2-propanol and pure DIPE were taken from our previous works [6, 18].

The V^E values of (2-propanol + DIPE) at different temperatures and pressures are represented in Figure 2, which shows calculated V^E calculated at each mole fraction as well as tendency curves. Figures 2(a) and 2(b) present the evolution of V^E with the mole fraction and pressure at 313.15 K and 393.28 K, respectively. Similarly, figures 2(c) and 2(d) show the behaviour of V^E in relation with composition and temperature at 10 MPa and 140 MPa, respectively.

In figure 2(a) it can be observed that the excess volumes of the binary mixture at 313.15 K are negative over the whole composition range at pressures from 0.1 MPa to 140 MPa. The binary mixture (2-propanol + DIPE) contains one strong self-associating component (2-propanol) and a non-self-associating component (DIPE) which, however, can form ether-alkanol complexes through hydrogen bonding. The chemical part of the excess volume is the combination of two contributions of opposite signs, namely, a positive term due to the destruction of alkanol-alkanol hydrogen bonds upon mixing and a negative term due to the formation of alkanol-ether complexes in the mixture. The negative term is due, first, to both interstitial accommodation of alkanol in ether aggregates and, second, to weak hydrogen-bonding interaction between unlike molecules. The breaking of hydrogen bonds in 2-propanol lead to a volume expansion, but the formation of new hydrogen bonds between the 2-propanol and DIPE presents a higher negative contribution, giving as a result negative excess molar volumes. When temperature increases, the excess volumes sign changes from negative to positive values, being the breaking of hydrogen bonds and the enlargement of the free volume the main contribution in the DIPE rich region. At higher temperatures, the physical forces are much greater than the chemical interactions, and the excess molar volumes become positive, as shown at 393.28 K. In both cases, figures 2(a) and 2(b), the absolute values of V^E decrease with an increase of pressure.

When representing the behaviour of V^E with respect to mole fraction and temperature at fixed pressure, figures 2(c) and 2(d), the curves are sigmoid-shaped. With increasing temperature, the sign changes from negative to positive values. The increase of pressure lead to lower absolute values of V^E, as expected.

Seven references of literature data for the same system at 298.15 K and at 0.1 MPa were found [7-12]. Figure 3 shows that our V^E data for the mixture (2-propanol + DIPE) agree with those reported in the literature. Only some data points of reference [7] present a small difference with respect to this work, but we have to take into account that measurements of [7] were taken by means of a pycnometer with no declared uncertainty.

Concerning the influence of the size of the alkanol in the mixture, figure 4 shows the comparison between the excess molar volume of (2-propanol + DIPE) and the one of (2-

butanol + DIPE), previously measured by our group [6]. Figure 4(a) represents the behaviour of both systems at 393.28 K as a function of the composition and pressure. We can observe that the values of V^E at high temperature are positive for the system (2-propanol + DIPE), while they are negative for the system (2-butanol + DIPE) at almost the same composition and pressure, showing the higher influence of the increase of the Van der Waals interactions when the length of the branched alcohol increase. At the pressure of 140 MPa, figure 4(b) shows that the sigmoid behaviour of both systems exist, but the $|V^E|$ also increase with longer chain of the alcohol, because the free volume between the ether and alcohol increase. Similar conclusions were appreciated in [10] for similar (alcohol + ether) mixtures at atmospheric pressure.

3.6. The derived thermodynamic properties.

More valuable than density data are the derived properties isothermal compressibility and isobaric expansivity. Those properties give more precise information on the dependence of the volumetric properties with respect to the temperature and pressure. The isothermal compressibility, κ_T, describes the influence of pressure on the density, as expressed by the equation:

$$\kappa_T = \left(\frac{1}{\rho}\right)\left(\frac{\partial \rho}{\partial p}\right)_T = \frac{C}{\left(1 - C\ln\left(\frac{B(T) + p}{B(T) + 0.1MPa}\right)\right)(B(T) + p)} \tag{5}$$

In parallel, by differentiating equation (1), we could obtain the isobaric thermal expansivity. Taking into account that $\rho_0(T)$ and $B(T)$ present temperature dependence. Concerning this calculation, Cerdeiriña et al. [19] and Troncoso et al. [20] have demonstrated that the estimated isobaric thermal expansivity depends on the form of functions $B(T)$ and $\rho_0(T)$. Then, as an alternative method, it seems to be more reliable to calculate the isobaric thermal expansivity from the isobaric densities. At every pressure, we propose that $\rho_p(T) = a_0 + a_1T + a_2T$ and, as a result, $(\partial\rho/\partial T)_p = a_1 + 2a_2T$. Therefore, we get a set (a_0, a_1, a_2). Once the calculated densities $\rho_p(T)$ and the differentiated density are included into $\alpha_p = -(1/\rho)(\partial\rho/\partial T)_p$, we can obtain, at the different T, p conditions, the isobaric thermal expansivity:

$$\alpha_p = -\frac{a_1 + 2a_2T + 3a_3T^2}{a_0 + a_1T + a_2T^2 + a_3T^3} \tag{6}$$

Some authors [21] point out that not only differences in density values are the explanation of the differences found in this coefficient in the literature references, but that they are also due frequently to the fitting equations.

After applying the above procedures for calculation, the estimated uncertainty is 1% for the isothermal compressibility, and 3 % for the isobaric thermal expansivity. The isobaric thermal expansivity, α_p, and the isothermal compressibility, κ_T, are reported in tables S1 and S2 as supplementary material, respectively. At fixed mole fraction, the values of κ_T and α_p increase with increasing temperature and decrease with increasing pressure.

Acknowledgements

List of symbols

AAD	Absolute Average Deviation
a_i	coefficients of isobaric thermal expansivity correlation
A_i, B_i, C	coefficients of density correlation
calc	calculated
exp	experimental
i	constituent identification
MD	Maximum Deviation
N	number of experimental data points which are in our p, T ranges
p	pressure
p_0	reference pressure
T	temperature
V	volume
V^E	excess molar volumes
x	molar fraction

Greek letters

σ	Standard deviation
α_p	isobaric thermal expansivity
ρ	density

ρ_0 density at a reference pressure p_0

κ_T isothermal compressibility

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Table 1. Purity and related data of chemicals.

Compound	Molecular formula	Molar Mass (g·mol^{-1})	Stated purity[a] (mol %)	CAS number
2-propanol[b]	C_3H_8O	60.095	99.8	67-63-0
DIPE[b]	$C_6H_{14}O$	102.17	99.5[c]	108-20-3

[a] Determined by gas chromatography (GC)
[b] Supplied by Sigma Aldrich
[c] The water content was checked to be less than 0.01% by titration method.

Table 2. Experimental Densities, ρ (g·cm^{-3}), for x 2-propanol + (1-x) DIPE at various Temperatures T and Pressures p^a.

x	p / MPa	T / K					
		298.15	313.15	333.15	353.19	373.24	393.28
0.1503	0.1	0.7255	0.7096	0.6874			
	1	0.7266	0.7108	0.6890	0.6658	0.6410	0.6141
	5	0.7313	0.7163	0.6954	0.6737	0.6507	0.6264
	10	0.7368	0.7224	0.7027	0.6823	0.6610	0.6390
	15	0.7421	0.7281	0.7093	0.6900	0.6700	0.6497
	20	0.7468	0.7334	0.7153	0.6969	0.6781	0.6589
	25	0.7514	0.7382	0.7209	0.7033	0.6853	0.6671
	30	0.7557	0.7431	0.7262	0.7092	0.6920	0.6747
	35	0.7597	0.7476	0.7311	0.7147	0.6981	0.6815
	40	0.7636	0.7517	0.7358	0.7198	0.7039	0.6878
	45	0.7674	0.7557	0.7402	0.7246	0.7092	0.6936
	50	0.7709	0.7595	0.7444	0.7294	0.7142	0.6991
	55	0.7744	0.7633	0.7484	0.7337	0.7191	0.7045
	60	0.7777	0.7668	0.7522	0.7378	0.7235	0.7092
	65	0.7809	0.7702	0.7560	0.7419	0.7278	0.7139
	70	0.7840	0.7735	0.7595	0.7457	0.7320	0.7184
	80	0.7899	0.7796	0.7663	0.7529	0.7397	0.7267
	90	0.7956	0.7856	0.7726	0.7597	0.7470	0.7344
	100	0.8008	0.7912	0.7785	0.7660	0.7537	0.7415
	110	0.8058	0.7964	0.7841	0.7720	0.7600	0.7483
	120	0.8105	0.8013	0.7894	0.7776	0.7659	0.7545
	130	0.8151	0.8062	0.7945	0.7829	0.7716	0.7604
	140	0.8195	0.8109	0.7993	0.7881	0.7769	0.7661
0.2979	0.1	0.7326	0.7169	0.6949			
	1	0.7336	0.7181	0.6964	0.6732	0.6483	0.6206
	5	0.7382	0.7233	0.7026	0.6807	0.6575	0.6324
	10	0.7436	0.7293	0.7096	0.6891	0.6676	0.6447
	15	0.7486	0.7348	0.7160	0.6965	0.6762	0.6551
	20	0.7532	0.7399	0.7218	0.7032	0.6841	0.6641
	25	0.7576	0.7446	0.7273	0.7093	0.6911	0.6722
	30	0.7619	0.7494	0.7324	0.7151	0.6976	0.6795
	35	0.7658	0.7536	0.7372	0.7205	0.7036	0.6863
	40	0.7696	0.7577	0.7417	0.7254	0.7092	0.6925
	45	0.7732	0.7616	0.7460	0.7302	0.7145	0.6982
	50	0.7767	0.7654	0.7502	0.7348	0.7193	0.7037
	55	0.7801	0.7690	0.7541	0.7390	0.7241	0.7089
	60	0.7833	0.7725	0.7578	0.7431	0.7285	0.7137
	65	0.7865	0.7758	0.7615	0.7471	0.7328	0.7183
	70	0.7895	0.7790	0.7650	0.7509	0.7368	0.7228

	80	0.7953	0.7851	0.7716	0.7580	0.7445	0.7310
	90	0.8008	0.7909	0.7778	0.7647	0.7517	0.7386
	100	0.8060	0.7963	0.7836	0.7708	0.7583	0.7456
	110	0.8110	0.8015	0.7892	0.7768	0.7645	0.7524
	120	0.8156	0.8064	0.7944	0.7823	0.7704	0.7585
	130	0.8201	0.8112	0.7994	0.7876	0.7760	0.7644
	140	0.8244	0.8158	0.8041	0.7927	0.7813	0.7700
0.4228	0.1	0.7394	0.7240	0.7024			
	1	0.7405	0.7251	0.7037	0.6807	0.6556	0.6279
	5	0.7448	0.7300	0.7095	0.6877	0.6642	0.6389
	10	0.7499	0.7357	0.7161	0.6955	0.6737	0.6505
	15	0.7546	0.7410	0.7223	0.7027	0.6821	0.6606
	20	0.7592	0.7460	0.7280	0.7092	0.6897	0.6695
	25	0.7635	0.7507	0.7333	0.7153	0.6966	0.6774
	30	0.7676	0.7551	0.7383	0.7209	0.7030	0.6846
	35	0.7715	0.7593	0.7430	0.7262	0.7089	0.6913
	40	0.7752	0.7634	0.7474	0.7312	0.7145	0.6974
	45	0.7788	0.7672	0.7517	0.7359	0.7196	0.7032
	50	0.7822	0.7709	0.7557	0.7403	0.7245	0.7086
	55	0.7855	0.7744	0.7596	0.7445	0.7292	0.7136
	60	0.7887	0.7778	0.7633	0.7486	0.7336	0.7184
	65	0.7918	0.7811	0.7669	0.7525	0.7378	0.7230
	70	0.7948	0.7843	0.7703	0.7562	0.7418	0.7273
	80	0.8005	0.7903	0.7768	0.7632	0.7493	0.7355
	90	0.8059	0.7960	0.7829	0.7697	0.7563	0.7429
	100	0.8109	0.8013	0.7886	0.7758	0.7628	0.7499
	110	0.8158	0.8064	0.7940	0.7815	0.7689	0.7564
	120	0.8204	0.8112	0.7991	0.7869	0.7747	0.7625
	130	0.8248	0.8158	0.8040	0.7921	0.7802	0.7683
	140	0.8290	0.8202	0.8086	0.7970	0.7853	0.7738
0.5000	0.1	0.7437	0.7285	0.7070			
	1	0.7447	0.7296	0.7084	0.6854	0.6604	0.6329
	5	0.7490	0.7344	0.7142	0.6924	0.6690	0.6437
	10	0.7540	0.7401	0.7207	0.7002	0.6783	0.6552
	15	0.7588	0.7453	0.7268	0.7072	0.6866	0.6651
	20	0.7632	0.7502	0.7323	0.7136	0.6940	0.6737
	25	0.7675	0.7546	0.7375	0.7195	0.7008	0.6814
	30	0.7715	0.7592	0.7424	0.7250	0.7070	0.6885
	35	0.7752	0.7633	0.7470	0.7301	0.7128	0.6951
	40	0.7789	0.7672	0.7514	0.7349	0.7181	0.7010
	45	0.7824	0.7709	0.7554	0.7395	0.7233	0.7066
	50	0.7858	0.7745	0.7594	0.7439	0.7280	0.7118
	55	0.7890	0.7781	0.7632	0.7480	0.7326	0.7169
	60	0.7921	0.7814	0.7668	0.7520	0.7369	0.7216

	65	0.7952	0.7847	0.7704	0.7558	0.7411	0.7260
	70	0.7982	0.7877	0.7737	0.7595	0.7450	0.7304
	80	0.8038	0.7936	0.7801	0.7663	0.7526	0.7385
	90	0.8091	0.7993	0.7862	0.7728	0.7594	0.7461
	100	0.8142	0.8045	0.7918	0.7789	0.7659	0.7529
	110	0.8189	0.8096	0.7973	0.7847	0.7720	0.7595
	120	0.8235	0.8144	0.8023	0.7901	0.7778	0.7655
	130	0.8279	0.8190	0.8072	0.7952	0.7833	0.7713
	140	0.8321	0.8235	0.8119	0.8002	0.7885	0.7768
0.6737	0.1	0.7549	0.7402	0.7194			
	1	0.7558	0.7413	0.7207	0.6983	0.6736	0.6459
	5	0.7599	0.7459	0.7261	0.7047	0.6814	0.6559
	10	0.7647	0.7511	0.7322	0.7119	0.6901	0.6665
	15	0.7691	0.7560	0.7379	0.7185	0.6979	0.6757
	20	0.7734	0.7607	0.7431	0.7245	0.7048	0.6839
	25	0.7774	0.7648	0.7480	0.7301	0.7112	0.6912
	30	0.7812	0.7692	0.7526	0.7353	0.7171	0.6980
	35	0.7848	0.7731	0.7570	0.7402	0.7226	0.7042
	40	0.7883	0.7768	0.7612	0.7448	0.7278	0.7101
	45	0.7917	0.7804	0.7651	0.7492	0.7327	0.7154
	50	0.7949	0.7839	0.7689	0.7535	0.7372	0.7205
	55	0.7981	0.7873	0.7726	0.7573	0.7417	0.7254
	60	0.8011	0.7905	0.7761	0.7611	0.7458	0.7299
	65	0.8040	0.7937	0.7794	0.7649	0.7498	0.7343
	70	0.8068	0.7966	0.7827	0.7684	0.7536	0.7385
	80	0.8123	0.8023	0.7889	0.7750	0.7609	0.7464
	90	0.8175	0.8078	0.7948	0.7814	0.7677	0.7537
	100	0.8224	0.8129	0.8002	0.7872	0.7740	0.7604
	110	0.8271	0.8179	0.8055	0.7929	0.7799	0.7668
	120	0.8315	0.8224	0.8104	0.7981	0.7855	0.7728
	130	0.8357	0.8269	0.8152	0.8031	0.7909	0.7784
	140	0.8398	0.8313	0.8197	0.8080	0.7960	0.7839
0.8483	0.1	0.7680	0.7540	0.7341			
	1	0.7689	0.7550	0.7353	0.7137	0.6896	0.6625
	5	0.7726	0.7592	0.7402	0.7195	0.6967	0.6713
	10	0.7771	0.7641	0.7458	0.7261	0.7045	0.6809
	15	0.7813	0.7687	0.7511	0.7322	0.7116	0.6894
	20	0.7852	0.7730	0.7559	0.7377	0.7180	0.6969
	25	0.7890	0.7769	0.7605	0.7429	0.7240	0.7038
	30	0.7926	0.7810	0.7649	0.7478	0.7295	0.7101
	35	0.7960	0.7847	0.7690	0.7524	0.7347	0.7160
	40	0.7993	0.7882	0.7729	0.7567	0.7396	0.7215
	45	0.8026	0.7917	0.7766	0.7608	0.7443	0.7266
	50	0.8056	0.7949	0.7803	0.7649	0.7486	0.7315

55	0.8086	0.7981	0.7838	0.7686	0.7527	0.7362
60	0.8115	0.8012	0.7870	0.7722	0.7567	0.7405
65	0.8143	0.8042	0.7903	0.7758	0.7605	0.7447
70	0.8171	0.8070	0.7935	0.7792	0.7642	0.7488
80	0.8223	0.8125	0.7993	0.7855	0.7712	0.7563
90	0.8273	0.8178	0.8050	0.7916	0.7777	0.7634
100	0.8320	0.8227	0.8102	0.7972	0.7838	0.7699
110	0.8366	0.8275	0.8153	0.8027	0.7895	0.7761
120	0.8408	0.8320	0.8201	0.8077	0.7950	0.7818
130	0.8449	0.8363	0.8247	0.8126	0.8002	0.7874
140	0.8489	0.8406	0.8291	0.8174	0.8051	0.7927

[a] Estimated expanded uncertainties (k = 2): temperature, $U(T)$ = 0.03 K; pressure, $U(P)$ = 0.04 MPa;

density, $U(\rho)$ = 0.7·10^{-3} g·cm^{-3}; mole fraction, $U(x)$ = 4·10^{-5}.

Table 3. Obtained Parameters and Deviations for Density Correlation by using equation 1 for x 2-propanol + (1-x) DIPE.

Parameters	x					
	0.1503	0.2979	0.4228	0.5000	0.6737	0.8483
A_0 / g cm^{-3}	1.179076	1.224077	1.235919	1.203348	1.295628	1.319241
A_1 / g cm^{-3} K^{-1}	-2.739215·10^{-3}	-3.162689·10^{-3}	-3.268437·10^{-3}	-2.970176·10^{-3}	-3.803582·10^{-3}	-4.004332·10^{-3}
A_2 / g cm^{-3} K^{-2}	6.567410·10^{-6}	8.082690·10^{-6}	8.563690·10^{-6}	7.756900·10^{-6}	1.050380·10^{-5}	1.133680·10^{-5}
A_3 / g cm^{-3} K^{-3}	-8.324630·10^{-9}	-1.007140·10^{-8}	-1.068660·10^{-8}	-9.941290·10^{-9}	-1.2283680·10^{-8}	-1.376940·10^{-8}
B_0 / MPa	320.0011	324.1750	330.1205	333.0718	330.6590	326.8512
B_1 / MPa K^{-1}	-1.285231	-1.280338	-1.285680	-1.285398	-1.222127	-1.138947
B_2 / MPa K^{-2}	1.300560·10^{-3}	1.266273·10^{-3}	1.248605·10^{-3}	1.234135·10^{-3}	1.103821·10^{-3}	9.394040·10^{-4}
C	0.08826689	0.08800502	0.08792216	0.08778054	0.08749022	0.08725911
AAD[a] / %	0.014	0.016	0.007	0.014	0.013	0.013
MD[b] / %	0.067	0.072	0.029	0.060	0.051	0.053
σ[c] / g·cm^{-3}	1.36·10^{-4}	1.50·10^{-4}	6.53·10^{-5}	1.34·10^{-4}	1.31·10^{-4}	1.33·10^{-4}

[a] Absolute Average Deviation, $\mathrm{AAD} = \dfrac{100}{N} \sum\limits_{i=1}^{N} \left| \dfrac{\rho_i^{\exp} - \rho_i^{\mathrm{calc}}}{\rho_i^{\exp}} \right|$; [b] Maximum Deviation, $\mathrm{MD} = \mathrm{Max}\left(100 \left| \dfrac{\rho_i^{\exp} - \rho_i^{\mathrm{calc}}}{\rho_i^{\exp}} \right| \right)$; [c] Standard

Deviation, $\sigma = \sqrt{\dfrac{\sum\limits_{i=1}^{N} (\rho_i^{\exp} - \rho_i^{\mathrm{calc}})^2}{N\text{-}m}}$;
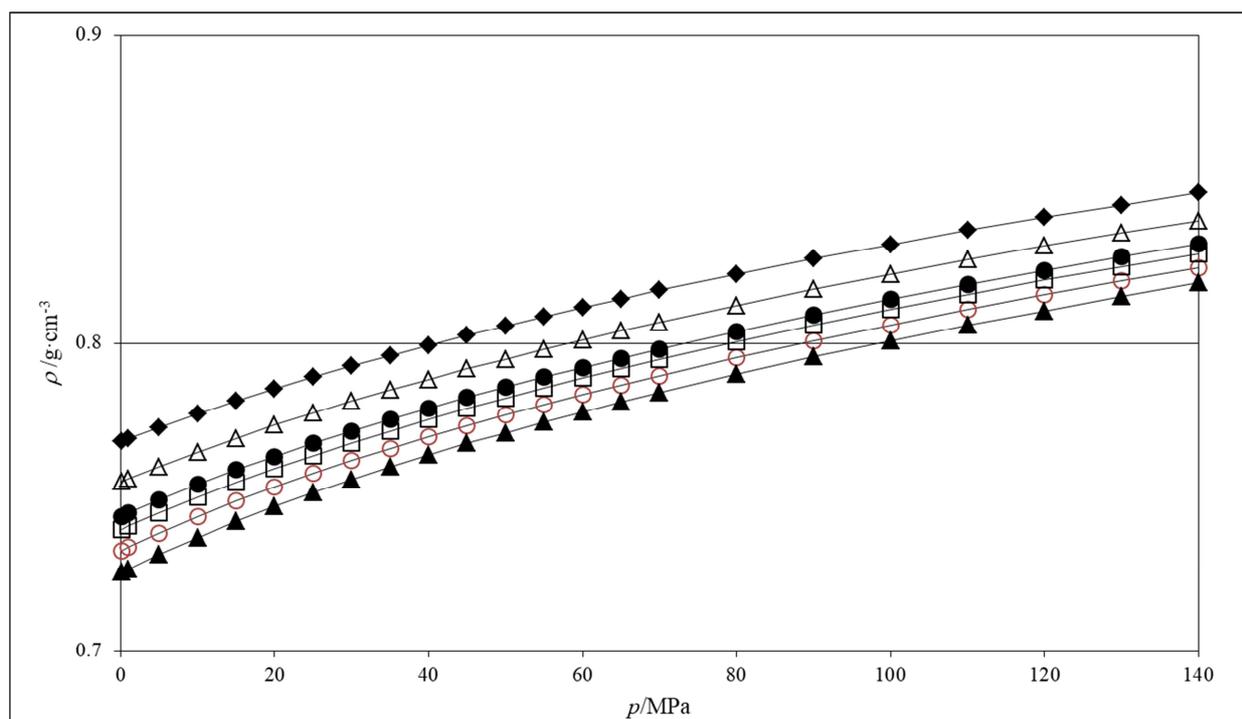
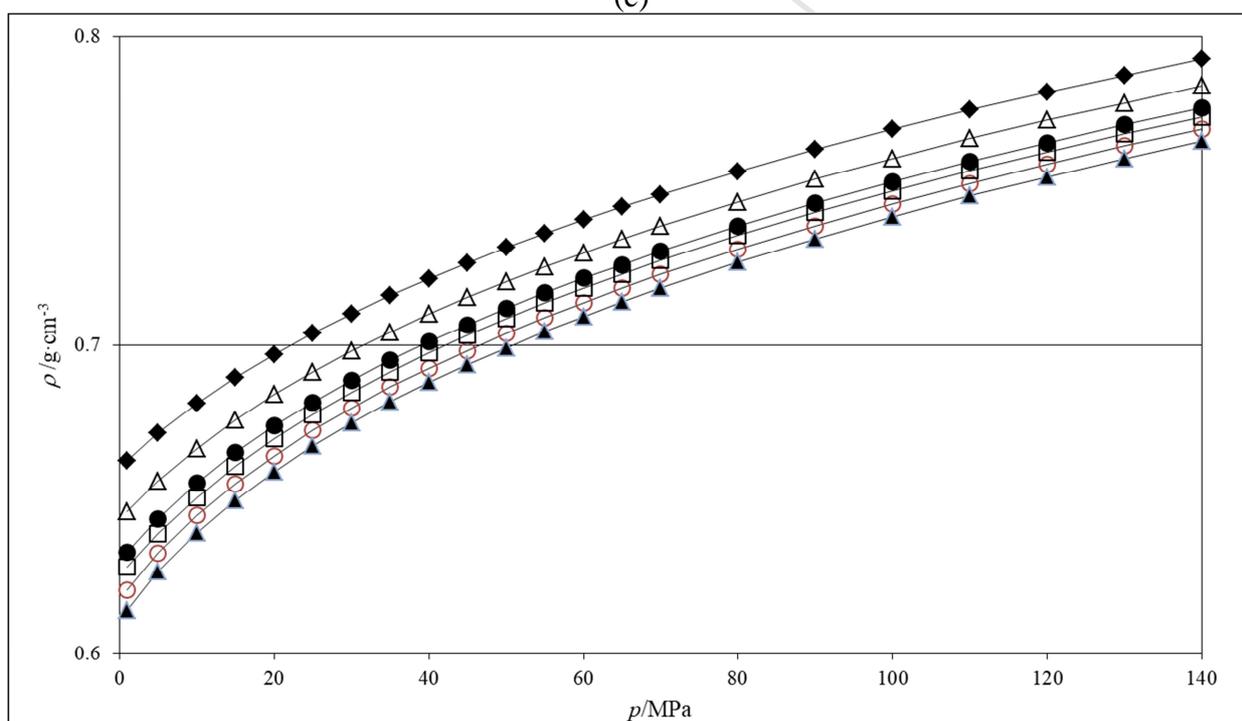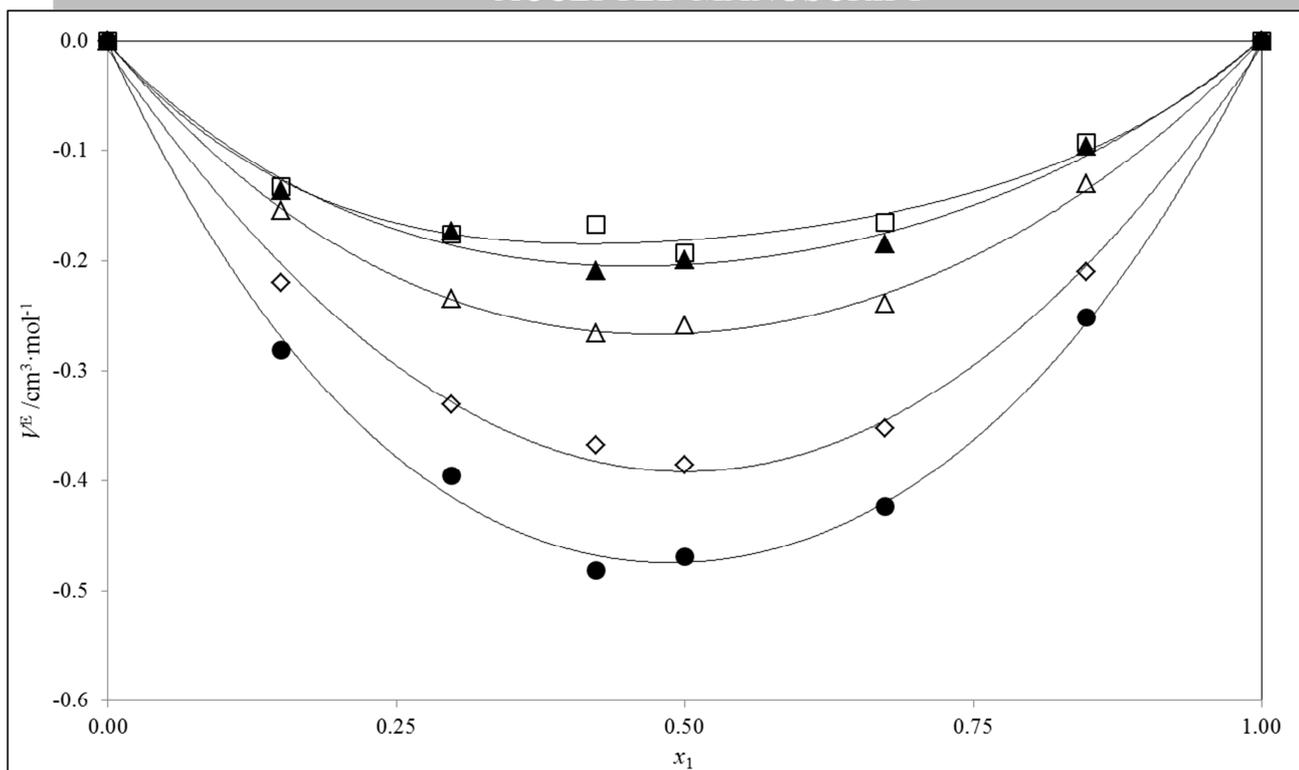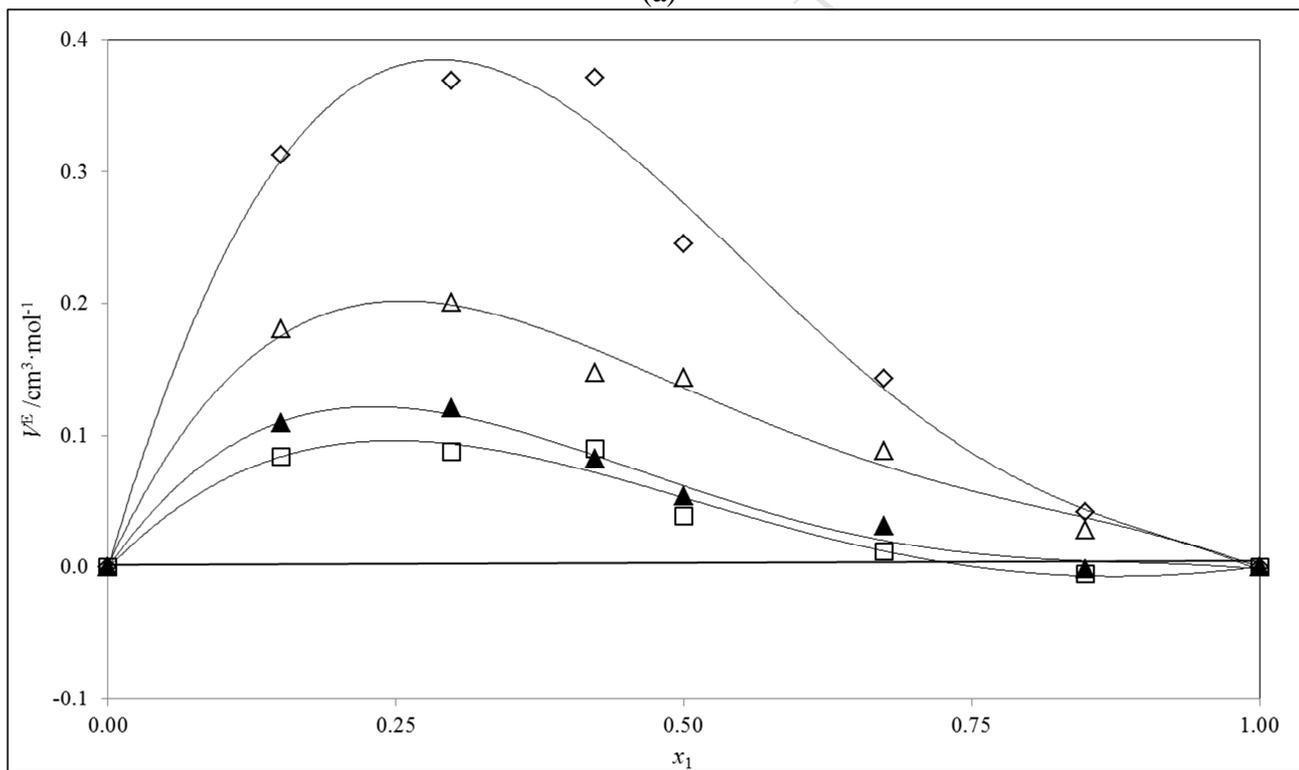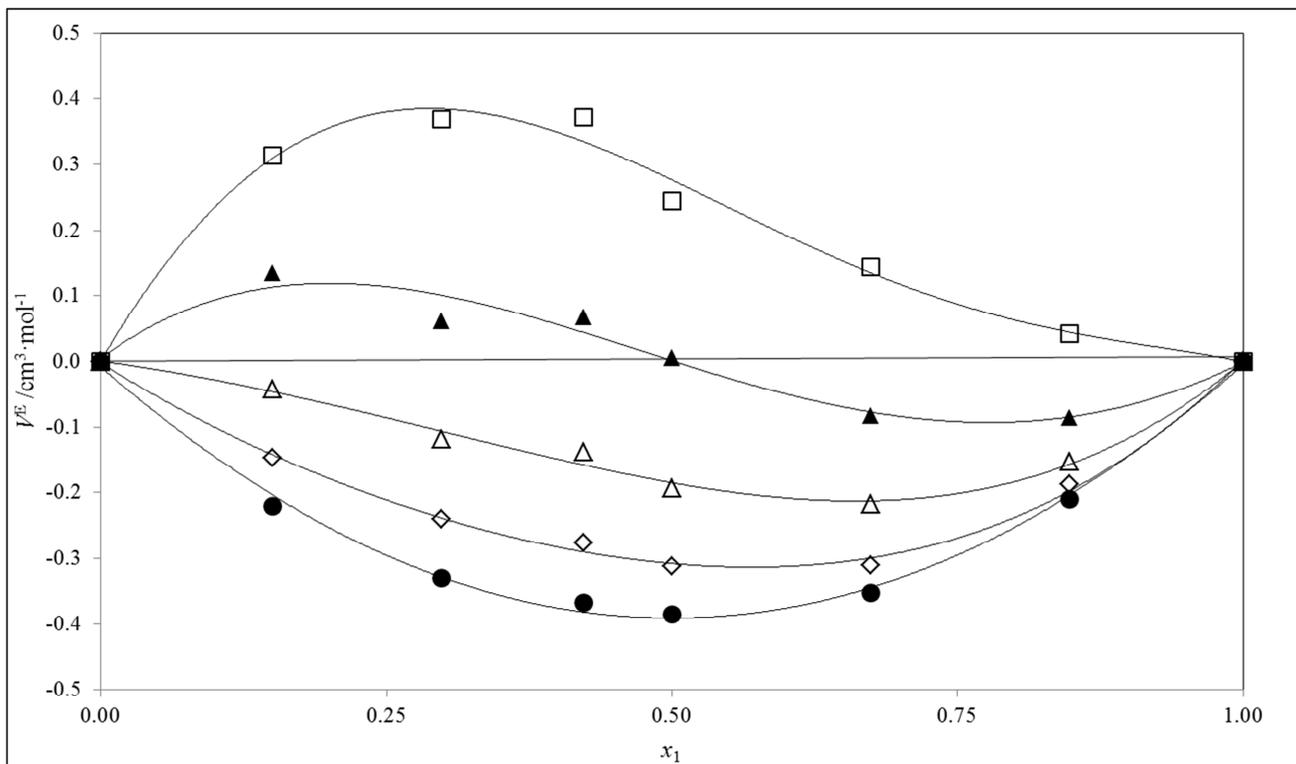N is the number of experimental data; m is the number of parameters.

(a)

(b)
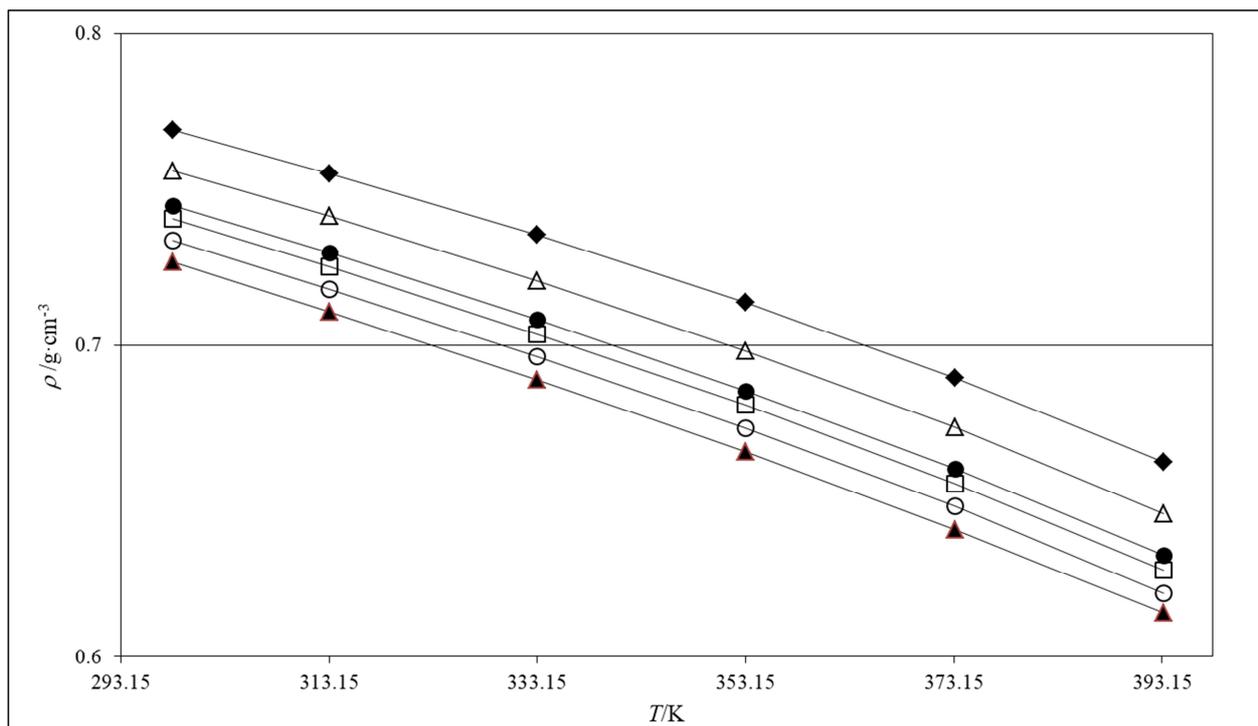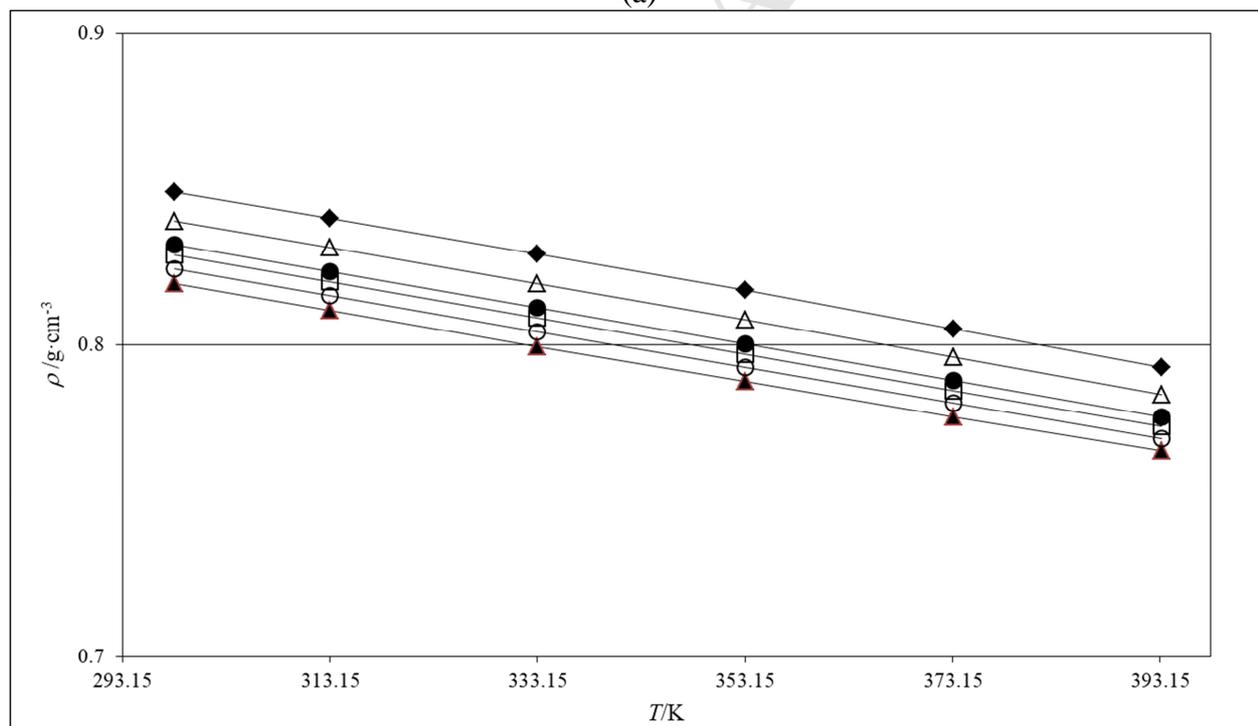
Fig. 1. Experimental values of densities, ρ, for different mole fractions of x 2-propanol + (1-x) DIPE vs. (a) the temperature, T at 1 MPa, (b) the temperature, T at 140 MPa, (c) the pressure, p at 298.15 K and (d) the pressure, p at 393.28 K: ▲, $x = 0.1503$; ○, $x = 0.2979$; □, $x = 0.4228$; ●, $x = 0.5000$; Δ, $x = 0.67375$; ♦, $x = 0.8483$; Tait equation (1).
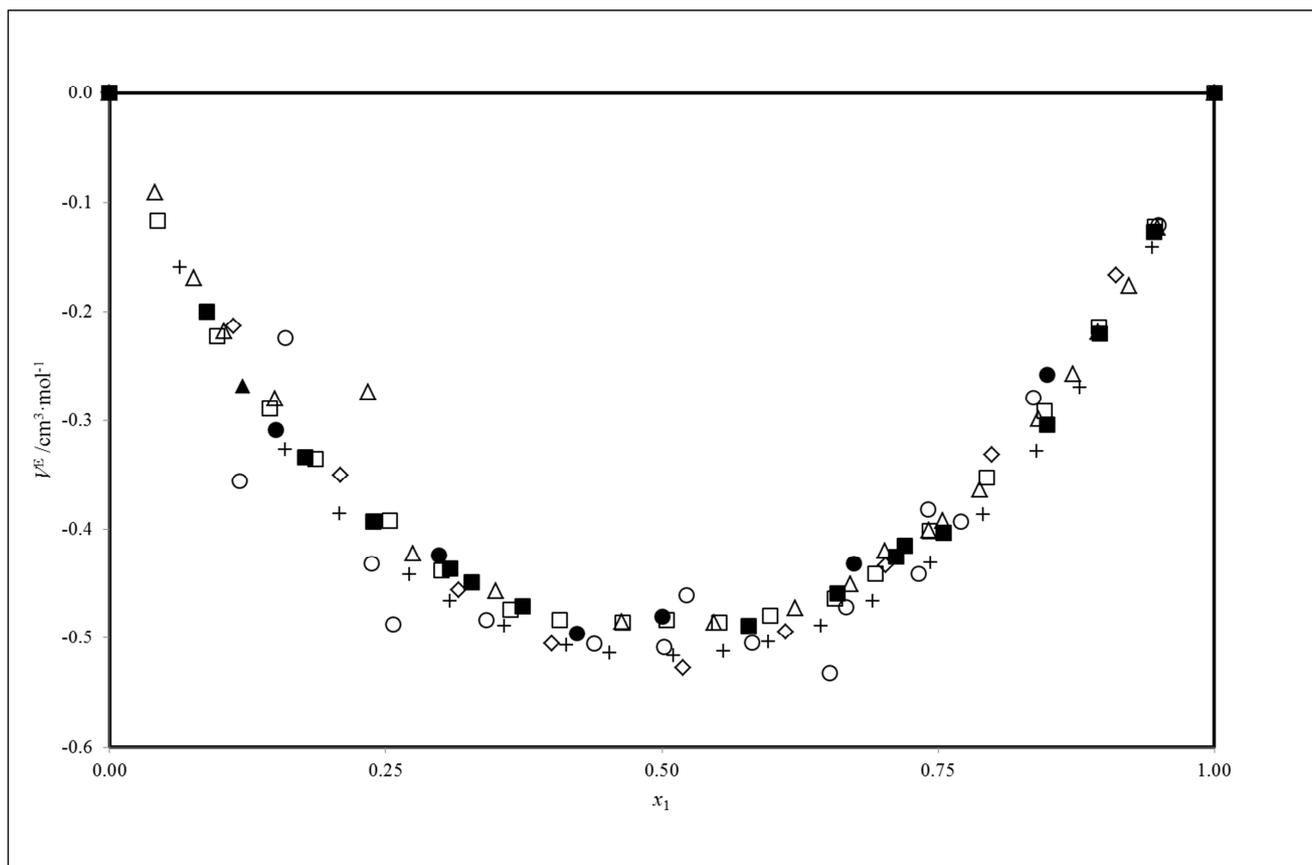
(a)

(b)
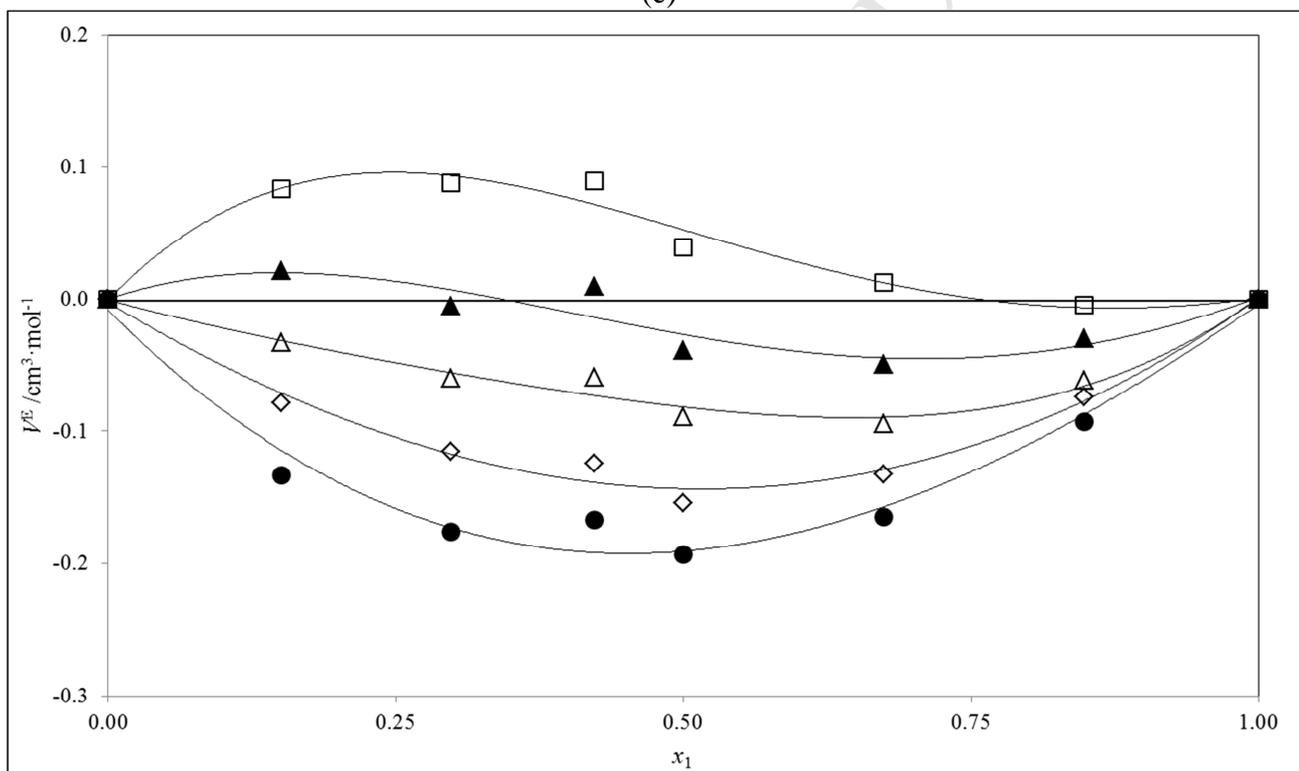
Fig 2. Experimental values of excess volumes, V^E, for the mixture x 2-propanol + (1-x) DIPE as a function of the mole fraction. (a) at 313.15 K for different pressure p: ●, 0.1 MPa; ◇, 10 MPa; Δ, 50 MPa; ▲, 100 MPa; □, 140 MPa; (b) at 393.28 K for different pressure p: ◇, 10 MPa; Δ, 50 MPa; ▲, 100 MPa; □, 140 MPa. (c) at 10 MPa for different temperature T: ●, 313.15K; ◇, 333.15 K; Δ, 353.19 K; ▲, 373.24 K; □, 393.28 K. (d) at 140 MPa for different temperature T: ●, 313.15K; ◇, 333.15 K; Δ, 353.19 K; ▲, 373.24 K; □, 393.28 K.
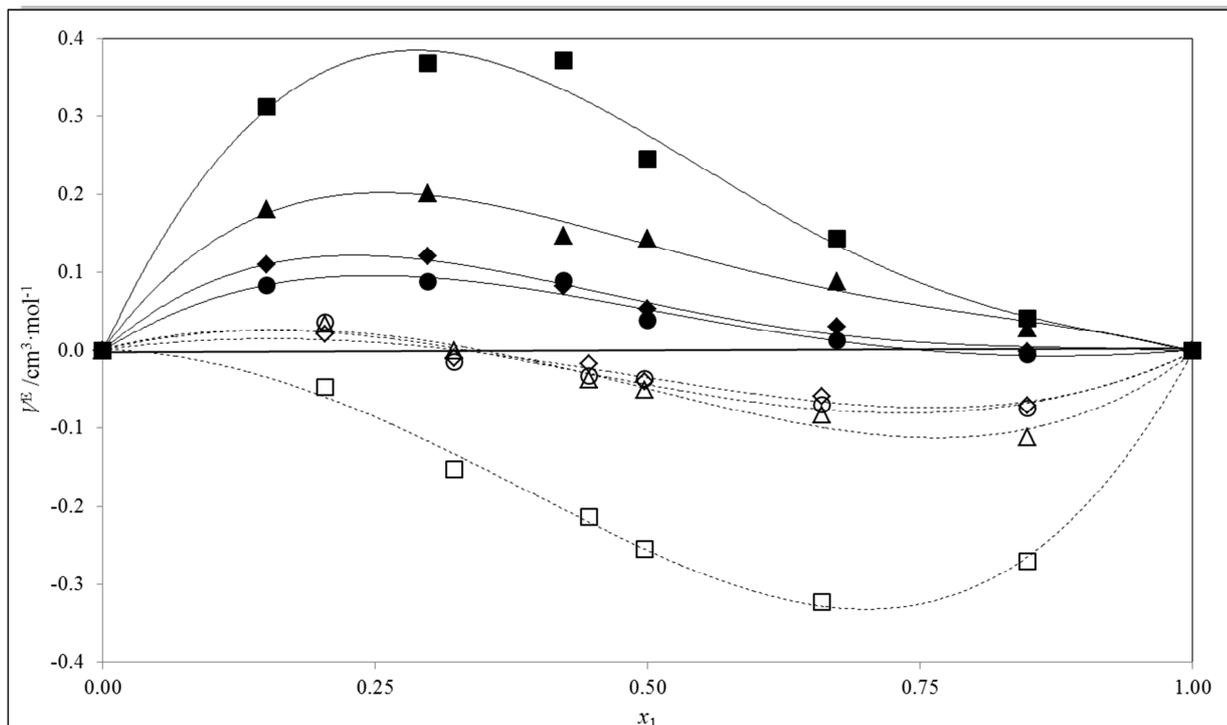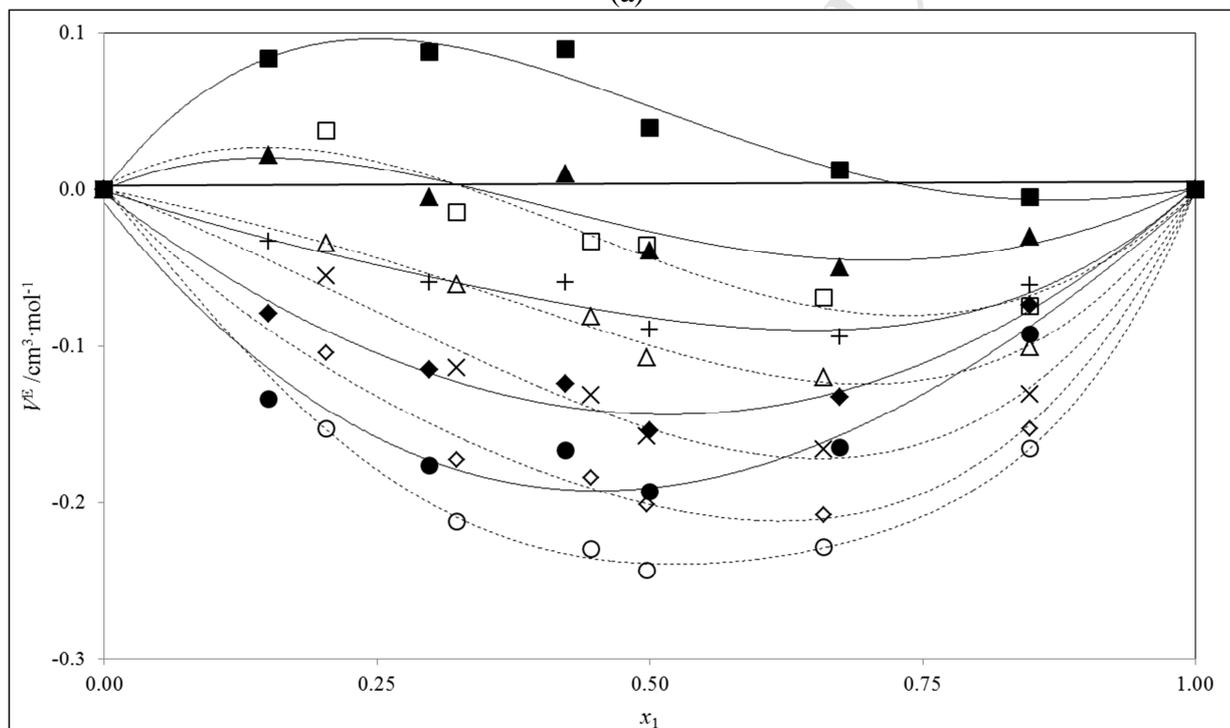
Fig 3. Experimental values of excess volumes, V^E, for the mixture x 2-propanol + $(1-x)$ DIPE as a function of the mole fraction. Comparison with literature values at 298.15 K and 0.1 MPa: ●, this work; ○, Miller and Bliss [7]; □, Blanco et al. [8]; Δ, Letcher and Govender [9]; ◇, Kammerer and Lichtenthaler [10]; ■, Wichterle [11]; ▲, Arce et al. [12].

Fig 4. Experimental values of excess volumes, V^E, for mixtures x 2-alkanol + ($1-x$) DIPE as a function of the mole fraction. Comparison between the system x 2-propanol + ($1-x$) DIPE (this work) and the system x 2-butanol + ($1-x$) DIPE [6]. (a) at 393.28 K for different pressure p. This work: ■, 10 MPa; ▲, 50 MPa; ◆, 100 MPa; ●, 140 MPa; Reference [6]: □ 10 MPa; Δ, 50 MPa; ◇, 100 MPa; O, 140 MPa. (b) at 140 MPa for different temperature T. This work ●, 313.15K; ◆, 333.15 K; +, 353.19 K; Δ, 373.24 K; ■, 393.28 K. Reference [6]: O, 313.15K; ◇, 333.15 K; X, 353.19 K; Δ, 373.24 K; □, 393.28 K

> New density data for binary mixtures of 2-propanol + DIPE are reported. > The pressure and temperature intervals are 0.1 - 140 MPa and 293.15 - 393.28 K. > 810 data points measured at 6 compositions were fitted to a Tait-like equation. > Excess volumes have been calculated from the experimental data. > The isobaric expansivity and the isothermal compressibility have been derived.