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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 ≤ 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.

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 multi-component 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 140 MPa. 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.

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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 (298.15–393.28) 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:

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

where

$$\rho_0(T) \quad = A_0 + A_1 T + A_2 T^2 + A_3 T^3 \tag{2}$$

$$B(T) = B_0 + B_1 T + B_2 T^2 \tag{3}$$

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 behaviour 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,

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

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

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.