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VOLUMETRIC PROPERTIES OF 1-IODOPERFLUOROHEXANE+ *n*-OCTANE BINARY SYSTEM AT SEVERAL TEMPERATURES

Experimental data and EoS prediction

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New densities are reported over the whole composition range for 1-iodoperfluorohexane+*n*-octane system at temperatures from 288.15 to 308.15 K at atmospheric pressure. These data have been used to compute the excess molar volumes, V_m^E. Large positive V_m^E values have been obtained over the entire range of composition, which increases when the temperature rises. The experimental data were used to calculate the isobaric thermal expansivity, and the quantities $(\partial V_m^E/\partial T)_p$ and $(\partial H_m^E/\partial p)_T$. Furthermore, the results have been used to investigate the volumetric prediction ability of the equations of state Soave–Redlich–Kwong, Peng–Robinson, Patel–Teja and Soave–Redlich–Kwong with volume translation.

Keywords: *density correlation, equation of state, excess molar volume, FIC, 1-iodoperfluorohexane*

Introduction

Fluoroiodocarbons (FICs) are considered as effective replacements for the chlorofluoro-carbons (CFCs) for cleaning aerospace components, due to these solvents have been shown to be effective in removing a wide variety of soils [1]. FIC solvents possess the unusual combination of attractive physical properties, excellent cleaning ability, nonflammability, low toxicity, and extremely low environmental impact [2]. FICs with six or fewer carbon atoms are odorless, colorless gases or liquids that evaporate quickly and cleanly, are nonflammable, and appear to have generally low toxicity and negligible environmental impact. Because the carbon-to-iodine bonds are photolyzed rapidly in sunlight, FICs have atmospheric lifetimes of about two days and very low global warming potential, GWPs, of about 6 (relative to CO_2). The ozone-depletion potential, ODPs, of FICs are lower than 0.0025 [1, 2]. Furthermore, some FICs are also being considered as promising alternative refrigerant, especially as components in mixtures, to replace CFCs or HCFCs, due to their excellent physical properties, zero ODP, low GWP and good thermal stability [3].

On the other hand, the reliable knowledge of the thermophysical properties of refrigerants and lubricants and their mixtures, including the volumetric ones is essential to the equipment design of the refrigeration machines. These data can be needed for solving material and energy balances required for the design and optimizations of chemical processes. Furthermore, to develop FICs as solvents their volumetric properties and those of their mixtures with other solvents are needed. In this sense, volumetric values as a function of temperature are needed for the development of both correlation and prediction models. In this sense studies on the prediction ability of different methods such as cubic Equations of State (EoS) are necessary. Cubic equations of state are widely used for different calculations of thermodynamic properties needed in many chemical and engineering applications of pure and mixtures of non-polar and slightly polar substances. Such equations inherently provide good information but, at present, their usefulness to polar substances is limited [4]. In spite of their theoretical shortcomings, the frequent use of cubic EoS is partly due to the fact that these equations can be transformed into cubic polynomials on the molar volume [5]. This reducibility to a cubic polynomial has an evident mathematical convenience: the calculation of the density or the molar volume from the given pressure and temperature (which is one of the most frequently performed operations in phase equilibrium calculations) can be performed for these cubic equations by Cardano´s method [5], with neither iterations and nor predetermined initial values. Nevertheless there are two challenges to overcome in the application of cubic EoS. First, a set of critical parameters and the acentric factor of the pure compounds are often needed, but these experimental data are not always available. Secondly, no single equation has been able to establish unrivalled supremacy. For these reasons, it is interesting to analyze the capability of the different equations of state to predict the volumetric

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Table 1 Experimental and literature densities ρ, and isobaric thermal expansivity α_p, for the pure compounds at atmospheric pressure

Compound		ρ/g cm^{-3}		$10^4\ \alpha_p$/K^{-1}	
	T/K	this work	literature	this work	literature
1-iodoperfluorohexane	288.15	2.06677	–		
	298.15	2.03963	–	13.2	–
	308.15	2.01294	–		
octane	288.15	0.70655	0.70669 [14]		
	298.15	0.69856	0.69861 [14], 0.69850 [15]		11.6 [14, 20]
			0.69845 [12], 0.69853 [13]	11.3	
			0.69854 [16]		
	308.15	0.69054	0.69046 [14]		

behavior, for several compounds and their mixtures. In addition, it is interesting to know which methods to estimate critical properties and acentric factor give better performances.

In this paper, experimental densities and excess molar volumes of (1-iodoperfluorohexane+octane) at the temperatures (288.15, 298.15 and 308.15 K), as well as their correlations with the temperature and composition, are reported. A set of critical parameters and acentric factor is given for 1-iodoperfluorohexane. The prediction goodness of four EoS, Peng-Robinson, Soave–Redlich–Kwong, Patel–Teja and Soave–Redlich–Kwong with volume translation, was studied for the same binary system. The experimental data were used to calculate, by analytical differentiations, the isobaric thermal expansivity, and the quantities $(\partial V_m^E/\partial T)_p$ and $(\partial H_m^E/\partial P)_T$. A literature review shows that thermophysical properties of pure 1-iodoperfluorohexane or systems including this FIC have not been studied nowadays.

Experimental

Materials

1-iodoperfluorohexane, $CF_3(CF_2)_4CF_2I$, (Interchim, puriss. 97%), octane (Fluka, puriss. >99.5%), heptane (Fluka, puriss. >99.5%) and dichloromethane (Aldrich, puriss. 99.6%), were used without purification except drying with Union Carbide 0.4 nm molecular sieves for several days. These chemicals were partially degassed with a Branson 2210 ultrasonic bath, before use.

Measurements

The densities were determined by means of an Anton-Paar 60/602HP vibrating-tube digital densimeter. This type of mechanical oscillator, widely used in the literature [6–10], is one of the most versatile and accurate instruments for density measurements. The temperature inside the cell block was controlled to within $\pm 1\cdot 10^{-3}$ K using a thermostat (Polyscience) and was measured with a digital thermometer CKT100 calibrated with an uncertainty of ±0.01 K. The temperature scale employed was ITS-90. The experimental procedure is similar to that applied in previous works [11–15]. Before each series of measurements, the densimeter was calibrated with *n*-heptane and dichloromethane. Liquid mixtures were prepared by mass using a precision digital Sartorius 210-P balance with an accuracy of $\pm 10^{-5}$ g. The uncertainties associated with the mole fraction, density and excess volumes are estimated to be less than $5\cdot 10^{-5}$, $1\cdot 10^{-4}$ g cm^{-3} and 2.10^{-3} cm^3 mol^{-1}, respectively. All molar quantities are based on the IUPAC relative atomic mass table.

Experimental results

Densities

The experimental densities, ρ, obtained from the measurements of the pure compounds at all the investigated temperatures are summarized in Table 1 together with some literature values for octane [11, 13–16]. As it has been commented before, no experimental density is available for 1-iodoperfluorohexane. Our values for octane are in very good agreement with those from literature, as it can be seen in Table 1. The density measurements of the x 1-iodoperfluorohexane+ $(1–x)$ octane binary mixtures are presented in Table 2 at 288.15, 298.15 and 308.15 K and at atmospheric pressure, whereas Fig. 1 shows the density experimental data for the same system *vs.* the composition. As it can be seen, the density data range from 0.7902 g cm^{-3} for pure *n*-octane to a high value, 1.9678 g cm^{-3}, for pure 1-iodoperfluorohexane, having a regular behavior with the mole fraction. The density dependence with the temperature is standard, ρ increases when the temperature decreases.

Table 2 Experimental densities, ρ, and excess molar volumes, V_m^E, of *x* 1-iodoperfluorohexane + (1–*x*) octane at several temperatures and atmospheric pressure

T/K	*x*	ρ/g cm^{-3}	V_m^E/cm^3 mol^{-1}
288.15	0.05050	0.79385	0.591
	0.12332	0.91433	1.329
	0.14069	0.94226	1.474
	0.20293	1.04024	1.873
	0.21915	1.06516	1.962
	0.30753	1.19734	2.295
	0.42742	1.36691	2.499
	0.53635	1.51255	2.461
	0.64222	1.64740	2.241
	0.77770	1.81181	1.690
	0.91191	1.96775	0.773
298.15	0.05379	0.79019	0.657
	0.11501	0.89047	1.263
	0.21342	1.04368	1.996
	0.32178	1.20248	2.505
	0.44027	1.36619	2.722
	0.61959	1.59742	2.500
	0.70487	1.70149	2.181
	0.80584	1.82097	1.587
	0.91132	1.94098	0.845
308.15	0.10535	0.86439	1.247
	0.20215	1.01408	2.003
	0.30750	1.16710	2.597
	0.44377	1.35320	2.873
	0.53675	1.47362	2.797
	0.59238	1.54348	2.655
	0.64253	1.60496	2.494
	0.79602	1.78577	1.739
	0.91283	1.91747	0.842

The reported densities have been represented as function of composition, *x*, by the following equation:

$$\rho(x)=\sum_{0}^{3}a_{\mathrm{i}}x^{\mathrm{i}} \qquad (1)$$

where *x* is the mole fraction of 1-iodoperfluorohexane. This type of correlation has been successfully used previously in literature [17–19]. The a_i parameters, obtained by a linear least squares fitting procedure, and the standard deviations, *s*, for each temperature are given in Table 3.

In order to analyze the change in the isobaric thermal expansivity, α_p, with the composition, a correlation of the density values with the temperature and mole fraction, i.e. $\rho(x, T)$, is needed. We must notice that in the broad literature on density behavior of liquids the best descriptions of the density tempera-

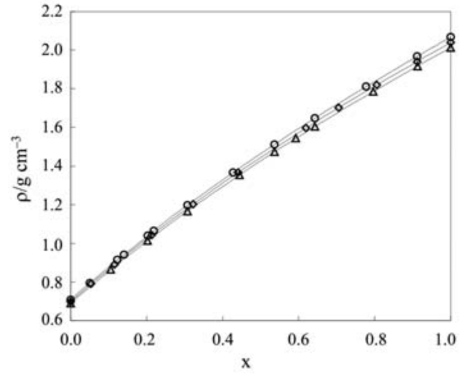

Fig. 1 Experimental densities for x 1-iodoperfluorohexane+ (1-x) octane system for several temperatures: (○) 288.15 K; ◇ – 298.15 K; △ – 308.15 K. Solid lines Eq. (2)

Table 3 Parameters a_i of Eq. (1), and b_{iA} and b_{iB} of Eq. (2), together with the standard deviation, s

T/K	a_i				s/g cm^{-3}
	a_0	a_1	a_2	a_3	
288.15	0.706898	1.74322	–0.52560	0.14246	0.0002
298.15	0.699077	1.71780	–0.52106	0.14411	0.0004
308.15	0.691015	1.69341	–0.51397	0.14284	0.0004
	i	b_{iA}	b_{iB}		
	0	0.93557	–0.0007934		
	1	2.46241	–0.0024976		0.0003
	2	–0.69984	0.0006064		
	3	0.14230	–		

ture dependence was obtained with temperature polynomial functions. Taking into account this fact a new correlation of the variation of the densities values with both the composition and the temperature has been studied in this work:

$$\rho(x, T)=\sum_{0}^{3} b_i(T)x^i \text{ with } b_i(T)=b_{iA}+b_{iB}T \qquad (2)$$

where x is the mole fraction of 1-iodoperfluorohexane and T is the absolute temperature. A simple multi-linear least squares fit has been performed to obtain the b_i parameters. Up to our knowledge this type of correlation has not been proposed in the literature. The values of the parameters b_{iA}, b_{iB} and the standard deviation, s, are shown in Table 3. As it can be seen the standard deviation, $3\cdot10^{-4}$ g cm^{-3}, is quite similar or even minor than those obtained using the Eq. (1), which are less or equal than $4\cdot10^{-4}$ (see Table 3). Hence, satisfactory results are obtained using Eq. (2). We must note that the proposed $b_i(T)$ polynomial function could be modified if a broader temperature range is studied.

Subsequently, according its definition, the isobaric thermal expansivities $\alpha_p=-(1/\rho)(\partial\rho/\partial T)_p$ were determined for the investigated system at 298.15 K using the b_i parameters from Table 3. The α_p values for the pure compounds at 298.15 K are presented in Table 1. As it can be seen, our data for octane agrees with the literature value at 298.15 K [14, 20] (relative deviation of 2%). In Fig. 2, the isobaric thermal expansivity has been plotted *vs.* the composition of the 1-iodoperfluorohexane at 298.15 K. In this figure it can be seen that α_p increases (from $11.3\cdot10^{-4}$ to $13.2\cdot10^{-4}$ K^{-1}) when the composition of the FIC raises.

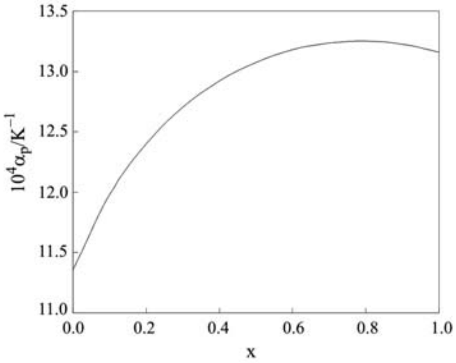

Fig. 2 Isobaric thermal expansivity, α_p, as a function of the mole fraction for x 1-iodoperfluorohexane+(1–x) octane at 298.15 K

Excess molar volumes

From the measured densities, the excess molar volumes V_m^E of the system have been determined at the referred temperatures according to:

$$V_m^E=xM_1\{(1/\rho)-(1/\rho_i)\}+(1-x)M_2\{(1/\rho)-(1/\rho_2)\} \quad (3)$$

where M_i and ρ_i denote, respectively, the molar mass and the density of the pure liquids and x and ρ the mole fraction and the density of the mixture. The obtained excess molar volumes are also listed in Table 2. A Redlich–Kister type relationship [21] was adjusted to the experimental values for each temperature, in a similar way as other authors [7–10, 22, 23]

$$V_m^E=x(1-x)\sum_i A_i(2x-1)^{i-1} \qquad (4)$$

where x is the mole fraction of 1-iodoperfluorohexane. The parameters A_i (obtained by a linear least squares fitting procedure) and the standard deviations, s, are summarized in Table 4. The experimental V_m^E data, at each studied temperature, are plotted in Fig. 3 *vs*. the composition, together with the curves fitted using the A_i parameters. As it can be seen, the excess molar volumes are large positive, over the whole range of composition, reaching values of up to 2.873 cm^3 mol^{-1}, so the mixture is less compact than the pure components. According to the simple interpretative scheme of Patterson [24], the largely positive V_m^E values can be qualitatively explained with a

Table 4 Values of A_i and A_{ij} parameters of Eqs (4) and (5), respectively, together with the standard deviation, *s*

T/K	A_i			s/cm^{-3} mol^{-1}
	A_0	A_1	A_2	
288.15	9.992795	–1.54426	1.83374	0.016
298.15	10.877331	–1.39714	0.75918	0.012
308.15	11.353687	–1.66881	0.74842	0.019

i	A_{ij}			s/cm^{-3} mol^{-1}
	A_{i1}	A_{i2}	A_{i3}	
1	7.89718335	0.17041853	–0.00204764	0.015
2	–2.55748316	0.09909058	–0.00210595	
3	5.44673993	–0.32090949	0.00533394	

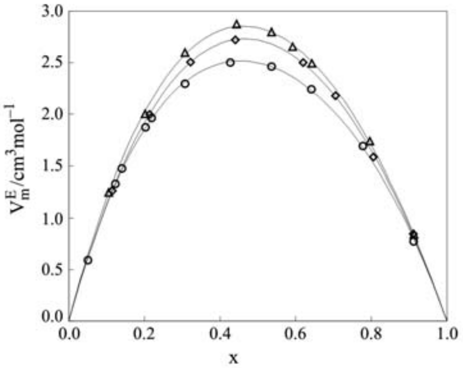

Fig. 3 Excess molar volume of *x* 1-iodoperfluorohexane+ (1–*x*) octane for several temperatures: ○ – 288.15 K; ◇ – 298.15 K; △ – 308.15 K. Solid lines Eq. (4)

net destruction, in the mixing process, of the structural order present in the pure liquids (hydrogen bonding, dipolar interaction, and orientational order). Thus, the high positive V_m^E values of the 1-iodoperfluorohexane+octane system is mainly due to major contribution of the effect due to the breaking of dipolar interactions in the pure fluoroiodocarbon, although the destruction of the orientational order of octane also gives positive contribution. It is likely that the unlike molecular interactions between the fluoroiodocarbon and the alkane are weak as those corresponding to the molecules of perfluorohydrocarbons and hydrocarbons [25–29]. Nevertheless, no LLE was found at ambient temperature for 1-iodoperfluorohexane+octane, contrary to the partial immiscibilities found for perfluorohexane+octane [28]. This could be an evidence that unlike molecular interactions between 1-iodoperfluorohexane and octane are not so weaker as those found in perfluorohexane+octane. In fact, this last system presents higher V_m^E values than those of 1-iodoperfluorohexane+*n*-octane. Hence, the packing loss during mixing diminishes when a iodine atom is introduced instead a fluor. This could be due to the iodine atom provokes an increase in the interactions energies of the unlike molecules.

We must note that the basic hypothesis that order destruction/formation produces positive/negative excess properties (enthalpy, entropy, Gibbs energy, and volumes) is evidently an oversimplification, due to the order is a no well-defined property. In spite of this, the Patterson scheme appears a useful tool for a qualitative interpretation of the sign of the excess quantities for most mixtures. In addition, we must add that in the case of V_m^E, different packing or steric effects could prevail over structural order changes, producing negative contribution to V_m^E values. On the other hand, the $V_m^E(x)$ curves for these mixtures are quite symmetric with the composition, with the maximum located near to x= 0.45, and the V_m^E values increase when the temperature rises at fixed composition. This behavior is similar to that of the perfluorohexane+*n*-octane system, that presents high and positive excess volumes and excess Gibbs energies [28, 29].

In order to obtain a general correlation, the excess molar volumes were also fitted to the following polynomial

$$V_m^E = x(1-x)\sum_{i=1}^{3}\sum_{j=1}^{3} A_{ij}(2x-1)^{i-1}(T-T_0)^{j-1} \qquad (5)$$

where T_0=273.15 K and T is the absolute temperature. The coefficients A_{ij} and the standard deviation *s* are given in Table 4. A simple multi-linear least squares optimization process has been used to obtain these parameters. This type of correlations has been broadly used in the literature in order to fit excess thermodynamic properties, $X_m^E(x, T)$, at constant pressure [12, 30–33]. As it can be seen in Table 4, the standard deviation (0.015 cm^3 mol^{-1}) is quite similar, even minor, that those obtained when Eq. (4) is used.

By analytical derivation of Eq. (5) the values of $(\partial V_m^E/\partial T)_p$ at 298.15 K were obtained. Figure 4a

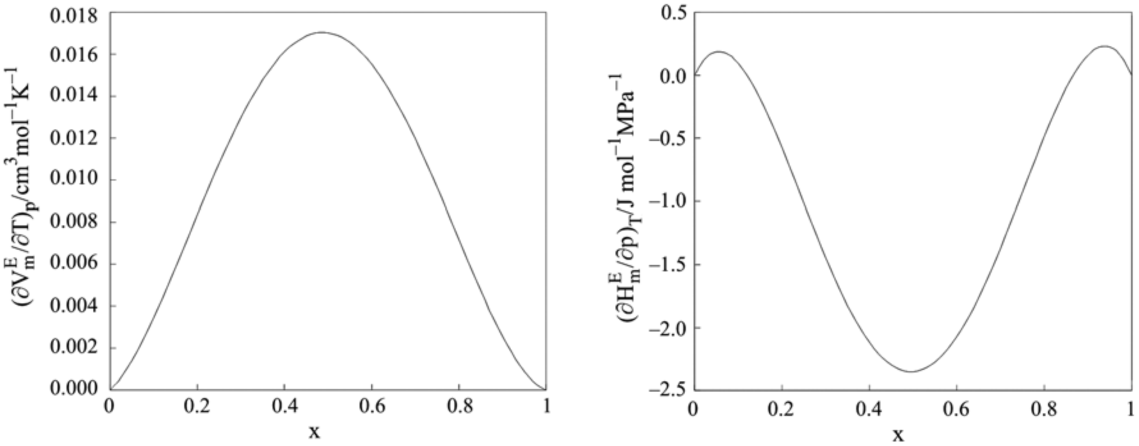

Fig. 4 $(\partial V_m^E/\partial T)_p$ and $(\partial H_m^E/\partial p)_T$ *vs*. the mole fraction for *x* 1-iodoperfluorohexane + (1–*x*) octane at 298.15 K

shows the $(\partial V_m^E/\partial T)_p$ behavior with the composition. The $(\partial V_m^E/\partial T)_p$ values are positive and the curve presents also a maximum near of x=0.45. The pressure dependence of the excess enthalpies determined from the excess volumes, by using the relation $(\partial H_m^E/\partial p)_T = V_m^E - T(\partial V_m^E/\partial T)_p$, has been determined at 298.15 K and it is showed in Fig. 4b. From this figure, we can conclude that the excess enthalpies change significantly, although no severely, with the pressure at this temperature. The symmetric curve $(\partial H_m^E/\partial p)_T$ *vs*. *x* presents a significant minimum of –2.4 J mol^{-1} MPa^{-1}. Due to both V_m^E and $T(\partial V_m^E/\partial T)_p$ are positive, the negative values of $(\partial H_m^E/\partial p)_T$, in almost all the concentration range, indicate that $T(\partial V_m^E/\partial T)_p > V_m^E$. Bhattacharyya and Patterson [34] and Costas *et al*. [35] have suggested that the properties $(\partial V_m^E/\partial T)_p$ and $(\partial H_m^E/\partial p)_T$ can be employed as indicators of changes of order in the solution. A destruction of orientational order during mixing process implies a negative contribution to $(\partial V_m^E/\partial T)_p$ and a positive contribution to V_m^E, H_m^E and $(\partial H_m^E/\partial p)_T$. It is interesting to note that in the present case V_m^E and $(\partial V_m^E/\partial T)_p$ are positive whereas $(\partial H_m^E/\partial p)_T$ is strongly negative (around the equimolar composition), so that effect does not seem to be very important in the studied system.

Theoretical results

Cubic EoS are extremely useful in the modelling of a large amount of actual applications and no single equation has been able to establish unrivalled supremacy [36, 37]. In previous papers [38–42] it was found that the most popular models for the phase equilibria, Soave–Redlich–Kwong [43] (SRK) and Peng–Robinson [44] (PR), give reasonable predictions for the volumetric behavior. Other equations that correlate the phase equilibria with accuracy similar to SRK or PR EoS, and improve the predictions of volumetric properties are Soave–Redlich–Kwong with volume translation [45] (SRK–VT) and Patel–Teja [46] (PT). The SRK–VT EoS is a modification to SRK EoS which does not affect the calculations of vapor pressures, and the PT EoS is an extension of the Soave [43], Peng–Robinson [44] and Schmidt and Wenzel [47] equations. These EoS (PR, SRK, SRK–VT and PT) can be applied if the critical parameters (critical temperature, T_c, and critical pressure, p_c) and the acentric factor (ω) of the pure components are available. The PT EoS requires in addition to T_c and p_c, two new parameters to characterize each particular fluid. Patel and Teja [46] have generalized their original equation correlating these new parameters as a function of the acentric factor.

The critical parameters and acentric factor of octane were taken from literature [48] whereas, unfortunately, these data are not available in the literature for 1-iodoperfluorohexane. For this reason they were estimated in this work. The critical pressure (p_c=15.63 bar) and the critical temperature (T_c=518.62 K) were calculated by means of the group contribution method of Lydersen [49], using for the estimation of T_c the boiling point, T_b=390.25 K [50]. The same contribution method was used in the literature [42, 51–54] for the estimation of the critical properties of polyol ethers, fluorinated ethers, fluorinated ketones, and amines with satisfactory results. The acentric factor for 1-iodoperfluorohexane (ω=0.5686), was determined by the Lee–Kesler method [55] taking into account the cited critical temperature and pressure and the boiling point due to no experimental vapor pressure values exist in the literature. The Lee–Kesler method has been selected because reproduces better the acentric factor value of the perfluorohexane, C_6F_{14}.

In order to assess and compare the performances of the different EoS, the absolute average percentual deviation, (AAD), the maximum percentual deviation, (MD), and the average percentual deviation, Bias, have

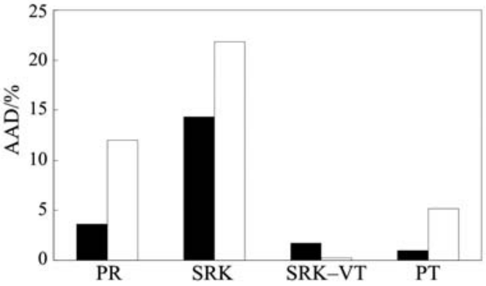

Fig. 5 AAD (%) between the experimental density data for the pure compounds and those predicted using several EoS: octane (black), 1-iodoperfluorohexane (white)

been used according to their definitions, given in a previous paper [39]. Figure 5 shows the AADs between the experimental densities reported in this work for the pure compounds and those predicted from the analyzed EoS. As it can be seen, the lowest AADs are obtained by using PT equation of state for octane (1%) and by using SRK–VT for 1-iodoperfluorohexane (0.3%). It must be emphasized the fine results were obtained by means of the SRK–VT EoS for 1-iodoperfluorohexane, in spite of its critical parameters have been estimated. The worse predictions for the densities of the pure compounds are obtained with SRK EoS (14% for octane and 22% for 1-iodoperfluorohexane).

The AAD, MD and Bias, obtained from PR, SRK, SRK–VT and PT density predictions for the 1-iodoperfluorohexane+octane system, over the studied temperature range, are listed in Table 5. This table shows that when the volume translation is considered for SRK EoS, the mixture density predictions are remarkably improved, as it happened for the pure components. Again, the best results are obtained with SRK–VT and PT equations of state (around 2%). From the Bias values [39], it can be concluded that the PT EoS underpredicts the density data, whereas the SRK with volume translation overpredicts the density values of the mixture. The predicted densities by the other analyzed EoS are always smaller than the experimental data and with maximum deviations (MD) higher than 10%. On the other hand, the trend with the temperature of the density is well predicted by all EoS.

The excess molar volume predictions have also been studied. All the analyzed equations of state reproduce the positive sign of this excess thermodynamic property. Nevertheless, whereas the maximum experimental values are between 2.5 and 2.9 $\mathrm{cm^3\ mol^{-1}}$, the corresponding V_m^E values predicted by the different EoS are in the (0.10–0.15 $\mathrm{cm^3\ mol^{-1}}$) interval. In addition, the trend with the temperature of the excess molar volumes for the 1-iodoperfluorohexane+octane system is represented correctly by the Patel–Teja EoS, but this is not the case of the other analyzed equations. For a satisfactory prediction of the magnitude of the excess molar volume, it is necessary to consider a binary interaction parameter. This parameter can be determined by fitting phase equilibrium values. Thus, in a previous paper [39], we have found that the predicted excess molar volumes by different EoS were also clearly lower than the experimental ones, for alkyl carbonate+alkane systems, which also presents positive V_m^E, when no binary interaction parameter was considered. For these systems, when interaction parameters determined from VLE data was used the EoS predictions have improved considerably [39]. Unfortunately VLE data are not available for 1-iodoperfluorohexane+*n*-octane

Conclusions

Experimental densities at atmospheric pressure are reported for the system 1-iodoperfluorohexane+*n*-octane over the temperature range between 288.15 and 308.15 K. From a new correlation $\rho(T,x)$ proposed in this work, with satisfactory results, the isobaric thermal expansivities were computed. We have found that the excess molar volumes are large positive (up to 2.9 $\mathrm{cm^3\ mol^{-1}}$) and increase when the temperature rises at fixed composition. The positive and high V_m^E values are mainly due to the breaking of dipolar interactions of the pure FIC, in the mixing process. Moreover, the V_m^E (x) curves are symmetric with the composition. In order to check the prediction ability of different equations of state the critical parameters and acentric factor of 1-iodoperfluorohexane were estimated in this work. The best density predictions for the pure compounds are obtained by using PT equation of state for octane (1%) and by using SRK–VT for 1-iodoperfluorohexane (0.3%). If volume translation is considered for SRK EoS, the density predic-

Table 5 AAD (%), MD (%) and Bias (%) between experimental density data for the *x* 1-iodoperfluorohexane+(1–*x*) octane mixture and those predicted using several EoS. N_p is the number of experimental points

	PR	SRK	SRK–VT	PT
AAD	7.1	17.4	1.7	2.2
MD	11.5	21.3	2.3	4.9
Bias	7.1	17.4	–1.7	2.2
N_p		29		

tions for pure compounds and mixtures are remarkably improved. The AADs between experimental density data for mixtures and those from SRK–VT and PT equation of state are around 2%, obtaining higher values if other equations of state are used. On the other hand, Patel–Teja EoS represents correctly the trends with the temperature of the excess molar volumes. But, it would be necessary experimental VLE data to determine a binary interaction parameter to improve estimation of the V_m^E magnitude.

Acknowledgements

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