High pressure volumetric properties of the binary mixtures (di-isopropyl ether + n-heptane, or methylcyclohexane)

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Abstract

This work reports the experimental density data for the binary mixtures of n-heptane, or methylcyclohexane + di-isopropyl ether, measured over the full composition range between 0.1 MPa up to 140 MPa, and for temperatures from 298.15 and 393.15 K, by means of a vibrating tube densitometer calibrated with an uncertainty of 0.0007 $g \cdot cm^{-3}$. Then, the experimental density data were fitted using a Tait-like equation to derive mixing thermodynamic coefficients including the isobaric expansivity and the isothermal compressibility. Finally, the excess volumes of the above-mentioned binary mixtures were calculated and their non-ideal behavior was investigated.

1. Introduction

Liquid biofuels are a suitable fuel alternative to fast depleting fossil fuel and oil reserves and in serious consideration of the environmental issues associated with the extensive use of fuels based on petrochemicals.[1] In order to reduce significantly life-cycle greenhouse-gas emissions, advanced biofuels from second- and third-generation feedstocks can be more environmentally friendly, compared to traditional fossil fuels or first-generation biofuels from food-based feedstocks. These advanced biofuels include alcohols, ethers, biodiesel, or synthetic hydrocarbons.[2] Amongst the ethers, di-isopropyl ether (DIPE), as a branched alkyl ether, seems to be a very good candidate from the environmental point of view, as it is non-toxic and non-polluting chemical,[3] and presents low solubility in water.[4] The volumetric interactions of DIPE with the rest of compounds of the fuel, mainly hydrocarbons, are of interest in the design and operation of biofuel storage and transport facilities. In order to check the volumetric interaction of DIPE with the hydrocarbons, we have selected in this work the n-heptane and methylcyclohexane as representatives, as they are used as reference compounds of the fuel.

This work reports the experimental densities, ρ, for the systems (n-heptane + DIPE) and (methylcyclohexane + DIPE) at pressures, p, from (0.1 to 140) MPa and temperatures, T, from (298.15 to 393.15) K over the full composition range. Previously, our team has reported density of DIPE and n-heptane at high pressure and high temperature as pure compounds[5,6]. This work contributes to broad the range of experimental data, as literature references at high pressure for the mixtures (DIPE + n-heptane) and (DIPE + methylcyclohexane) are very scarce. With respect to the system (n-heptane + DIPE) only data at 101.3 kPa and 298.15 K[7-9] and 303.15 K[10] are reported. In relation with the system (methylcyclohexane + DIPE, reference 11 reports data at 101.3 kPa and 288.15K, 298.15 and 308.15 K. In this article, besides densities, we report excess molar volumes, isobaric thermal expansion coefficient and the isothermal compressibility coefficient for the binary mixtures (n-heptane, or methylcyclohexane + DIPE) at high pressures and temperatures.

2. Experimental

2.1 Materials

Data related to di-isopropyl ether n-heptane and methyl cyclohexane are shown in Table 1. The liquids were stored over a molecular sieve to avoid any moisture and were carefully degassed before use, without any further purification.

2.2. Measurement technique. Experimental procedure

A Mettler Toledo balance model MS2045 with an estimated expanded uncertainty of $1 \cdot 10^{-4}$ g was used to weigh the liquid mixtures. The pure fluids were degassed by means of an ultrasonic bath PSelecta, model Ultrason-H for at least 15 min at room temperature. The mole fraction estimated expanded uncertainty is $5 \cdot 10^{-4}$ for the prepared mixtures.

Reference 6 describes the Anton Paar DMA HPM vibrating-tube densitometer used to measure the density. Densitiy, ρ, was measured at several pressures, p (from 0.1 up to 140 MPa) and temperatures, T (from 298.15 to 393.15 K). Our previous works[5,6] report the operating procedure and the set-up calibration of the vibrating-tube densitometer. The recommended guide EA-4/02[12] is used to estimate the standard uncertainty (coverage factor k = 2) of density. The fluids used as reference to calibrate the densitometer, following the procedures cited in 13 and 14, are vacuum and water. For the water, the equation of state reported by Wagner and Pruss[15] was used to obtain the density values for 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, 1 MPa is the reference pressure for water density instead of 0.1 MPa.

Taking into account the uncertainties of the temperature, pressure and period of oscillation measurements, the expanded uncertainty on densities was estimated to be 0.0007 $g \cdot cm^{-3}$ (i.e. around ± 0.07% for density close to water density) for pressure up to 140 MPa, The estimated expanded uncertainty of the temperature measured with a Pt 100 calibrated probe was 0.03 K, while the same for the pressure measured with a pressure transducer WIKA CPH 6000 was 0.04 MPa.

3. Results and Discussion

3.1. Density

The measured densities of n-heptane + DIPE (n-heptane mole fractions x: 0.1505, 0.3233, 0.4994, 0.6732, and 0.8486) and methylcyclohexane + DIPE (methylcyclohexane mole fractions x: 0.1507, 0.3254, 0.5000, 0.6735, 0.8480 and 1.0000) are given in Tables 2 and 3 respectively, from (298.15 to 393.15) K at pressures up to 140 MPa (23 isobars). The density of DIPE and n-heptane as pure compounds

were previously reported.[5,6] As the boiling point of DIPE is 341.5 K, no mixtures measurements were made at p = 0.1 MPa and 373.15 K and 393.15 K.

3.2. Tait representation

The relation between our density values and the temperature and pressure values was established by means of the well-known Tait-like equation[14,16]

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

where

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

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

At each composition, we correlate simultaneously the experimental densities values versus pressure and temperature to obtain the A_i, B_i and C parameter values. Table 4 presents the Tait-correlation parameters with the Absolute Average Deviation (AAD), Maximum Deviation (MD) and standard deviation (σ) obtained for each mole fraction.

As the average deviation parameters (AAD and the standard deviation) are lower than the experimental uncertainty, eqs 1 to 3 allow the interpolation of the density at any T, p conditions. The evolution of density with the temperature at p = (0.1 and 140) MPa of the system n-heptane + DIPE at different mole fractions of n-heptane is shown in Figures 1(a) and 1(b). These figures reveal that when temperature increases density decreases. This non-linear behavior of density with temperature (particularly at low pressure) justifies the use of eq 2, as shown by Figure 1. Besides, Figures 1(c) and 1(d) show the dependence of density of n-heptane + DIPE with the pressure at T = (298.15 and 393.15) K as a function of the composition. In this case, density increases when pressure increases. In summary, we can conclude that the logarithmic Tait-type equation is very adequate to represent the dependence of density with respect to the pressure, as shown by the shape of the isothermal curves. With respect to the influence of mole fraction, Figures 1 show that density increases as the DIPE mole fraction increases.

A similar behavior can be observed in Figure 2 for the system methylcyclohexane + DIPE at several pressures and temperatures. As density of pure methylcyclohexane is higher than those of n-heptane, density results for the mixture methylcyclohexane + DIPE occur also at higher values than those of n-heptane + DIPE for similar mole fraction. Concerning the system methylcyclohexane + DIPE, Figures 2(a) and 2(b) represent the variation of density with the temperature at p = (0.1 and 140) MPa, while

Figures 2(c) and 2(d) present the evolution of density with the pressure at T = (298.15 and 393.15) K.

New density data of pure methylcyclohexane are reported in this article, then comparison with previous literature data at high pressure and temperature[17-24] in our p, T ranges is shown in Table 5. Comparison between the values generated using the Tait-like equation at exactly the same experimental p, T sets given by references 17-19 show a huge AAD deviation, over 10%, but it must be noticed that the data reported in these articles were measured in broad ranges of pressure, by means of experimental apparatus (self-design compression bench, dilatometer bellows) with no declared accuracy or uncertainty. The density data of the rest of references[20-24] were measured in low-medium pressure ranges with different models of vibrating-tube densitometers, the same physical principle as in this article. For these references, the AAD deviation is well under the estimated expanded uncertainty of the present article (0.7%), with exception of the data coming from reference 20, where the difference reaches AAD of 0.15%.

3.3. Excess Molar Volumes

The excess molar volumes, V^E, are used to be calculated by the following equation

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

where ρ and ρ_i are the measured densities of the mixture and pure component i, respectively; x_i is the mole fraction of component i in the mixture while M_i is its molar mass, and n is the number of components.

The Redlich–Kister polynomial equation was used to fit the data for the binary mixtures,

$$V^E = x(1-x)\sum_i z_i (2x-1)^{i-1} \tag{5}$$

where z_i are the parameters and x is the mole fraction of n-heptane o methylcyclohexane. Density values of pure DIPE and n-heptane were previously published.[5,6] Table 6 gives the obtained values of the adjustable parameters z_i of the fits at several pressures and temperatures and the corresponding fitting parameter. As shown in Table 6, z_i parameters are pressure and temperature dependent.

The V^E values of n-heptane + DIPE are presented in Figure 3 at different temperatures and pressures. The figures show V^E calculated data points at every composition as well as the Redlich-Kister curves. Concerning Figure 3, the curves show positive V^E and a parabolic shape over the full composition range at temperatures from (298.15 to 353.15)

K. In our case, DIPE shows a non-self-associating behaviour, while n-heptane is a non-polar compound. The excess volume is the result of two contributions of opposite signs: the negative contribution of the geometrical fitting between components and the positive contribution of the dispersive interactions between unlike molecules. Actually, the absolute values of V^E decrease with the increase of temperature at constant pressure (Figure 3(a)). This may be due to the increase in the intermolecular spacing between heptane molecules with increasing temperature, which allows the DIPE molecules largely adapt to these spaces at higher temperatures. In relation with the pressure, the increase of pressure at constant temperature (Figure 3(b)) at fixed composition leads to a decrease in V^E. The free volume reduction observed when a fluid is pressurized can be explained by means of the reduction of the inter-molecular distance. This trends of influence of pressure and temperature on the excess molar volume are in accordance with some literature references reporting mixtures of oxygenated compounds with hydrocarbons.[6,11]

Several references of V^E at 0.1 MPa were found for the mixture n-heptane + DIPE. References 7-9 report V^E data at 298.15 K, while reference 10 gives data at 303.15 K. Comparison of literature data at 0.1 MPa with this work is also presented in Figure 3(a), which shows that our work gives V^E values slightly over the literature values at 298.15 K.[7-9] It must be taken into account that the measurements reported by the literature are performed by means of high precision atmospheric devices, while our work is done with a high pressure device with a higher uncertainty at low pressures. Moreover, small differences in density values lead to greater differences in excess volume, as excess properties use to be one three order of magnitude smaller than the mixture properties. Nevertheless, comparison with data at 303.15 K of reference 10, even this temperature is not measured in this work, shows a quite higher deviation when compared with the close temperatures of 298.15 and 313.15 K.

With respect to the system methylcyclohexane + DIPE, V^E values are presented in Figure 4. It can be observed in Figure 4(a) that the curves show negative V^E and a parabolic shape over the full composition range at 0.1 MPa and at temperatures from (298.15 to 353.15) K, showing the stronger negative contribution due to the geometrical fitting between different components. The absolute values of V^E decrease with the decrease of temperature (Figure 4(a)). At high temperature (Figure 4(b)), the V^E values change from negative to positive values with the increase of pressure due to the increase contribution of the dispersive interactions, showing a sigmoid behaviour.

Only one reference of V^E at 0.1 MPa was found for the mixture methylcyclohexane + DIPE. Reference 11 reports V^E data at 288.15, 298.15 and 308.15 K. It must be said that reference 11 reports positive V^E values in its Table 2, but when calculating the corresponding V^E data from its reported composition and density data at the respective *p, T* sets with its V^E equation (2) (the same as our equation (5)), the results give negative values. Comparison of our present data with those newly calculated V^E data of reference 11 are presented in Figure 4(a). At 298.15 K the agreement is quite good, while data at 308.15 K seems to be plausibly placed between our 298.15 and 313.15 K data.

3.4. The derived thermodynamic properties.

The derived properties isothermal compressibility and isobaric expansivity can be obtained from the experimental densities through the Tait equation. These properties are very important because of the information they give on the dependence of the volumetric properties with temperature and pressure. The effect of pressure on the density is given by the isothermal compressibility, κ_T:

$$\kappa_T = \left(\frac{1}{\rho}\right)\left(\frac{\partial\rho}{\partial p}\right)_T = \frac{C}{\left(1 - C\ln\left(\frac{B(T)+p}{B(T)+0.1MPa}\right)\right)\left(B(T)+p\right)} \tag{6}$$

By differentiation of eq 1, the isobaric thermal expansivity, α_p, could also be obtained,

$$\alpha_p = -\left(\frac{1}{\rho}\right)\left(\frac{\partial\rho}{\partial T}\right)_p \tag{7}$$

Some authors[25,26] have demonstrated that the calculated isobaric thermal expansivity depends on the formulation of functions *B(T)* and $\rho_0(T)$. Thus, the fitting equation $\rho_0(T)$ is subjective, as two different equations may represent the same $\rho_0(T)$ but lead to a different temperature dependence of $\alpha_p(T)$. Jacquemin et al.[27] have found that differences reported for this coefficient in the literature can be due to the fitting equations, besides differences in density values. As an alternative, at each pressure, we can suppose that $\rho_p(T) = a_0+a_1T+a_2T^2$ and consequently $(\partial\rho/\partial T)_p = a_1 + 2a_2T$. Then, the isobaric thermal expansivity can be derived from the isobaric densities and get a set (a_0, a_1, a_2). By substituting the differentiated density and the calculated densities $\rho_p(T)$ into $\alpha_p = -(1/\rho(\partial\rho/\partial T)_p$ the isobaric thermal expansivity has been derived at the different *T, p* conditions:

$$\alpha_p = -\frac{a_1 + 2a_2T}{a_0 + a_1T + a_2T^2} \tag{8}$$

Then, the calculated values of the isothermal compressibility, κ_T, and the isobaric thermal expansivity, α_p, are given in Tables S1 and S2 of the supporting information for the system n-heptane + DIPE and S3 and S4 for the system methylcyclohexane + DIPE, respectively. The respective uncertainties are 1 % and 3%. These values are of the same order as those of high-pressure density studies.[28,29] For both systems, values of κ_T increase when temperature increases and decrease when pressure increases at fixed mole fraction. For α_p, the influence of the temperature leads to an increase at low pressures (close to 50 MPa) and to a decrease at high pressures, while the increase of pressure always lead to a decrease in α_p. The impact of pressure and temperature in the behavior of is similar to other references.[6,11,23,26] Concerning the influence of mole fraction, Tables S1 to S4 show that κ_T and α_p increase as the DIPE mole fraction increases.

4. Conclusions

1749 experimental density data for the compressed liquid phase of the binary systems n-heptane, or methylcyclohexane + di-isopropyl ether have been measured at 298.15, 313.15, 333.15, 353.15, 373.15 and 393.15 K and at pressures up to 140 MPa (23 isobars), with an absolute uncertainty of $0.7 \cdot 10^{-3}$ g.cm.$^{-3}$ Moreover, from these density values, derived properties, as the isothermal compressibility and the isobaric thermal expansivity, and excess molar volumes were calculated.

The work is a contribution of new data for both binary systems. To correlate experimental densities with temperature and pressure a Tait-type equation was used. As the AAD is lower than 0.015 % for both binary mixtures, the agreement between experimental and calculated data is quite good. The new data on densities of the systems n-heptane, or methylcyclohexane + DIPE were compared with the literature data available at 0.1 MPa. Excess molar volumes show positive values in the case of n-heptane + DIPE, as the dispersive interactions between unlike molecules dominates the interaction. At the opposite, in the case of methylcyclohexane + DIPE, excess molar volumes show negative values due to the geometrical fitting between different components.

Acknowledgements

The authors acknowledge support for this research to the Ministerio de Ciencia e Innovación, Spain, Project ENE2009-14644-C02-02, and to the University of Burgos (M. Dakkach, staff mobility program 2011). Gabriel Rubio-Pérez wishes to

acknowledge the Ministerio de Ciencia, Innovación y Universidades, Spain, for the funding of his doctoral scholarship FPU18/02975.

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Table 1. Purity and related data of chemicals.

Compound		Molecular formula	Molar Mass ($g \cdot mol^{-1}$)	Stated purity[a] (mol %)	CAS number
DIPE	Sigma Aldrich	$C_6H_{14}O$	102.17	99.5	108-20-3
n-Heptane	Sigma Aldrich	C_7H_{16}	100.21	99.5	142-82-5
Methylcyclohexane	Sigma Aldrich	C_7H_{14}	98.20	99.9	108-87-2

[a] Determined by gas chromatography (GC) by the supplier Sigma Aldrich

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

x	p / MPa	T / K					
		298.15	313.15	333.15	353.15	373.15	393.15
0.1505	0.1	0.7116	0.6965	0.6751			
	1	0.7127	0.6977	0.6767	0.6549	0.6317	0.6067
	5	0.7175	0.7031	0.6831	0.6625	0.6412	0.6184
	10	0.7230	0.7093	0.6903	0.6710	0.6513	0.6306
	15	0.7282	0.7149	0.6968	0.6786	0.6599	0.6410
	20	0.7329	0.7202	0.7029	0.6855	0.6679	0.6500
	25	0.7374	0.7252	0.7085	0.6917	0.6750	0.6580
	30	0.7417	0.7296	0.7136	0.6976	0.6815	0.6653
	35	0.7457	0.7343	0.7184	0.7029	0.6875	0.6720
	40	0.7497	0.7384	0.7231	0.7081	0.6930	0.6782
	45	0.7534	0.7424	0.7274	0.7128	0.6983	0.6839
	50	0.7569	0.7462	0.7316	0.7174	0.7032	0.6893
	55	0.7604	0.7499	0.7356	0.7217	0.7079	0.6942
	60	0.7638	0.7534	0.7393	0.7258	0.7125	0.6991
	65	0.7669	0.7568	0.7431	0.7299	0.7167	0.7036
	70	0.7699	0.7601	0.7466	0.7336	0.7207	0.7080
	80	0.7759	0.7663	0.7532	0.7407	0.7284	0.7161
	90	0.7814	0.7721	0.7596	0.7475	0.7354	0.7238
	100	0.7866	0.7776	0.7654	0.7536	0.7420	0.7306
	110	0.7916	0.7828	0.7710	0.7595	0.7482	0.7372
	120	0.7965	0.7878	0.7762	0.7652	0.7541	0.7433
	130	0.8010	0.7925	0.7812	0.7704	0.7596	0.7492
	140	0.8053	0.7971	0.7860	0.7753	0.7649	0.7547
0.3233	0.1	0.7044	0.6898	0.6694			
	1	0.7054	0.6910	0.6708	0.6498	0.6277	0.6038
	5	0.7100	0.6962	0.6769	0.6571	0.6365	0.6148
	10	0.7153	0.7021	0.6837	0.6651	0.6460	0.6263
	15	0.7202	0.7075	0.6899	0.6724	0.6542	0.6361
	20	0.7248	0.7126	0.6958	0.6789	0.6618	0.6446
	25	0.7291	0.7173	0.7011	0.6848	0.6686	0.6522
	30	0.7332	0.7216	0.7061	0.6906	0.6748	0.6592
	35	0.7372	0.7261	0.7108	0.6957	0.6806	0.6656
	40	0.7410	0.7301	0.7152	0.7007	0.6860	0.6715
	45	0.7446	0.7339	0.7194	0.7052	0.6911	0.6770
	50	0.7480	0.7376	0.7235	0.7096	0.6958	0.6822
	55	0.7514	0.7412	0.7273	0.7138	0.7003	0.6871
	60	0.7546	0.7445	0.7310	0.7178	0.7047	0.6918
	65	0.7577	0.7479	0.7346	0.7217	0.7087	0.6961
	70	0.7606	0.7510	0.7380	0.7254	0.7127	0.7005
	80	0.7664	0.7571	0.7445	0.7323	0.7201	0.7083
	90	0.7717	0.7627	0.7505	0.7388	0.7270	0.7157
	100	0.7768	0.7681	0.7562	0.7448	0.7334	0.7224

	110	0.7817	0.7731	0.7616	0.7505	0.7394	0.7288
	120	0.7864	0.7780	0.7667	0.7559	0.7451	0.7347
	130	0.7908	0.7826	0.7716	0.7610	0.7505	0.7404
	140	0.7951	0.7871	0.7763	0.7659	0.7557	0.7458
0.4994	0.1	0.6974	0.6834	0.6637			
	1	0.6984	0.6846	0.6651	0.6450	0.6237	0.6010
	5	0.7028	0.6894	0.6708	0.6518	0.6319	0.6112
	10	0.7078	0.6951	0.6773	0.6593	0.6410	0.6219
	15	0.7126	0.7002	0.6833	0.6663	0.6488	0.6312
	20	0.7169	0.7051	0.6888	0.6725	0.6559	0.6393
	25	0.7212	0.7097	0.6940	0.6782	0.6624	0.6466
	30	0.7250	0.7138	0.6987	0.6836	0.6684	0.6532
	35	0.7288	0.7181	0.7032	0.6886	0.6739	0.6594
	40	0.7325	0.7219	0.7075	0.6934	0.6790	0.6651
	45	0.7360	0.7256	0.7116	0.6978	0.6840	0.6704
	50	0.7393	0.7292	0.7155	0.7020	0.6885	0.6753
	55	0.7426	0.7326	0.7192	0.7061	0.6929	0.6801
	60	0.7457	0.7360	0.7227	0.7100	0.6972	0.6846
	65	0.7487	0.7392	0.7262	0.7136	0.7011	0.6888
	70	0.7515	0.7422	0.7295	0.7172	0.7049	0.6928
	80	0.7572	0.7481	0.7358	0.7239	0.7120	0.7005
	90	0.7623	0.7536	0.7417	0.7303	0.7187	0.7076
	100	0.7673	0.7587	0.7472	0.7361	0.7249	0.7142
	110	0.7720	0.7637	0.7524	0.7416	0.7308	0.7204
	120	0.7765	0.7684	0.7574	0.7469	0.7363	0.7262
	130	0.7808	0.7729	0.7621	0.7519	0.7416	0.7317
	140	0.7850	0.7772	0.7667	0.7566	0.7466	0.7369
0.6732	0.1	0.6909	0.6774	0.6584			
	1	0.6918	0.6785	0.6597	0.6403	0.6200	0.5984
	5	0.6959	0.6831	0.6651	0.6468	0.6278	0.6078
	10	0.7009	0.6885	0.6713	0.6539	0.6363	0.6179
	15	0.7054	0.6934	0.6770	0.6605	0.6437	0.6267
	20	0.7096	0.6981	0.6823	0.6665	0.6506	0.6344
	25	0.7136	0.7025	0.6872	0.6719	0.6568	0.6413
	30	0.7174	0.7064	0.6918	0.6772	0.6624	0.6477
	35	0.7210	0.7106	0.6961	0.6819	0.6678	0.6535
	40	0.7245	0.7142	0.7002	0.6865	0.6726	0.6590
	45	0.7279	0.7178	0.7042	0.6908	0.6774	0.6640
	50	0.7311	0.7213	0.7080	0.6948	0.6818	0.6689
	55	0.7343	0.7246	0.7115	0.6988	0.6860	0.6734
	60	0.7373	0.7278	0.7149	0.7025	0.6901	0.6778
	65	0.7402	0.7309	0.7183	0.7060	0.6939	0.6818
	70	0.7429	0.7339	0.7215	0.7096	0.6975	0.6858
	80	0.7484	0.7396	0.7275	0.7160	0.7045	0.6932
	90	0.7534	0.7449	0.7333	0.7221	0.7110	0.7001
	100	0.7582	0.7499	0.7386	0.7278	0.7170	0.7064
	110	0.7628	0.7547	0.7437	0.7332	0.7227	0.7125

	120	0.7673	0.7593	0.7485	0.7383	0.7281	0.7181
	130	0.7714	0.7636	0.7532	0.7432	0.7332	0.7235
	140	0.7754	0.7678	0.7576	0.7477	0.7380	0.7285
0.8486	0.1	0.6846	0.6716	0.6533			
	1	0.6855	0.6726	0.6545	0.6359	0.6163	0.5957
	5	0.6895	0.6770	0.6596	0.6419	0.6236	0.6044
	10	0.6941	0.6821	0.6655	0.6488	0.6316	0.6139
	15	0.6985	0.6868	0.6709	0.6550	0.6386	0.6221
	20	0.7025	0.6913	0.6760	0.6607	0.6451	0.6294
	25	0.7063	0.6956	0.6807	0.6659	0.6511	0.6361
	30	0.7100	0.6993	0.6852	0.6709	0.6565	0.6421
	35	0.7135	0.7033	0.6892	0.6754	0.6616	0.6477
	40	0.7169	0.7070	0.6932	0.6799	0.6663	0.6530
	45	0.7201	0.7103	0.6970	0.6840	0.6709	0.6579
	50	0.7232	0.7137	0.7007	0.6879	0.6752	0.6626
	55	0.7263	0.7169	0.7041	0.6916	0.6792	0.6669
	60	0.7292	0.7199	0.7074	0.6953	0.6832	0.6711
	65	0.7320	0.7230	0.7107	0.6987	0.6868	0.6750
	70	0.7346	0.7258	0.7137	0.7021	0.6903	0.6789
	80	0.7399	0.7313	0.7196	0.7083	0.6971	0.6860
	90	0.7448	0.7365	0.7252	0.7142	0.7033	0.6927
	100	0.7495	0.7414	0.7303	0.7198	0.7092	0.6989
	110	0.7539	0.7460	0.7353	0.7250	0.7147	0.7047
	120	0.7582	0.7505	0.7399	0.7299	0.7199	0.7101
	130	0.7622	0.7547	0.7444	0.7346	0.7249	0.7153
	140	0.7661	0.7588	0.7487	0.7391	0.7296	0.7202

[a] Estimated expanded uncertainties (k = 2): temperature, $U(T)$ = 0.03 K; pressure, $U(P)$ = 0.04 MPa; density, $U(\rho) = 0.7 \cdot 10^{-3}$ g·cm^{-3}; mole fraction, $U(x) = 5 \cdot 10^{-4}$.

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

x	p / MPa	T / K					
		298.15	313.15	333.15	353.15	373.15	393.15
0.1507	0.1	0.7250	0.7098	0.6884			
	1	0.7261	0.7111	0.6900	0.6681	0.6450	0.6198
	5	0.7308	0.7164	0.6962	0.6757	0.6542	0.6314
	10	0.7363	0.7224	0.7033	0.6839	0.6641	0.6433
	15	0.7414	0.7280	0.7097	0.6915	0.6727	0.6535
	20	0.7460	0.7332	0.7158	0.6982	0.6805	0.6624
	25	0.7505	0.7382	0.7213	0.7043	0.6875	0.6703
	30	0.7548	0.7426	0.7264	0.7102	0.6940	0.6776
	35	0.7588	0.7472	0.7312	0.7155	0.6999	0.6842
	40	0.7627	0.7513	0.7358	0.7206	0.7054	0.6903
	45	0.7665	0.7553	0.7402	0.7254	0.7107	0.6959
	50	0.7699	0.7591	0.7444	0.7299	0.7156	0.7014
	55	0.7734	0.7628	0.7483	0.7342	0.7202	0.7064
	60	0.7767	0.7663	0.7521	0.7384	0.7248	0.7113
	65	0.7799	0.7696	0.7558	0.7423	0.7289	0.7157
	70	0.7829	0.7729	0.7594	0.7461	0.7330	0.7202
	80	0.7889	0.7792	0.7660	0.7532	0.7407	0.7282
	90	0.7944	0.7850	0.7723	0.7600	0.7478	0.7358
	100	0.7996	0.7905	0.7781	0.7662	0.7543	0.7428
	110	0.8046	0.7957	0.7836	0.7720	0.7606	0.7494
	120	0.8094	0.8007	0.7889	0.7777	0.7664	0.7555
	130	0.8139	0.8054	0.7939	0.7829	0.7720	0.7614
	140	0.8183	0.8100	0.7988	0.7879	0.7773	0.7669
0.3254	0.1	0.7329	0.7182	0.6977			
	1	0.7339	0.7194	0.6990	0.6781	0.6561	0.6320
	5	0.7383	0.7243	0.7049	0.6850	0.6643	0.6424
	10	0.7435	0.7301	0.7115	0.6927	0.6735	0.6533
	15	0.7484	0.7353	0.7176	0.6997	0.6814	0.6628
	20	0.7528	0.7403	0.7233	0.7062	0.6889	0.6711
	25	0.7571	0.7450	0.7285	0.7119	0.6955	0.6786
	30	0.7612	0.7492	0.7334	0.7175	0.7016	0.6855
	35	0.7650	0.7536	0.7380	0.7225	0.7073	0.6917
	40	0.7687	0.7576	0.7423	0.7275	0.7124	0.6976
	45	0.7723	0.7614	0.7465	0.7320	0.7176	0.7031
	50	0.7757	0.7650	0.7506	0.7363	0.7223	0.7082
	55	0.7791	0.7686	0.7544	0.7405	0.7267	0.7131
	60	0.7822	0.7719	0.7580	0.7445	0.7311	0.7177
	65	0.7854	0.7753	0.7616	0.7483	0.7352	0.7221
	70	0.7882	0.7784	0.7650	0.7520	0.7390	0.7263
	80	0.7941	0.7845	0.7714	0.7589	0.7465	0.7342
	90	0.7994	0.7901	0.7775	0.7654	0.7534	0.7416
	100	0.8045	0.7955	0.7832	0.7715	0.7597	0.7484

	110	0.8094	0.8006	0.7886	0.7771	0.7658	0.7547
	120	0.8141	0.8054	0.7938	0.7826	0.7715	0.7607
	130	0.8185	0.8101	0.7987	0.7877	0.7770	0.7664
	140	0.8228	0.8145	0.8033	0.7926	0.7822	0.7718
0.5000	0.1	0.7410	0.7268	0.7070			
	1	0.7419	0.7279	0.7083	0.6882	0.6671	0.6449
	5	0.7461	0.7325	0.7137	0.6945	0.6747	0.6540
	10	0.7510	0.7379	0.7199	0.7017	0.6831	0.6640
	15	0.7555	0.7428	0.7256	0.7083	0.6906	0.6727
	20	0.7598	0.7476	0.7309	0.7142	0.6975	0.6804
	25	0.7638	0.7521	0.7359	0.7198	0.7037	0.6874
	30	0.7677	0.7560	0.7406	0.7250	0.7094	0.6938
	35	0.7714	0.7602	0.7449	0.7298	0.7149	0.6999
	40	0.7749	0.7641	0.7491	0.7346	0.7198	0.7054
	45	0.7784	0.7677	0.7531	0.7389	0.7247	0.7106
	50	0.7817	0.7712	0.7570	0.7430	0.7292	0.7155
	55	0.7850	0.7746	0.7606	0.7470	0.7335	0.7201
	60	0.7880	0.7779	0.7641	0.7509	0.7378	0.7246
	65	0.7910	0.7810	0.7676	0.7546	0.7416	0.7288
	70	0.7938	0.7841	0.7709	0.7581	0.7453	0.7329
	80	0.7995	0.7900	0.7771	0.7647	0.7526	0.7405
	90	0.8046	0.7955	0.7831	0.7710	0.7592	0.7476
	100	0.8095	0.8006	0.7886	0.7769	0.7654	0.7542
	110	0.8143	0.8056	0.7938	0.7825	0.7713	0.7604
	120	0.8189	0.8103	0.7987	0.7878	0.7768	0.7662
	130	0.8232	0.8148	0.8036	0.7928	0.7821	0.7718
	140	0.8273	0.8192	0.8082	0.7976	0.7872	0.7770
0.6735	0.1	0.7491	0.7354	0.7163			
	1	0.7500	0.7364	0.7175	0.6982	0.6781	0.6570
	5	0.7539	0.7408	0.7225	0.7041	0.6850	0.6652
	10	0.7585	0.7458	0.7283	0.7107	0.6927	0.6743
	15	0.7628	0.7505	0.7337	0.7169	0.6996	0.6824
	20	0.7668	0.7550	0.7387	0.7225	0.7061	0.6895
	25	0.7707	0.7592	0.7434	0.7277	0.7120	0.6961
	30	0.7744	0.7630	0.7478	0.7327	0.7174	0.7022
	35	0.7779	0.7670	0.7520	0.7372	0.7226	0.7079
	40	0.7813	0.7707	0.7560	0.7417	0.7273	0.7132
	45	0.7847	0.7741	0.7598	0.7459	0.7319	0.7180
	50	0.7878	0.7775	0.7636	0.7498	0.7362	0.7228
	55	0.7910	0.7808	0.7670	0.7537	0.7404	0.7273
	60	0.7939	0.7839	0.7704	0.7574	0.7445	0.7315
	65	0.7968	0.7870	0.7738	0.7609	0.7481	0.7355
	70	0.7995	0.7900	0.7769	0.7643	0.7518	0.7395
	80	0.8049	0.7957	0.7830	0.7708	0.7587	0.7468
	90	0.8099	0.8010	0.7888	0.7769	0.7651	0.7537
	100	0.8147	0.8059	0.7940	0.7826	0.7712	0.7601
	110	0.8194	0.8108	0.7991	0.7879	0.7768	0.7661

	120	0.8238	0.8153	0.8040	0.7931	0.7823	0.7718
	130	0.8280	0.8197	0.8086	0.7979	0.7874	0.7772
	140	0.8321	0.8240	0.8131	0.8026	0.7923	0.7823
0.8480	0.1	0.7575	0.7442	0.7258			
	1	0.7583	0.7452	0.7270	0.7084	0.6892	0.6691
	5	0.7619	0.7492	0.7315	0.7137	0.6955	0.6766
	10	0.7663	0.7539	0.7370	0.7199	0.7026	0.6848
	15	0.7703	0.7583	0.7420	0.7256	0.7090	0.6923
	20	0.7742	0.7625	0.7467	0.7309	0.7150	0.6989
	25	0.7778	0.7666	0.7512	0.7357	0.7205	0.7051
	30	0.7813	0.7702	0.7554	0.7405	0.7257	0.7108
	35	0.7847	0.7740	0.7593	0.7448	0.7305	0.7161
	40	0.7880	0.7774	0.7631	0.7491	0.7350	0.7211
	45	0.7912	0.7808	0.7668	0.7531	0.7395	0.7258
	50	0.7942	0.7840	0.7704	0.7569	0.7435	0.7304
	55	0.7972	0.7872	0.7736	0.7606	0.7475	0.7346
	60	0.8000	0.7902	0.7770	0.7640	0.7514	0.7387
	65	0.8028	0.7931	0.7802	0.7675	0.7549	0.7426
	70	0.8054	0.7960	0.7832	0.7708	0.7585	0.7463
	80	0.8107	0.8015	0.7890	0.7770	0.7651	0.7534
	90	0.8155	0.8067	0.7945	0.7829	0.7713	0.7601
	100	0.8202	0.8115	0.7997	0.7884	0.7771	0.7662
	110	0.8246	0.8162	0.8047	0.7936	0.7827	0.7720
	120	0.8291	0.8206	0.8094	0.7986	0.7879	0.7775
	130	0.8330	0.8249	0.8139	0.8034	0.7929	0.7829
	140	0.8371	0.8290	0.8183	0.8079	0.7977	0.7878
1.0000	0.1	0.7648	0.7519	0.7342			
	1	0.7655	0.7528	0.7352	0.7173	0.6988	0.6797
	5	0.7690	0.7567	0.7395	0.7222	0.7046	0.6864
	10	0.7731	0.7611	0.7445	0.7280	0.7113	0.6941
	15	0.7770	0.7652	0.7493	0.7334	0.7172	0.7010
	20	0.7806	0.7692	0.7538	0.7384	0.7229	0.7073
	25	0.7841	0.7731	0.7580	0.7430	0.7281	0.7131
	30	0.7875	0.7765	0.7620	0.7476	0.7330	0.7185
	35	0.7907	0.7803	0.7658	0.7516	0.7376	0.7235
	40	0.7938	0.7835	0.7694	0.7557	0.7419	0.7283
	45	0.7969	0.7868	0.7729	0.7595	0.7461	0.7328
	50	0.7997	0.7899	0.7764	0.7631	0.7501	0.7371
	55	0.8027	0.7929	0.7796	0.7667	0.7538	0.7411
	60	0.8054	0.7958	0.7827	0.7701	0.7576	0.7451
	65	0.8082	0.7986	0.7858	0.7733	0.7610	0.7488
	70	0.8106	0.8014	0.7888	0.7766	0.7644	0.7525
	80	0.8158	0.8067	0.7944	0.7826	0.7708	0.7593
	90	0.8205	0.8117	0.7998	0.7883	0.7769	0.7658
	100	0.8250	0.8164	0.8048	0.7936	0.7825	0.7717
	110	0.8293	0.8210	0.8096	0.7987	0.7879	0.7774
	120	0.8336	0.8253	0.8142	0.8036	0.7930	0.7827

130	0.8376	0.8295	0.8186	0.8082	0.7979	0.7879
140	0.8414	0.8336	0.8229	0.8126	0.8026	0.7928

[a] Estimated expanded uncertainties (k = 2): temperature, $U(T)$ = 0.03 K; pressure, $U(P)$ = 0.04 MPa; density, $U(\rho) = 0.7 \cdot 10^{-3}$ g·cm^{-3}; mole fraction, $U(x) = 5 \cdot 10^{-4}$.

Table 4. Obtained Parameters and Deviations for Density Correlation by using equation 1 for *x* n-heptane, or methylcyclohexane + (1-*x*) DIPE.

Parameters	A_0 / g cm^{-3}	A_1 / g cm^{-3} K^{-1}	A_2 / g cm^{-3} K^{-2}	A_3 / g cm^{-3} K^{-3}	B_0 / MPa	B_1 / MPa K^{-1}	B_2 / MPa K^{-2}	C	AAD[a] / %	MD[b] / %	σ[c] / g·cm^{-3}
					x n-heptane + (1-*x*) DIPE						
x											
0.1505	1.033187	$-1.545747\cdot10^{-3}$	$2.855447\cdot10^{-6}$	$-4.319508\cdot10^{-9}$	310.3305	-1.246057	$1.268105\cdot10^{-3}$	0.08864049	0.015	0.082	$1.36\cdot10^{-4}$
0.3233	0.9682871	$-1.070847\cdot10^{-3}$	$1.475635\cdot10^{-6}$	$-2.858099\cdot10^{-9}$	312.2786	-1.240304	$1.249756\cdot10^{-3}$	0.08876722	0.013	0.085	$1.23\cdot10^{-4}$
0.4994	0.9242808	$-7.663976\cdot10^{-4}$	$5.645542\cdot10^{-7}$	$-1.829419\cdot10^{-9}$	317.7093	-1.253726	$1.258401\cdot10^{-3}$	0.08881196	0.013	0.080	$1.19\cdot10^{-4}$
0.6732	0.9285521	$-8.799163\cdot10^{-4}$	$8.691370\cdot10^{-7}$	$-1980630\cdot10^{-9}$	323.5153	-1.269089	$1.269836\cdot10^{-3}$	0.08876676	0.014	0.072	$1.21\cdot10^{-4}$
0.8486	0.898709	$-6.996252\cdot10^{-4}$	$3.510443\cdot10^{-7}$	$-1.381912\cdot10^{-9}$	328.5831	-1.279794	$1.274150\cdot10^{-3}$	0.08860404	0.012	0.052	$1.05\cdot10^{-4}$
					x methylcyclohexane + (1-*x*) DIPE						
x											
0.1507	1.053999	$-1.599768\ 10^{-3}$	$2.981293\cdot10^{-6}$	$-4.413644\cdot10^{-9}$	314.7250	-1.255433	$1.269498\cdot10^{-3}$	0.08849268	0.015	0.098	$1.38\cdot10^{-4}$
0.3254	1.066921	$-1.664784\cdot10^{-3}$	$3.139953\cdot10^{-6}$	$-4.404449\cdot10^{-9}$	318.8070	-1.243084	$1.228656\cdot10^{-3}$	0.08845976	0.014	0.086	$1.33\cdot10^{-4}$
0.5000	0.9605515	$-6.286583\cdot10^{-4}$	$-6.559707\cdot10^{-8}$	$-9.894573\cdot10^{-10}$	338.1132	-1.316696	$1.311728\cdot10^{-3}$	0.0884548	0.013	0.061	$1.19\cdot10^{-4}$
0.6735	0.9776970	$-7.307579\cdot10^{-4}$	$2.155668\cdot10^{-7}$	$-1.124748\cdot10^{-9}$	344.1968	-1.311858	$1.281326\cdot10^{-3}$	0.08836144	0.012	0.046	$1.10\cdot10^{-4}$
0.8480	0.9727383	$-6.227597\cdot10^{-4}$	$-1.531977\cdot10^{-7}$	$-6.004894\cdot10^{-10}$	357.3852	-1.342901	$1.300003\cdot10^{-3}$	0.08844635	0.011	0.053	$1.01\cdot10^{-4}$
1.0000	0.9789955	$-6.296108\cdot10^{-4}$	$-1.528671\cdot10^{-7}$	$-4.851429\cdot10^{-10}$	366.5443	-1.359978	$1.305718\cdot10^{-3}$	0.08794217	0.011	0.033	$1.08\cdot10^{-4}$

[a] Absolute Average Deviation, $\mathrm{AAD} = \frac{100}{N}\sum_{i=1}^{N}\left|\frac{\rho_i^{\mathrm{exp}} - \rho_i^{\mathrm{calc}}}{\rho_i^{\mathrm{exp}}}\right|$; [b] Maximum Deviation, $\mathrm{MD} = \mathrm{Max}\left(100\left|\frac{\rho_i^{\mathrm{exp}} - \rho_i^{\mathrm{calc}}}{\rho_i^{\mathrm{exp}}}\right|\right)$; [c] Standard Deviation, $\sigma = \sqrt{\frac{\sum_{i=1}^{N}(\rho_i^{\mathrm{exp}} - \rho_i^{\mathrm{calc}})^2}{N\text{-}m}}$;

N is the number of experimental data; *m* is the number of parameters.

Table 5. Literature comparison between the values generated using the Tait-like equation at exactly the same experimental *p, T* sets given for methylcyclohexane at high pressure for several literature references.

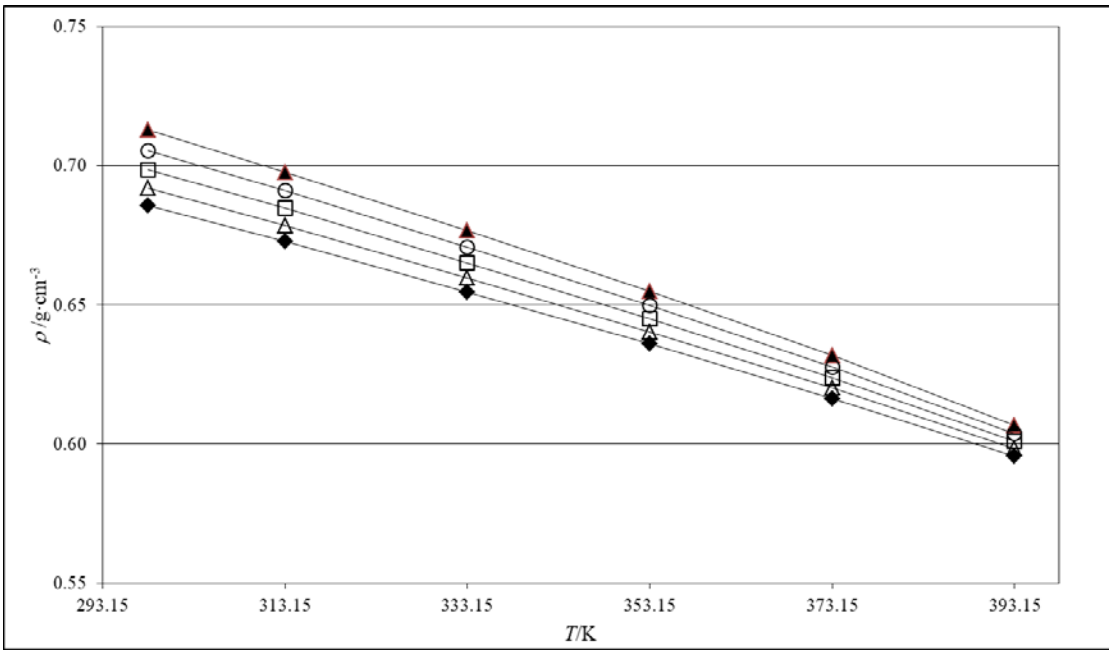
Reference	Year	N_P	T_{min} / K	T_{max}/ K	P_{min}/ MPa	P_{max}/ MPa	AAD / %	MD / %	Bias / %
Bridgman[17]	1949	3	298.15	298.15	0.1	400	13.0	21.7	-13.0
Brazier and Freeman[18]	1969	3	298.15	298.15	0.1	450	11.7	17.9	-8.60
Jonas *et al.*[19]	1979	3	203.10	298.15	0.1	500	12.5	20.9	-12.5
Et-Tahir *et al.* [20]	1995	42	298.15	363.15	0.1	40	0.05	0.13	-0.02
Baylaucq *et al.*[21]	1997	18	303.15	343.15	0.1	100	0.15	0.24	-0.15
Zeberg-Mikkelsen *et al.*[22]	2003	32	293.15	353.15	0.1	100	0.04	0.10	-0.04
Zeberg-Mikkelsen *et al.*[23]	2005	60	283.15	353.15	0.1	45	0.06	0.30	-0.06
Laesecke *et al.*[24]	2008	75	270	470	0.1	40	0.04	0.10	0.04

N_P Number of data points which are in our *p, T* ranges.

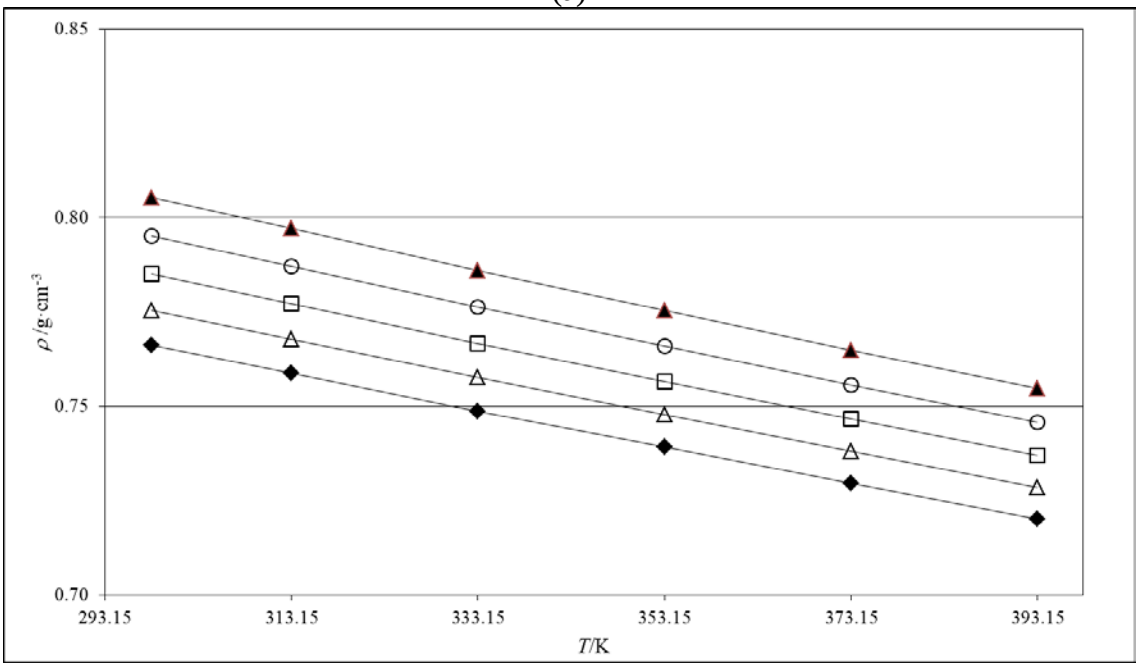
Table 6. Values of parameters z_i of equation (5) and the corresponding standard deviation, σ, for binary mixtures x n-heptane, or methylcyclohexane + (1-x) DIPE at 298.15 K and 393.15 K for different pressures, and at 0.10, 1.00 and 100.00 MPa for the temperatures measured.

	z_1	z_2	z_3	$\sigma (V^E)$/ cm^3·mol^{-1}
		x n-heptane + (1-x) DIPE		
p / MPa		(T = 313.15 K)		
0.10	0.7299	-0.1162	-0.3913	0.01
1.00	0.7251	-0.1887	-0.0520	0.01
10.00	0.6835	-0.0814	-0.1210	0.01
25.00	0.5855	-0.1270	-0.5354	0.01
50.00	0.6578	-0.0500	-0.2705	0.01
100.00	0.5282	-0.1065	-0.1926	0.01
p / MPa		(T = 393.15 K)		
1.00	0.5099	-0.2988	0.2240	0.01
10.00	0.7637	-0.3551	0.4190	0.02
25.00	0.7527	-0.3548	0.1502	0.01
50.00	0.7449	-0.2701	-0.2126	0.01
100.00	0.6338	-0.1186	-0.0120	0.01
T / K		(p = 0.10 MPa)		
298.15	1.0520	-0.1252	0.2711	0.01
313.15	0.7251	-0.1887	-0.0520	0.01
333.15	0.6864	-0.2144	-0.1368	0.01
353.15	0.6930	-0.1398	-0.0694	0.01
T / K		(p = 100.00 MPa)		
298.15	0.7473	-0.0842	0.2141	0.01
313.15	0.5160	-0.0833	-0.3859	0.01
333.15	0.5019	-0.0931	-0.1158	0.01
353.15	0.4269	-0.1736	-0.1941	0.01
373.15	0.6486	-0.2384	-0.0261	0.01
393.15	0.5975	-0.2111	0.1929	0.01
		x methylcyclohexane + (1-x) DIPE		
p / MPa		(T = 313.15 K)		
0.10	-0.7268	0.1014	-0.2157	0.01
1.00	-0.6614	0.0819	-0.2930	0.01
10.00	-0.4400	0.0794	-0.0405	0.01
25.00	-0.2962	0.1383	-0.2770	0.01
50.00	-0.0391	0.1049	-0.1113	0.01
100.00	0.0062	-0.0017	-0.2150	0.01
p / MPa		(T = 393.15 K)		
1.00	-2.6777	-0.5283	0.9513	0.03
10.00	-1.1364	-0.4921	0.6237	0.02
25.00	-0.3652	-0.3286	0.3484	0.01

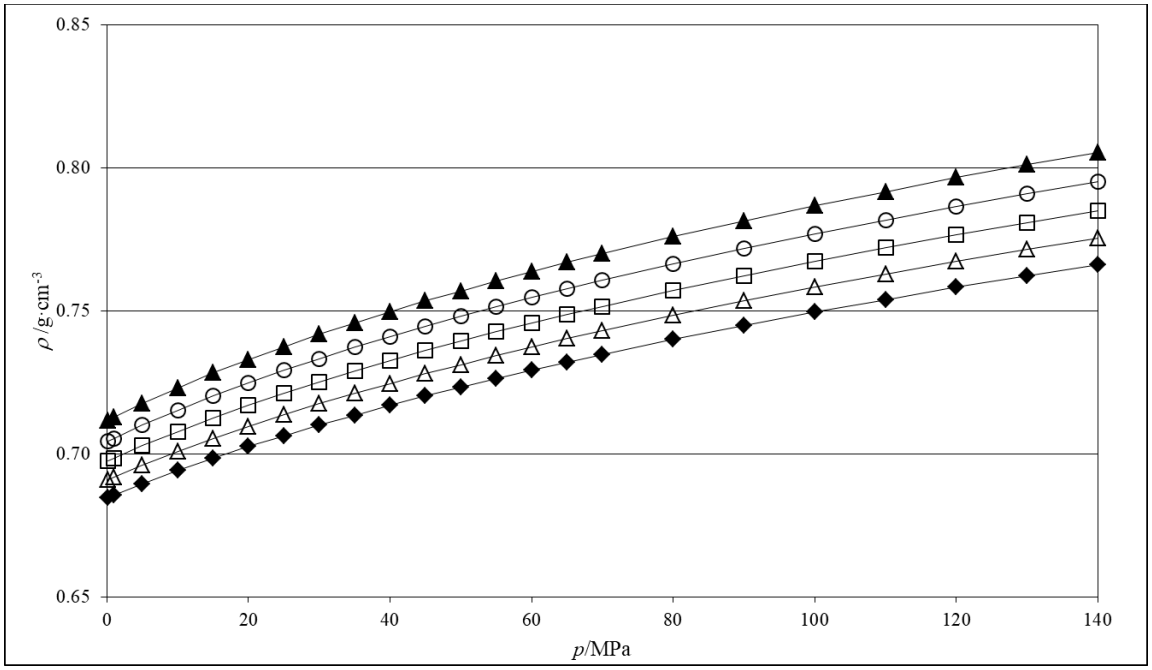
50.00	-0.0045	-0.2914	0.0991	0.01
100.00	0.1529	-0.2261	0.2724	0.01
T / K		(p = 1.00 MPa)		
298.15	-0.3716	-0.1888	-0.0260	0.01
313.15	-0.6614	0.0819	-0.2930	0.01
333.15	-0.8911	0.0291	-0.2443	0.01
353.15	-1.3254	0.0567	0.0159	0.01
373.15	-1.8444	-0.0153	0.0554	0.01
393.15	-2.6777	-0.5283	0.9513	0.03
T / K		(p = 100.00 MPa)		
298.15	0.1748	-0.1084	-0.0022	0.01
313.15	0.0413	0.1148	-0.2669	0.01
333.15	0.0485	0.0369	-0.0351	0.01
353.15	0.0145	0.0628	-0.2042	0.01
373.15	0.1228	-0.1981	0.2632	0.01
393.15	0.1044	-0.1901	0.2733	0.01


0.75
0.70
0.65
0.60
0.55
ρ /g·cm-3
293.15
313.15
333.15
353.15
373.15
393.15
T/K

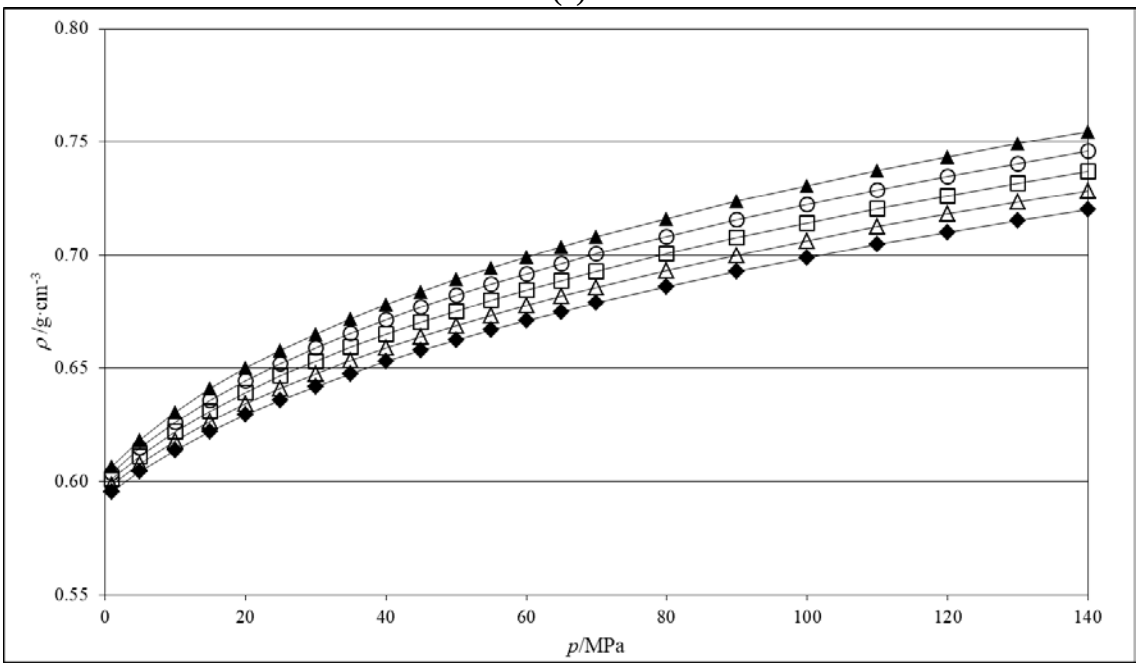
(a)


0.85
0.80
0.75
0.70
ρ /g·cm-3
293.15
313.15
333.15
353.15
373.15
393.15
T/K

(b)

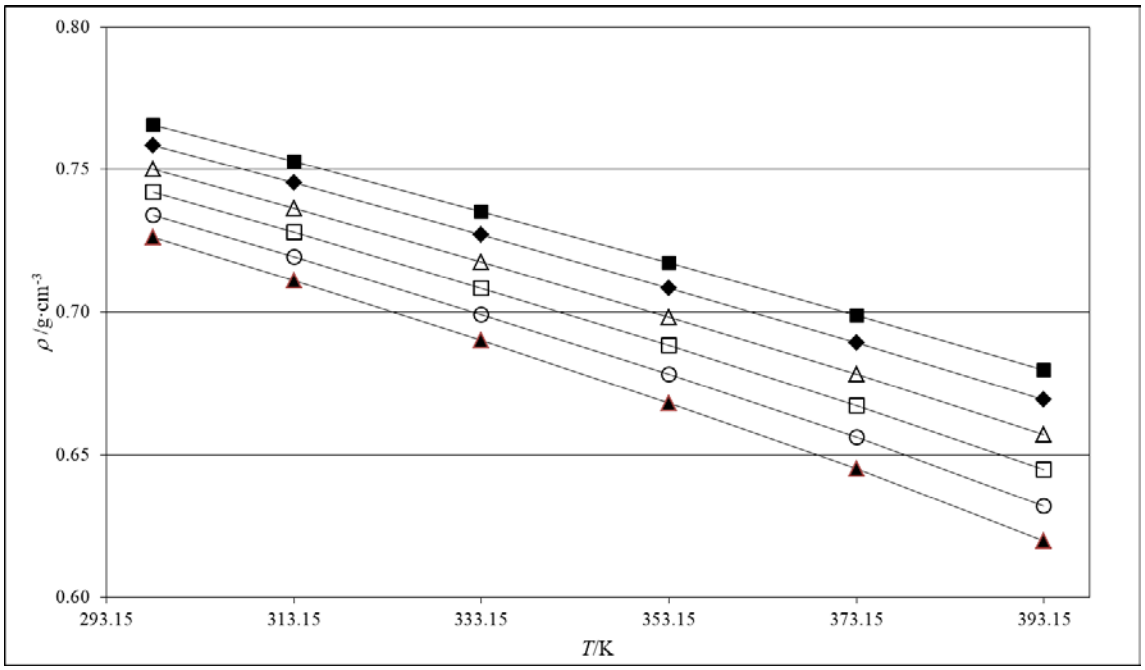


(c)

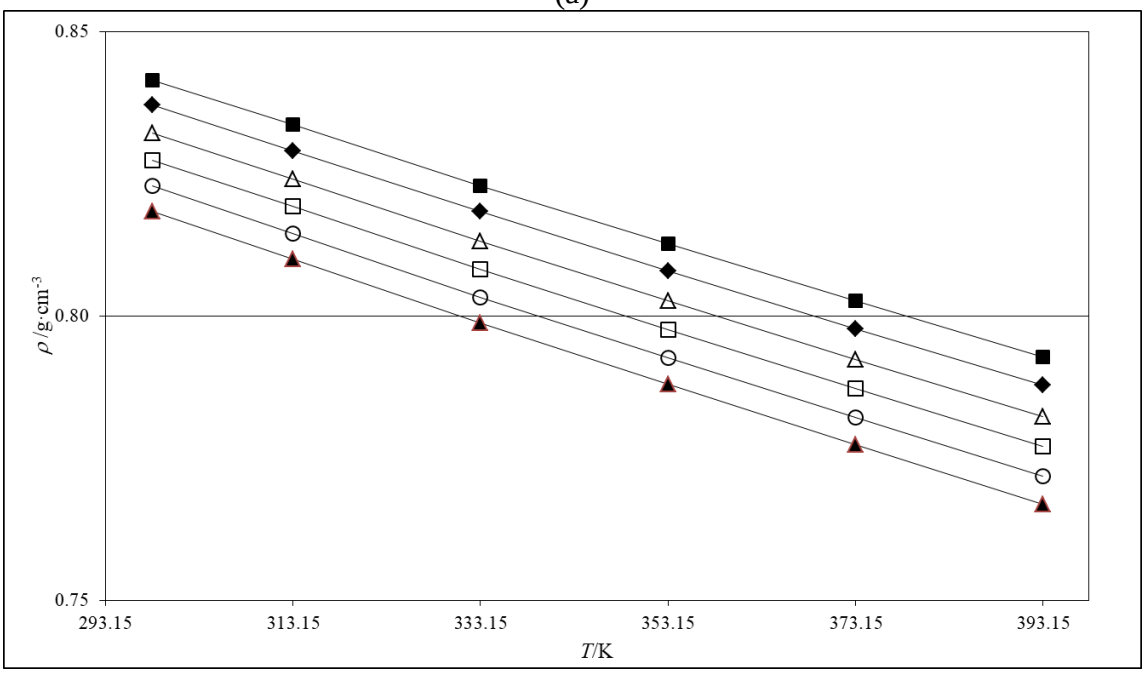


(d)

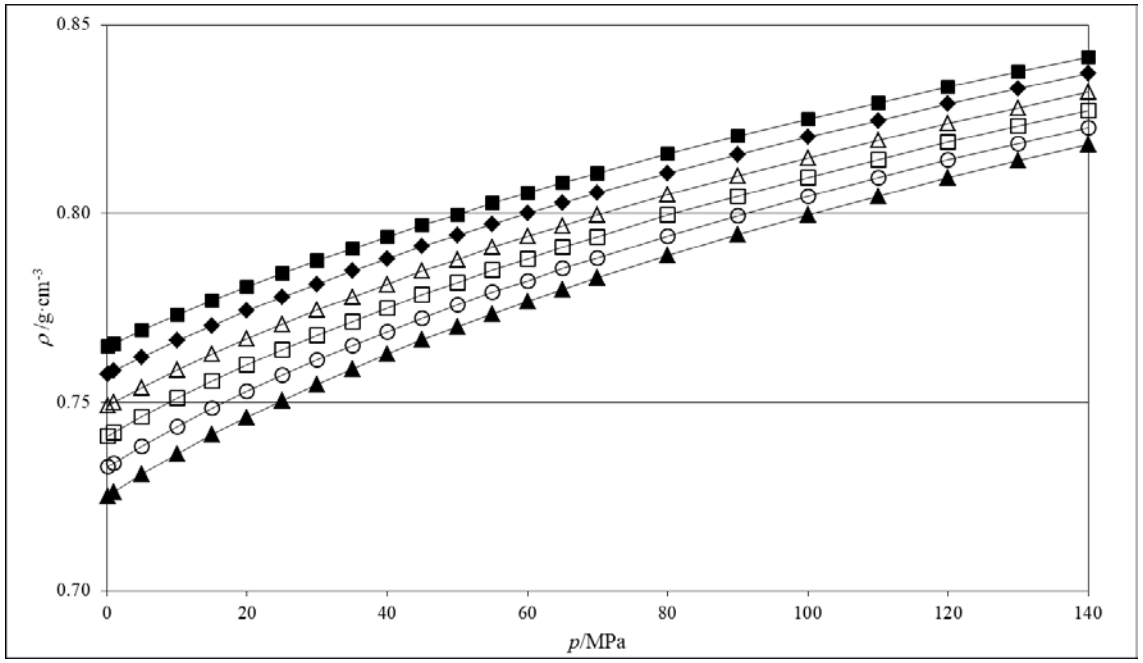
Fig. 1. Experimental values of densities, ρ, for different mole fractions of x n-heptane + (1-x) DIPE vs. (a) the temperature, T at 1 MPa, (b) the temperature, T at 140 MPa, (c) the pressure, p at 298.15 K and (d) the pressure, p at 393.15 K: ▲, x = 0.1505; ○, x = 0.3233; □, x = 0.4994; Δ, x = 0.6732; ♦, x = 0.8486; (-)Tait equation (1).


0.80
0.75
0.70
0.65
0.60
ρ /g·cm-3
293.15
313.15
333.15
353.15
373.15
393.15
T/K

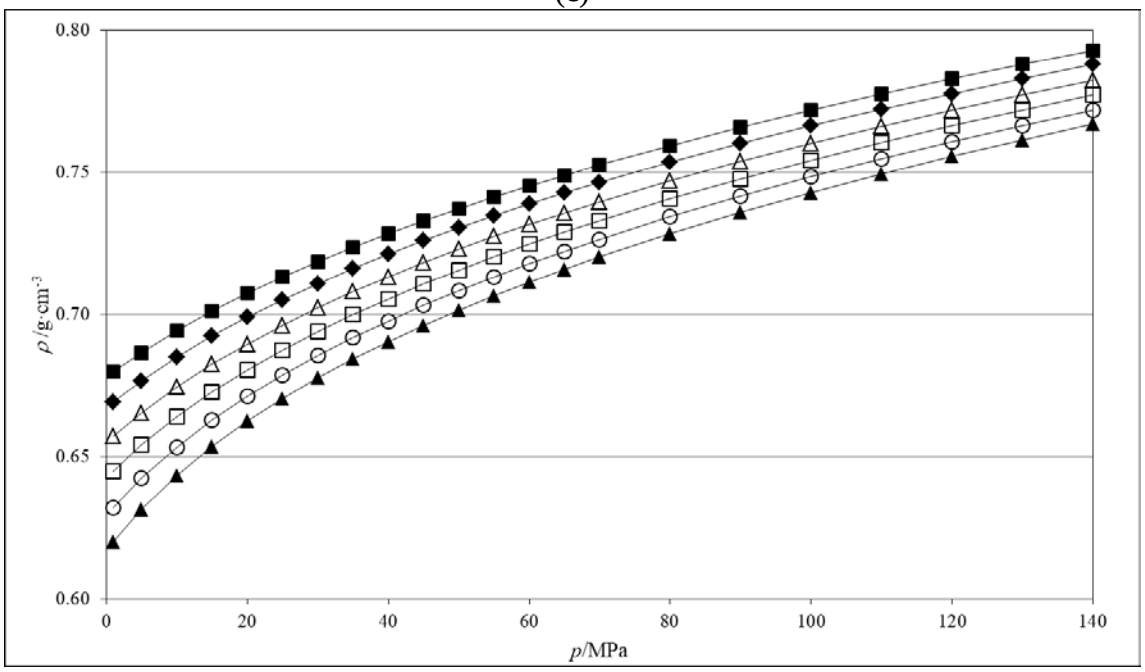
(a)


0.85
0.80
0.75
ρ /g·cm-3
293.15
313.15
333.15
353.15
373.15
393.15
T/K

(b)

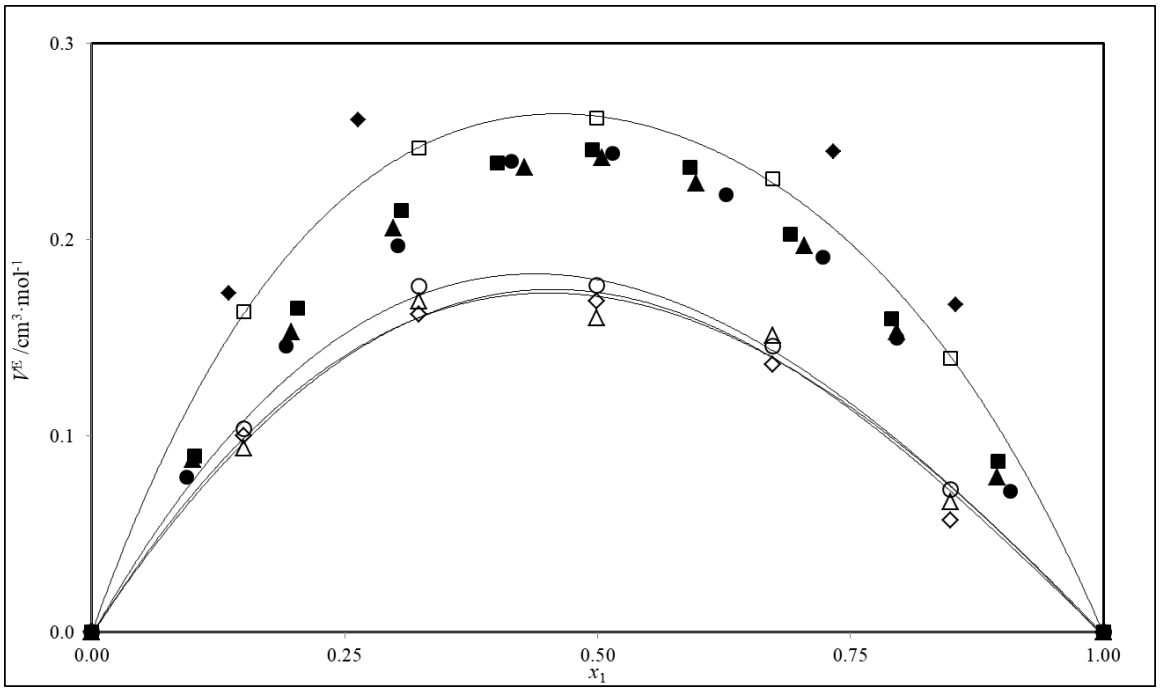


(c)

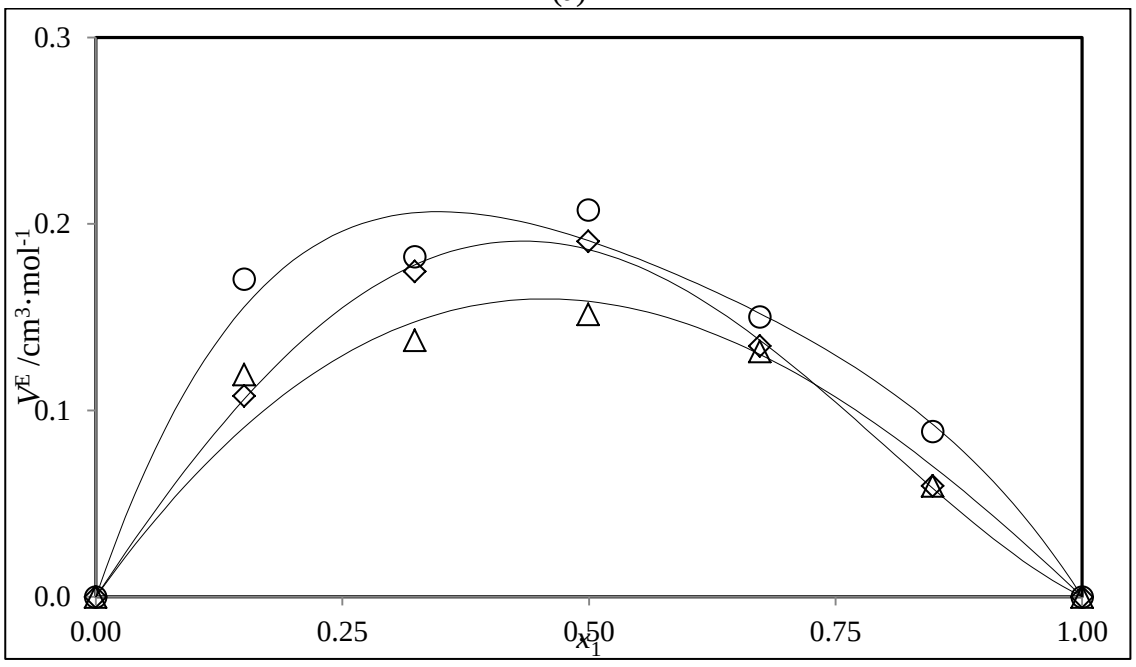


(d)

Fig. 2. Experimental values of densities, ρ, for different mole fractions of x methylcyclohexane + (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 393.15 K: ▲, x = 0.1507; ○, x = 0.3254; □, x = 0.5000; Δ, x = 0.6735; ♦, x = 0.8480; ■, x = 1.0000; (-)Tait equation (1).

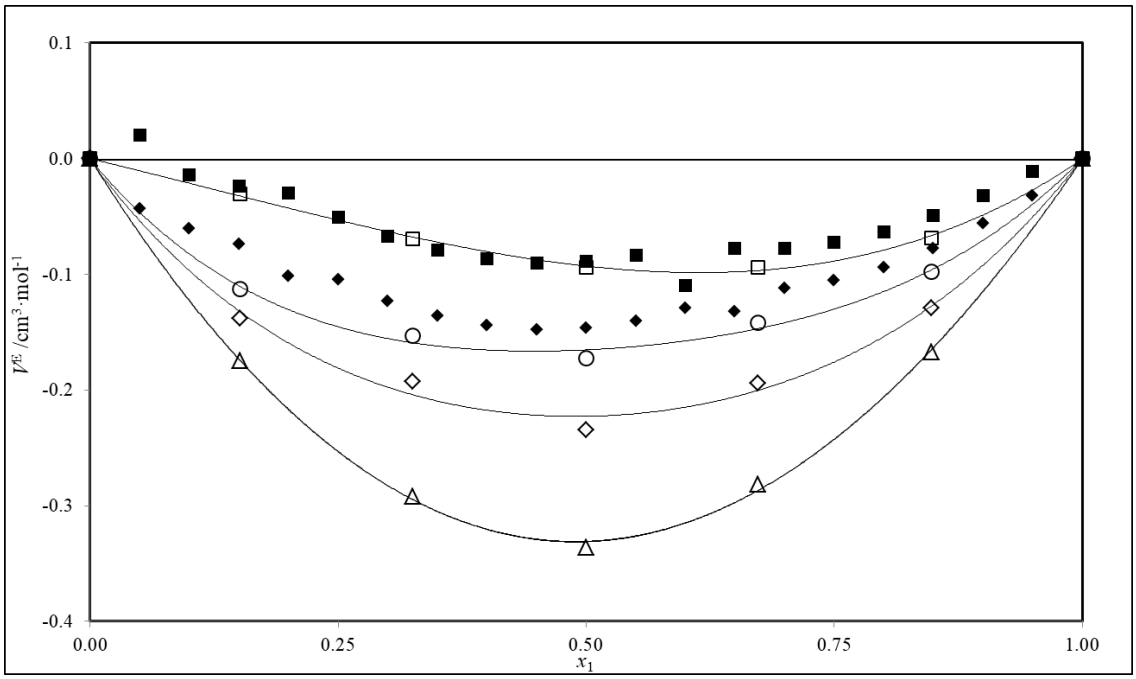


(a)

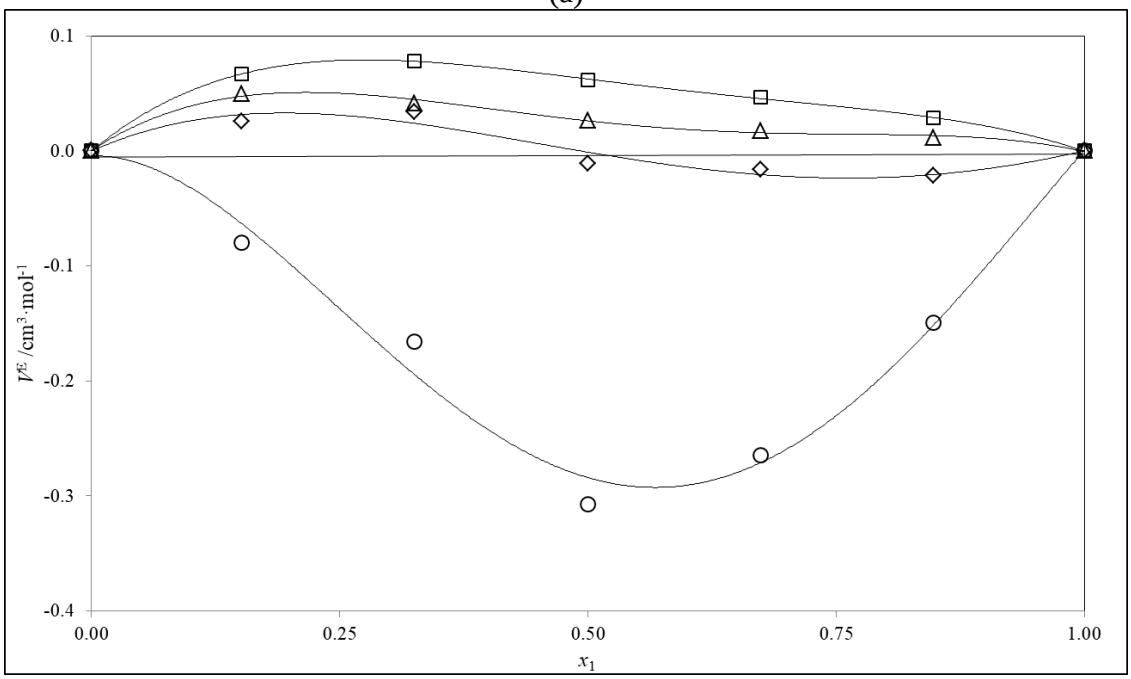


(b)

Fig 3. Experimental values of excess volumes, V^E, for the mixture *x* n-heptane + (*1*-*x*) DIPE as a function of the mole fraction. (a) at 0.1 MPa for different temperature *T*: □, 298.15K; ○, 313.15 K; ◇, 333.15 K; Δ, 353.15 K; ●, 298.15 K reference [7]; , ■, 298.15 K reference 8; ▲, 298.15 K reference [9]; ♦, 303.15 K reference 10. (b) at 393.15 K for different pressure *p*: ○, 10 MPa; ◇, 50 MPa; Δ, 100 MPa. (-) Redlich-Kister equation (5).



(a)



(b)

Fig 4. Experimental values of excess volumes, V^E, for the mixture *x* methylcyclohexane + (*1*-*x*) DIPE as a function of the mole fraction. (a) at 0.1 MPa for different temperature *T*: □, 298.15K; ○, 313.15 K; ◇, 333.15 K; Δ, 353.15 K; ■, 298.15 K reference [11]; ●, 308.15 K reference [11]. (b) at 393.15 K for different pressure *p*: ○, 10 MPa; ◇, 50 MPa; Δ, 100 MPa; □, 140 MPa. (-) Redlich-Kister equation (5).

TOC Graphic

