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**Densities and Excess Molar Volumes of the Ternary System (1,4-Dioxane + 2-Propanol + 1,1,2,2-Tetrachloroethane) at  $T = 288.15\text{--}318.15$  K and at Atmospheric Pressure: Experimental Measurements and Prigogine–Flory–Patterson Modeling**

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**Densities and Excess Molar Volumes of the ternary system (1,4-Dioxane + 2-Propanol + 1,1,2,2-Tetrachloroethane) at  $T = [288.15 \text{ to } 318.15]$  K and at atmospheric pressure. Experimental Measurements and Prigogine-Flory-Patterson Modelling.**

Houda Benabida<sup>1</sup>; Christophe Coquelet<sup>2</sup>, Farid Brahim Belaribi<sup>1,\*</sup>

<sup>1</sup>*Thermodynamic and Molecular Modelisation Laboratory, Faculty of Chemistry, University of Sciences and Technology Houari Boumediene (USTHB) B.P. 32 El-Alia, Bab-Ezzouar, Algiers, Algeria.*

<sup>2</sup>*MINES ParisTech, PSL University, CTP - Centre of Thermodynamic of Processes, 35 rue Saint Honoré 77305 Fontainebleau, France.*

\*Corresponding author: e-mail: (bbelaribi@usthb.dz; faridbrahimbelaribi@yahoo.com), Tel/fax: +(213)21248008

Houda Benabida : e-mail : benabidahouda16@gmail.com

Christophe Coquelet : e-mail : christophe.coquelet@mines-paristech.fr

**Abstract**\_\_\_\_\_ Excess molar volumes for 1,4-dioxane + 2-propanol + 1,1,2,2-tetrachloroethane ternary mixture and for the constituent binaries, were determined from density measurements, over the entire composition range, at four temperatures comprising between [288.15 and 318.15] K and at atmospheric pressure. The ether containing binary mixtures present positive excess molar volume,  $V^E$ , with the alkanol, and negative  $V^E$  values, with the chloroalkane, over the whole composition and working temperature ranges. As the temperature increases, the  $V^E$  magnitude increases, for 1,4-dioxane + 2-propanol, whereas it decreases for 1,4-dioxane + 1,1,2,2-tetrachloroethane. For 2-propanol + 1,1,2,2-tetrachloroethane mixture, sigmoidal- $V^E$  curves are observed and the  $V^E$  increases as the temperature increases. Sigmoidal- $V_{123}^E$  curves are observed, also, for 1,4-dioxane + 2-propanol + 1,1,2,2-tetrachloroethane ternary mixture. The equations of Redlich-Kister and of Cibulka, were used to fit the experimental excess molar volume data, for the investigated binary and ternary mixtures, respectively. In order to provide more informations on solute-solvent interactions, for the studied binary mixtures, the partial molar volumes and excess partial molar volumes, are calculated over the entire composition range and at infinite dilution, at (288.15 K and 318.15) K. The Prigogine-Flory-Patterson theory (PFP model) was applied to the 1,1,2,2-tetrachloroethane containing binary mixtures.

*Keywords: Density, Excess volume, 1,4-Dioxane, 1,1,2,2-Tetrachloroethane, 2-Propanol, PFP model.*

## 1. Introduction

Study of the thermodynamic behaviour of a liquid mixture, requires not only a theoretical model, but also numerous and reliable experimental data on thermodynamic excess properties of this mixture. Literature survey shows that excess volume and Prigogine-Flory-Patterson theory, the so-called PFP model,<sup>1-5</sup> are useful tools for investigating liquid mixtures.

Continuing our investigation on volumetric properties of liquid mixtures,<sup>6,7</sup> we are presently focused on 1,4-dioxane + 2-propanol + 1,1,2,2-tetrachloroethane ternary system with the aim to provide new experimental data on volumetric properties for these mixtures and to test the PFP model.<sup>1-5</sup> A survey of the open literature shows that, for 1,4-dioxane + 2-propanol mixture, there is few  $V^E$  data at temperatures inside [288.15 to 318.15] K<sup>7-11</sup> whereas, for 1,4-dioxane + 1,1,2,2-tetrachloroethane mixture, there is only two reports, once at 303.15 K<sup>12</sup> and the other, at 293.15 K.<sup>13</sup> For 2-propanol + 1,1,2,2-tetrachloroethane binary

mixture, and 1,4-dioxane + 2-propanol + 1,1,2,2-tetrachloroethane ternary one, there is no  $V^E$  data report.

## 2. Experimental

### 2.1. Materials

CAS registry number, supplier and purity of 1,4-dioxane, 1,1,2,2-tetrachloroethane and 2-propanol are reported in Table 1. The chemicals were used without further purification. Density measurements for the pure liquids were carried out at the temperature range  $T = [283.15 \text{ to } 318.15] \text{ K}$  and at atmospheric pressure, and well compared with open literature data<sup>14-27</sup> in Table 1. The observed deviations between our experimental density values and the literature data are small and would probably be due to the difference in the origin and purity of the compounds and also to other conditions such as humidity and pressure

### 2.2. Apparatus and procedure

As in our previous work<sup>7</sup>, densities of binary and ternary mixtures and pure liquids, were measured using an Anton Paar vibrating U-tube densimeter (Model DMA-5000), where the temperature was automatically regulated to  $\pm 0.01 \text{ K}$ . All the mixtures were carried out by mass using a Metler balance. The ternary mixtures were prepared by adding the third component (1,1,2,2-tetrachloroethane) to fixed mole ratio of 1,4-dioxane (1) + 2-propanol (2) binary mixture. The mole fraction ratio,  $x_1/x_2$ , has the values; 3, 1 and 1/3. Uncertainties of masse, and density measurements were estimated to be  $\pm 1.10^{-3} \text{ g}$ , and  $\pm 10^{-5} \text{ g cm}^{-3}$ , respectively. For the molar fractions and the excess molar volumes, the calculated uncertainties are of the order  $\pm 10^{-3}$  and  $\pm 4 \cdot 10^{-3} \text{ cm}^3 \text{ mol}^{-1}$ , respectively.

## 3. Results and discussion

### 3.1. Binary mixtures

The experimental values of density for pure components and for binary mixtures were used to calculate the excess molar volumes, using the following equation:

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

Where,  $x_i$ ,  $M_i$  and  $\rho_i$  are the mole fraction, the molecular weight and the density of the component  $i$ . respectively.  $\rho$  is the mixture density.  $n$  stands for the number of components.

The experimental values of density,  $\rho$ , and of excess molar volumes,  $V^E$ , for 1,1,2,2-tetrachloroethane containing binary mixtures, at all studied temperatures, over the whole mole fraction range, are reported in Table 2. Those for 1,4-dioxane + 2-propanol mixture were reported in our previous work.<sup>7</sup>

The experimental  $V^E$  values are fitted to the Redlich-Kister equation:<sup>28</sup>

$$V^E = x_1 x_2 \sum_{i=0}^{i=n} A_i (x_1 - x_2)^i \quad (2)$$

The parameters  $A_i$  in eq 2 are reported in Table 3 along with standard deviations,  $\sigma$ , calculated by using eq 3:

$$\sigma = \left[ \frac{\sum_{i=1}^{i=N} (V_{(\text{expt.},i)}^E - V_{(\text{calc.},i)}^E)^2}{N - p} \right]^{1/2} \quad (3)$$

Where  $N$  is the number of experiments and  $p$  the number of adjusted parameters  $A_i$

Other volumetric properties such as partial molar volumes and excess partial molar volumes of the components, for all the investigated binary mixtures, were calculated over the entire composition range and at infinite dilution, at  $T = (288.15 \text{ and } 318.15) \text{ K}$ .

The partial molar volume,  $V_i$ , of a component  $i$ , is given by the following equation:

$$V_i = V_i^0 + V_i^E + (1 - x_i) (\partial V^E / \partial x_i)_{P,T} \quad (4)$$

Where  $V_i^0$  is the molar volume of pure component  $i$

The derivative  $(\partial V^E / \partial x_i)$  was obtained by differentiation of eq 2, which leads to the following equations for the partial molar volumes of the components 1 and 2, respectively:

$$V_1 = V_1^0 + (1 - x_1)^2 \left[ \sum_{k=0}^{k=n} A_k (2x_1 - 1)^{k-1} [2(k+1)x_1 - 1] \right] \quad (5)$$

$$V_2 = V_2^0 + x_1^2 \left[ \sum_{k=0}^{k=n} A_k (2x_1 - 1)^{i-1} [2(i+1)x_1 - (2k+1)] \right] \quad (6)$$

The excess partial molar volumes,  $V_1^E = V_1 - V_1^0$  and  $V_2^E = V_2 - V_2^0$  are also calculated.

Setting  $(x_1 = 0)$  in eq (5) and  $(x_2 = 0)$  in eq (6), leads to eqs (7) and (8), for the partial molar volumes at infinite dilution,  $V_1^\infty$  and  $V_2^\infty$  of the component (1) and (2) respectively:

$$V_1^\infty = V_1^0 + \sum_{k=0}^{k=n} A_k (-1)^k \quad (7)$$

$$V_2^\infty = V_2^0 + \sum_{k=0}^{k=n} A_k \quad (8)$$

Rearrangement of eqs 7 and 8 leads to eqs 9 and 10, for the excess partial molar volumes of components at infinite dilution,

$$V_1^{E,\infty} = \sum_{k=0}^{k=n} A_k (-1)^k \quad (9)$$

$$V_2^{E,\infty} = \sum_{k=0}^{k=n} A_k \quad (10)$$

For all the binary mixtures, the  $V_i$ ,  $V_i^\infty$ ,  $V_i^E$  and  $V_1^{E,\infty}$  calculated values, for each component i, at  $T = (288.15 \text{ and } 318.15) \text{ K}$ , are reported in Tables 4 and 5.

### 3.2 Ternary mixture

For the ternary mixture 1,4-dioxane (1) + 2-propanol (2) + 1,1,2,2-tetrachloroethane (3), the excess molar volumes,  $V_{123}^E$ , were determined also from density measurements, at  $T = (288.15; 298.15; 308.15 \text{ and } 318.15) \text{ K}$  and at atmospheric pressure. The experimental density and excess molar volume values are reported together in Table 6.

The experimental  $V_{123}^E$  values were correlated with the Cibulka equation:<sup>29</sup>

$$V_{123}^E/\text{cm}^3 \text{ mol}^{-1} = V_{\text{bin}}^E/\text{cm}^3 \text{ mol}^{-1} + x_1 x_2 (1 - x_1 - x_2) (B_0 + B_1 x_1 + B_2 x_2) \quad (11)$$

Where the binary contribution to excess molar volume,  $V_{\text{bin}}^E/\text{cm}^3 \text{ mol}^{-1}$ , is given by:

$$V_{\text{bin}}^E = V_{12}^E + V_{13}^E + V_{23}^E \quad (12)$$

Where  $V_{jk}^E$  is given by eq 2. The  $B_i$  adjusted values along with the standard deviations are reported in Table 7.

Our experimental binary  $V^E$  results, for 1,1,2,2-tetrachloroethane containing binary mixtures, were also illustrated graphically. The  $V^E$  values, for 1,4-dioxane + 1,1,2,2-tetrachloroethane are reported in Fig. 1 together with the literature  $V^E$  data<sup>12,13</sup> for comparison. Fig. 1 shows that this mixture presents negative  $V^E$  values, over the mole fraction range and at all working temperatures. It can be seen also, that the  $V^E$ -curves are asymmetrical, slightly skewed toward the chloroalkane high mole fraction, and the  $V^E$  magnitude decreases as the temperature rises. Fig. 1, shows a good agreement between our  $V^E$  values and those reported in literature at 293.15 and 303.15 K.<sup>12,13</sup> The  $V^E$  values, for 2-propanol + 1,1,2,2-tetrachloroethane mixture, are reported in Fig. 2. This mixture presents sigmoidal- $V^E$  curves. As the temperature increases, the positive  $V^E$  values increase whereas negative  $V^E$  values decrease. As far as we know, there is no  $V^E$  report, for this mixture, in the open literature. The experimental  $V^E$  results, for 1,4-dioxane + 2-propanol mixture, have been reported in our previous work [7] and well compared with corresponding literature  $V^E$  data.<sup>[8-10]</sup> In another hand, various thermo-physical and thermodynamic property data, reported in the literature,<sup>[8-11]</sup> shown that the dispersive forces between unlike molecules predominate in the mixture behavior.

It can be seen from Table 6 and in Figs 3 and 4, that ternary mixture of 1,4-dioxane (1) + 2-propanol (2) + 1,1,2,2-tetrachloroethane (3) presents positive  $V_{123}^E$  values, in the 1,1,2,2-tetrachloroethane poor region, and negative  $V_{123}^E$  values for  $x_3 > 0.15$ , at working temperatures. For the chloroalkane-poor region, as the alcohol ratio increases, the  $V_{123}^E$  magnitude decreases in the following sequence:  $V_{123}^E$  (for 25% of alcohol)  $>$   $V_{123}^E$  (for 50% of alcohol)  $>$   $V_{123}^E$  (for 75% of alcohol). For the chloroalkane-rich region, in contrary, the  $V_{123}^E$  magnitude decreases in the following sequence:  $V_{123}^E$  (75 % of alcohol)  $>$   $V_{123}^E$  (50 % of alcohol)  $>$   $V_{123}^E$  (25 % of alcohol). Also, the  $V_{123}^E$  presents minimums, at  $x_3 = 0.415, 0.50$  and  $0.55$ , for the fixed mole ratio  $x_1/x_2$  values equal to  $1/3, 1$  and  $3$ , respectively. The corresponding minimum  $V_{123}^E$  values are equal to  $(-0.356, -0.346, -0.322$  and  $-0.28) \text{ cm}^3 \text{ mol}^{-1}$ ,  $(-0.248, -0.267, -0.275$  and  $-0.272) \text{ cm}^3 \text{ mol}^{-1}$  and  $(-0.2433, -0.285, -0.320$  and  $-0.348) \text{ cm}^3 \text{ mol}^{-1}$ , at the temperatures  $T = (288.15, 298.15, 308.15$  and  $318.15) \text{ K}$ , respectively. The lines of the ‘‘constant ternary contribution’’,  $(V_{123}^E - V_{bin}^E)$ , calculated using eq 11, at  $T = 298.15 \text{ K}$ , are reported in Fig. 5. As it can be seen, the ternary contribution presents a minimum, at  $x_1 =$

0.135 and  $x_2 = 0.45$ , for a value of  $-0.196 \text{ cm}^3 \text{ mol}^{-1}$  and a maximum, for  $0.005 \text{ cm}^3 \text{ mol}^{-1}$ , at  $x_1 = 0.75$  and  $x_2 = 0.25$ .

The excess molar volume values are the result of several opposing effects and, also, mainly depends upon the balance between a negative contribution to  $V^E$ , due to the interactions between unlike molecules or to structural effects such as interstitial accommodation or changes in free volume, and a positive contribution to  $V^E$ , due to the interactions between like molecules or changes in the molecule self-association. So, the negative  $V^E$  values, presented by the 1,4-dioxane + 1,1,2,2-tetrachloroethane mixture, over the whole composition and working temperature ranges, is due to the predominance of the negative contribution to  $V^E$  which results from specific intermolecular interactions between unlike molecules in this mixture. It should be pointed out, that this behaviour was reported, for mixtures of 1,4-dioxane with numerous chloroalkanes, by several other authors.<sup>12,13,30-37</sup> The sigmoidal- $V^E$  curves, observed in Fig. 2, for 2-propanol + 1,1,2,2-tetrachloroethane mixture, result from the balance between two main contributions to  $V^E$  values. Once, positive, probably due to the break-up of associates in the pure state, such as the self-association in the pure alcohol and dipole-dipole in the chloroalkane, which is more significant in the chloroalkane-rich region. The second one, the negative contribution, results from the possible formation of specific interactions (OH...Cl) between unlike molecules, and the geometrical fitting of one molecule in the structure of the other, due to the difference in molecular size of the components; the molar volume of 2-propanol, equal to  $76.94 \text{ cm}^3 \cdot \text{mol}^{-1}$ , is lower than 1,1,2,2-tetrachloroethane molar volume, equal to  $105.75 \text{ cm}^3 \cdot \text{mol}^{-1}$ , at  $T = 298.15 \text{ K}$ . The negative contribution predominated the  $V^E$  values in the alcohol rich region. The  $V^E$  values for the binary mixture of 2-propanol with 1,1,2,2-tetrachloroethane increase as the temperature increases. This may be explained by a possible breaking up of the associations between like and unlike molecules in the mixture as the temperature increases, which produces an expansion in the mixture volume and makes more positive the  $V^E$  values.

Knowledge of the volumetric properties is of great interest for a better comprehension of intermolecular interactions in liquid mixtures. The volumetric properties at infinite dilution, especially, are more informative concerning the solute-solvent interactions in these mixtures. As it can be seen in Tables 4 and 5, for 1,4-dioxane + 2-propanol mixture, both of the components had the same behavior when mixing. So, the partial molar volume values increase. Also, the  $V_i^\infty$  values rise by comparison with  $V_i^0$  values. Then  $V_i^E$  and  $V_i^{E,\infty}$  values are positives. For the binary mixture of 1,4-dioxane + 1,1,2,2-tetrachloroethane, the  $V_i$  values



decrease, and the  $V_i^E$  values are negatives, especially at dilute region, where strong negative  $V_i^{E,\infty}$  values are observed for both components of this mixture. For 2-propanol + 1,1,2,2-tetrachloroethane binary mixture, the components had several behaviors as the composition mixture changes. The partial molar volume values of 2-propanol decrease when this component is mixed with 1,1,2,2-tetrachloroethane, which leads to negative excess partial molar volume values of 2-propanol in this mixture. However, at dilute region, the  $V_i^\infty$  values are higher than  $V_i^0$  values and the  $V_i^{E,\infty}$  values, for 2-propanol, are positives. The partial molar volume values of 1,1,2,2-tetrachloroethane decrease in the 2-propanol rich region and increase with the molar fraction of 1,1,2,2-tetrachloroethane in the mixture. So, the excess partial molar volume values for 1,1,2,2-tetrachloroethane are positives at the 1,1,2,2-tetrachloroethane rich region and became negatives for the 2-propanol high mole fraction region, and the  $V_i^{E,\infty}$  values are strongly negatives. As the temperature increases, the  $V_i$ , and  $V_i^\infty$  values change in the same way and increase for all binary mixtures. However, the  $V_i^E$  and  $V_i^{E,\infty}$  values became more negatives for 1,4-dioxane + 1,1,2,2-tetrachloroethane mixture, and increase, for 1,4-dioxane + 2-propanol and 2-propanol + 1,1,2,2-tetrachloroethane binary mixtures, when the temperature rises.

#### 4. Analysis in terms of the Prigogine-Flory-Patterson theory (PFP model)

Prediction of excess molar volumes, for the presently investigated binary mixtures, was carried out by the Prigogine-Flory-Patterson theory (PFP model)<sup>1-5</sup> in order to test this model.

From the PFP model, the excess molar volume  $V^E$  expression is given by:

$$\begin{aligned} \frac{V_m^E}{(x_1V_1^* + x_2V_2^*)} = & \left[ \frac{(\tilde{V}^{1/3} - 1)\tilde{V}^{2/3}}{(4/3)\tilde{V}^{1/3} - 1} \right] \Psi_1 \theta_2 \left[ \frac{\chi_{12}}{P_1^*} \right] \quad (\text{interactional contribution}) \\ & - \frac{(\tilde{V}_1 - \tilde{V}_2)^2 [(14/9)\tilde{V}^{1/3} - 1]}{[(4/3)\tilde{V}^{1/3} - 1]} \Psi_1 \Psi_2 \quad (\text{curvature contribution}) \\ & + \frac{(\tilde{V}_1 - \tilde{V}_2)^2 (P_1^* - P_2^*)}{P_1^* \Psi_2 + P_2^* \Psi_1} \Psi_1 \Psi_2 \quad (\text{internal pressure effect}) \end{aligned} \quad (13)$$

$\tilde{V}$ , is the reduced volume of the solution, and is estimated in eq (13) by:

$$\tilde{V} = \Psi_1 \tilde{V}_1 + \Psi_2 \tilde{V}_2 \quad (14)$$

Where the molecular contact energy fractions,  $\Psi_1$  and  $\Psi_2$ , are calculated by:

$$\Psi_1 = 1 - \Psi_2 = \frac{\phi_1 P_1^*}{(\phi_1 P_1^* + \phi_2 P_2^*)} \quad (15)$$

The hard-core volume fractions,  $\phi_1$  and  $\phi_2$ , given by:

$$\phi_1 = 1 - \phi_2 = \frac{x_1 V_1^*}{(x_1 V_1^* + x_2 V_2^*)} \quad (16)$$

The molecular surface fraction  $\theta_2$  is defined by:

$$\theta_2 = 1 - \theta_1 = \frac{\phi_2}{(\phi_1 (\frac{S_1}{S_2}) + \phi_2)} \quad (17)$$

Where the ratios  $\frac{S_1}{S_2}$  are approximated by  $\frac{S_1}{S_2} = \left( \frac{V_2^*}{V_1^*} \right)^{(1/3)}$

The reduced volume,  $\tilde{V}_i$ , of a constituent  $i$ , is given by:

$$\tilde{V}_i = \left[ \frac{1 + (4/3)\alpha_i T}{1 + \alpha_i T} \right]^3 \quad (18)$$

Where the thermal expansion coefficient,  $\alpha_i$ , is defined by

$$\alpha_i = \left( \frac{1}{V_i^0} \right) \left( \frac{\partial V_i^o}{\partial T} \right)_P \quad (19)$$

The characteristic pressure and volume,  $P_i^*$  and  $V_i^*$  are defined by:

$$V_i^* = V_i / \tilde{V}_i \quad (20)$$

$$P_i^* = T \tilde{V}_i^2 \alpha_i / \kappa_{Ti} \quad (21)$$

Where the isothermal compressibility  $\kappa_{T_i}$  of a constituent  $i$  is given by:

$$\kappa_{T_i} = -\left(\frac{1}{V_i^0}\right) \left(\frac{\partial V_i^0}{\partial P}\right)_T \quad (22)$$

The values of the parameters,  $\alpha_i$ ,  $V_i^*$  and  $P_i^*$ , for pure components were estimated from the Flory theory, whereas the thermal compressibility,  $\kappa_{T_i}$  values were obtained using the equation:

$$\kappa_T = \kappa_S + (\alpha^2 V_m T / C_{p,m}) \quad (23)$$

The Newton-Laplace equation was used to estimate the isentropic compressibility values,  $\kappa_S$ , for pure components:

$$\kappa_S = \frac{1}{\rho u^2} \quad (24)$$

The  $\kappa_{T_i}$  values, for pure components, were calculated using our experimental density values,  $\rho$ , whereas those of speed of sound,  $u_i$ , and those of heat capacity,  $C_{pi}$ , were calculated from literature data.<sup>9, 12, 18, 22, 38-52</sup> All the  $\alpha_i$ ,  $\kappa_{T_i}$ ,  $V_i^*$  and  $P_i^*$  values, which were used in PFP calculation, are summarized in Table 8. The interchange parameter,  $\chi_{12}$ , was derived by fitting the  $V^E$  expression (eq 13) to our experimental  $V^E$  values, at  $T = 298.15$  K. The adjusted values of  $\chi_{12}$  and the calculated three contributions to the  $V^E$  values at equimolar fraction, are reported in Table 9. It appears, from this table, that the interactional contribution value is negative for the two systems and is predominant in the case of 1,4-dioxane containing mixture. Graphical comparison of experiment with PFP calculation is given in Fig. 6, for 1,4-dioxane + 1,1,2,2-tetrachloroethane mixture, and in Fig. 7, for 1,1,2,2-tetrachloroethane + 2-propanol. One can be seen that the agreement is acceptable for 1,1,2,2-tetrachloroethane + 1,4-dioxane whereas the PFP model was failed for 1,1,2,2-tetrachloroethane + 2-propanol.

## 5. Conclusion

Densities and excess molar volumes for 1,4-dioxane + 2-propanol + 1,1,2,2-tetrachloroethane ternary mixture and constituent binaries were determined over the whole composition range, at four temperatures inside  $T = (288.15 \text{ to } 318.15)$  K. 1,1,2,2-

tetrachloroethane containing binary mixtures presents negative  $V^E$  values, over the whole composition and temperature ranges, with the 1,4-dioxane, and present sigmoidal- $V^E$  curves with 2-propanol. As the temperature increases, the  $V^E$  magnitude for 1,4-dioxane containing binary mixtures decreases with 1,1,2,2-tetrachloroethane and increases with 2-propanol, The  $V^E$  values for 2-propanol + 1,1,2,2-tetrachloroethane mixture increase as the temperature increase. The experimental binary and ternary excess molar volume values, were fitted to the empirical equations of Redlich-Kister and of Cibulka, respectively. The Prigogine-Flory-Patterson theory (PFP model) was tested, and the graphical comparison of experiment with PFP calculations, shows an acceptable agreement for the mixture of 1,1,2,2-tetrachloroethane with 1,4-dioxane but the model failed for the mixture of 1,1,2,2-tetrachloroethane with 2-propanol.

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**Table 1. CAS Registry Number, Purity and Density ( $\rho$ ) of the Chemicals**

				T/K	$\rho / \text{g}\cdot\text{cm}^{-3}$ <sup>q</sup>	
Component	CAS Reg. No	suppliers	purity (%)		this work	literature
1,4-dioxane	123-91-1	Sigma-Aldrich	> 99.5	288,15	<b>1,03912</b> <sup>p</sup>	1.0391 <sup>b</sup>
				298,15	<b>1,02784</b> <sup>p</sup>	1.02780 <sup>c</sup> ; 1.02786 <sup>d</sup>
				308,15	<b>1,01657</b> <sup>p</sup>	1.01657 <sup>e</sup>
				318,15	<b>1,00529</b> <sup>p</sup>	1.005279 <sup>f</sup>
1,1,2,2-tetrachloroethane	79-34-5	Merck	> 97.0	288,15	1,60277	1.601447 <sup>g</sup>
				298,15	1,58720	1.58665 <sup>h</sup> , 1.5876 <sup>i</sup>
				308,15	1,57163	1.570266 <sup>g</sup> ; 1.5729 <sup>j</sup> ; 1.5724 <sup>k</sup>
				318,15	1,55607	1, 5526 <sup>l</sup> ; 1.5642 <sup>l</sup> , 1.55704 <sup>o</sup>
2-Propanol	67-63-0	Prolabo	> 99.7	288,15	<b>0,78968</b> <sup>p</sup>	0.7893 <sup>m</sup>
				298,15	<b>0,78108</b> <sup>p</sup>	0.781073 <sup>a</sup> ; 0.78109 <sup>n</sup>
				308,15	<b>0,77248</b> <sup>p</sup>	0.772434 <sup>a</sup>
				318,15	<b>0,76388</b> <sup>p</sup>	

<sup>a</sup>Ref 9. <sup>b</sup>Ref 14. <sup>c</sup>Ref 15. <sup>d</sup>Ref 16. <sup>e</sup>Ref 17. <sup>f</sup>Ref 18. <sup>g</sup>Ref 19. <sup>h</sup>Ref 20. <sup>i</sup>Ref 21. <sup>j</sup>Ref 22. <sup>k</sup>Ref 23. <sup>l</sup>Ref 24. <sup>m</sup>Ref 25. <sup>n</sup>Ref 26. <sup>o</sup>Ref 27. <sup>p</sup> **Ref 7**. <sup>q</sup>The pressure for the density measurement was 101.3 kPa; the standard uncertainties,  $u$ , are  $u(T) = 0.01$  K,  $u(p) = 5$  kPa and  $u_r(\rho) = 0.0005$ .

**Table 2. Densities,  $\rho$ , in ( $\text{g}\cdot\text{cm}^{-3}$ ) and Molar Excess Volumes,  $V^E$ , in ( $\text{cm}^3\cdot\text{mol}^{-1}$ ), for the binary mixtures 1,4-Dioxane (1) + 1,1,2,2-Tetrachloroethane (2) and 2-Propanol (1) + 1,1,2,2-Tetrachloroethane (2) and, at Pressure  $P = 101.3$  kPa and Temperature  $T = (288.15 \text{ to } 318.15)$  K.<sup>a</sup>**

$x_1$	$\rho$	$V^E$	$\rho$	$V^E$	$\rho$	$V^E$	$\rho$	$V^E$
	$T/\text{K} = 288.15$		$T/\text{K} = 298.15$		$T/\text{K} = 308.15$		$T/\text{K} = 318.15$	
1,4-Dioxane (1) + 1,1,2,2-Tetrachloroethane (2)								
0.000	1.60277	0.000	1.58720	0.000	1.57163	0.000	1.55607	0.000
0.025	1.59150	-0.022	1.57615	-0.032	1.56075	-0.039	1.54531	-0.044
0.050	1.58046	-0.053	1.56524	-0.067	1.54997	-0.078	1.53466	-0.088
0.150	1.53437	-0.137	1.51970	-0.169	1.50496	-0.198	1.49018	-0.225
0.250	1.48614	-0.208	1.47199	-0.254	1.45777	-0.297	1.44347	-0.337
0.350	1.43496	-0.232	1.42131	-0.289	1.40758	-0.342	1.39376	-0.392
0.452	1.38012	-0.224	1.36695	-0.287	1.35369	-0.347	1.34034	-0.402
0.500	1.35363	-0.211	1.34067	-0.276	1.32762	-0.337	1.31448	-0.393
0.550	1.32503	-0.182	1.31228	-0.246	1.29944	-0.307	1.28650	-0.363
0.650	1.26613	-0.137	1.25377	-0.198	1.24131	-0.254	1.22878	-0.307
0.750	1.20448	-0.076	1.19245	-0.126	1.18036	-0.173	1.16819	-0.216
0.850	1.14050	-0.042	1.12879	-0.077	1.11702	-0.108	1.10518	-0.135
0.950	1.07365	-0.012	1.06228	-0.029	1.05084	-0.041	1.03934	-0.048
1.000	<b>1.03912<sup>b</sup></b>	0.000	<b>1.02784<sup>b</sup></b>	0.000	<b>1.01657<sup>b</sup></b>	0.000	<b>1.00529<sup>b</sup></b>	0.000
2-Propanol (1) + 1,1,2,2-Tetrachloroethane (2)								
0.000	1.60277	0.000	1.58720	0.000	1.57163	0.000	1.55607	0.000
0.050	1.57223	0.048	1.55686	0.051	1.54144	0.056	1.52599	0.065
0.150	1.50952	0.048	1.49438	0.067	1.47918	0.092	1.46392	0.121
0.250	1.44436	-0.013	1.42956	0.018	1.41465	0.057	1.39964	0.105
0.350	1.37515	-0.085	1.36078	-0.047	1.34627	0.003	1.33162	0.066
0.450	1.30200	-0.174	1.28816	-0.131	1.27415	-0.074	1.25996	-0.001
0.500	1.26378	-0.223	1.25024	-0.178	1.23651	-0.118	1.22259	-0.041
0.550	1.22385	-0.262	1.21065	-0.217	1.19724	-0.155	1.18362	-0.074
0.650	1.14046	-0.358	1.12799	-0.315	1.11530	-0.252	1.10237	-0.166
0.750	1.05044	-0.403	1.03887	-0.366	1.02706	-0.307	1.01497	-0.221
0.850	0.95306	-0.370	0.94259	-0.348	0.93184	-0.300	0.92080	-0.223
0.950	0.84657	-0.182	0.83749	-0.190	0.82812	-0.171	0.81841	-0.118
1.000	<b>0.78968<sup>b</sup></b>	0.000	<b>0.78108<sup>b</sup></b>	0.000	<b>0.77248<sup>b</sup></b>	0.000	<b>0.76388<sup>b</sup></b>	0.000

<sup>a</sup> Standard uncertainties  $u$  are  $u(T) = 0.01\text{K}$ ,  $u(p) = 5$  kPa,  $u(x_1) = 0.001$ ,  $u_r(\rho) = 0.0005$  and  $u(v^E) = 0.004$   $\text{cm}^3$   $\text{mol}^{-1}$ . <sup>b</sup> Ref 7.

**Table 3. Parameters  $A_i$  of Equation 2 and their Standard Deviations  $\sigma A_i$  and Standard Deviations  $\sigma$  in ( $\text{cm}^3 \cdot \text{mol}^{-1}$ ), for 1,1,2,2-Tetrachloroethane containing (2) Binary Systems, at Pressure  $P = 101.3$  kPa and Temperature  $T = (288.15$  to  $318.15)$  K.**

$T/\text{K}$	$A_0$	$\sigma A_0$	$A_1$	$\sigma A_1$	$A_2$	$\sigma A_2$	$A_3$	$\sigma A_3$	$A_4$	$\sigma A_4$	$\sigma / \text{cm}^3 \cdot \text{mol}^{-1}$
1,4-Dioxane (1) + 1,1,2,2-Tetrachloroethane (2)											
288.15	-0.830	0.008	0.776	0.033	0.251	0.037	-0.432	0.082			0.003
298.15	-1.086	0.009	0.750	0.038	0.226	0.042	-0.412	0.093			0.004
308.15	-1.328	0.009	0.722	0.041	0.230	0.046	-0.382	0.101			0.004
318.15	-1.555	0.009	0.695	0.037	0.270	0.042	-0.332	0.093			0.004
2-Propanol (1) + 1,1,2,2-Tetrachloroethane (2)											
288.15	-0.879	0.008	-1.863	0.031	-1.043	0.089	-0.987	0.08	0.511	0.154	0.003
298.15	-0.707	0.013	-1.790	0.050	-0.846	0.143	-1.149	0.128	-0.022	0.248	0.005
308.15	-0.468	0.014	-1.701	0.054	-0.717	0.153	-1.066	0.136	-0.132	0.263	0.005
318.15	-0.155	0.009	-1.594	0.035	-0.670	0.099	-0.667	0.088	0.267	0.171	0.003

**Table 4. Partial molar volumes,  $V_i$ , and excess molar partial volumes,  $V_i^E$ , at  $T = (288.15$  and  $318.15)$  K, for 1,4-Dioxane (1) + 2-Propanol,<sup>a</sup> + 1,1,2,2-Tetrachloroethane (2), and 2-Propanol (1) + 1,1,2,2-Tetrachloroethane (2), at Temperature  $T = (288.15$  and  $318.15)$  K.**

$x_1$	$T/K = 288,15$				$T/K = 318,15$			
	$V_1$	$V_1^E$	$V_2$	$V_2^E$	$V_1$	$V_1^E$	$V_2$	$V_2^E$
1,4-Dioxane (1) + 2-Propanol (2)								
0,000	86,08	1,286	76,11	0,000	89,68	2,035	78,68	0,000
0,050	85,78	0,988	76,11	0,007	89,21	1,564	78,69	0,012
0,150	85,45	0,658	76,15	0,041	88,65	1,003	78,75	0,070
0,250	85,31	0,518	76,18	0,075	88,38	0,729	78,81	0,137
0,350	85,23	0,441	76,21	0,108	88,22	0,573	78,88	0,203
0,449	85,16	0,364	76,27	0,160	88,09	0,446	78,96	0,288
0,500	85,11	0,316	76,31	0,203	88,02	0,378	79,03	0,350
0,550	85,06	0,265	76,37	0,260	87,96	0,310	79,10	0,426
0,651	84,95	0,157	76,53	0,424	87,82	0,175	79,31	0,629
0,750	84,86	0,067	76,74	0,635	87,71	0,068	79,55	0,878
0,850	84,81	0,012	76,96	0,849	87,66	0,009	79,79	1,111
0,950	84,79	-0,001	77,05	0,948	87,64	-0,002	79,86	1,181
1,000	84,79	0,000	77,01	0,900	87,65	0,000	79,76	1,086
1,4-Dioxane (1) + 1,1,2,2-Tetrachloroethane (2)								
0,000	83,87	-0,923	104,72	0,000	86,00	-1,648	107,87	0,000
0,025	83,83	-0,964	104,73	0,000	86,01	-1,638	107,87	0,000
0,050	83,82	-0,977	104,73	0,001	86,04	-1,606	107,87	-0,001
0,150	83,95	-0,842	104,71	-0,017	86,31	-1,334	107,83	-0,034
0,250	84,23	-0,563	104,64	-0,088	86,69	-0,960	107,74	-0,128
0,350	84,51	-0,283	104,52	-0,207	87,05	-0,599	107,59	-0,283
0,452	84,72	-0,076	104,38	-0,345	87,33	-0,313	107,39	-0,473
0,500	84,78	-0,013	104,32	-0,401	87,43	-0,215	107,31	-0,562
0,550	84,82	0,029	104,28	-0,448	87,51	-0,136	107,22	-0,650
0,650	84,85	0,057	104,24	-0,487	87,61	-0,041	107,08	-0,789
0,750	84,83	0,039	104,28	-0,441	87,64	-0,007	107,00	-0,866
0,850	84,80	0,012	104,39	-0,332	87,65	-0,001	106,98	-0,886
0,950	84,79	0,000	104,49	-0,235	87,65	-0,001	106,97	-0,894
1,000	84,79	0,000	104,49	-0,234	87,65	0,000	106,95	-0,923
2-Propanol (1) + 1,1,2,2-Tetrachloroethane (2)								
0,000	77,55	1,439	104,72	0,000	80,38	1,703	107,87	0,000
0,050	76,67	0,563	104,75	0,021	79,69	1,013	107,88	0,017
0,150	75,82	-0,283	104,83	0,106	78,91	0,234	107,97	0,098
0,250	75,57	-0,541	104,89	0,167	78,56	-0,115	108,05	0,182
0,350	75,48	-0,623	104,93	0,201	78,38	-0,295	108,13	0,258
0,450	75,43	-0,671	104,96	0,233	78,27	-0,404	108,20	0,330
0,500	75,42	-0,685	104,97	0,246	78,24	-0,437	108,23	0,360

**Table 4** (to be continued)

$x_I$	$V_1$	$T = 288,15 \text{ K}$			$T = 318,15$			
		$V_1^E$	$V_2$	$V_2^E$	$V_1$	$V_1^E$	$V_2$	$V_2^E$
0,550	75,42	-0,686	104,97	0,246	78,22	-0,454	108,25	0,378
0,650	75,49	-0,620	104,87	0,142	78,25	-0,429	108,20	0,335
0,750	75,65	-0,453	104,46	-0,263	78,36	-0,321	107,94	0,073
0,850	75,88	-0,222	103,51	-1,218	78,52	-0,160	107,28	-0,591
0,950	76,07	-0,032	101,73	-2,996	78,65	-0,023	105,99	-1,876
1,000	76,11	0,000	100,46	-4,261	78,68	0,000	105,05	-2,819

<sup>a</sup> Ref 7.

**Table 5. Molar volumes,  $V_i^0$ , partial molar volumes at infinite dilution,  $V_i^\infty$ , and excess partial molar volumes at infinite dilution,  $V_i^{E,\infty}$ , for 1,4-Dioxane (1) + 2-Propanol, + 1,1,2,2-Tetrachloroethane (2), and 2-Propanol (1) + 1,1,2,2-Tetrachloroethane (2) at Temperature  $T = (288.15 \text{ and } 318.15) \text{ K}$ .**

$T/\text{K}$	$V_1^0$	$V_1^\infty$	$V_1^{E,\infty}$	$V_2^0$	$V_2^\infty$	$V_2^{E,\infty}$
1,4-Dioxane (1) + 2-Propanol (2)						
288,15	84,79	86,08	1,286	76,11	77,01	0,900
318,15	87,65	89,68	2,035	78,68	79,76	1,086
1,4-Dioxane (1) + 1,1,2,2-Tetrachloroethane (2)						
288,15	84,79	83,87	-0,923	104,72	104,49	-0,234
318,15	87,65	86,00	-1,648	107,87	106,95	-0,923
2-Propanol (1) + 1,1,2,2-Tetrachloroethane (2)						
288,15	76,11	77,55	1,439	104,72	100,46	-4,261
318,15	78,68	80,38	1,703	107,87	105,05	-2,819

**Table 6. Densities,  $\rho$ , in ( $\text{g}\cdot\text{cm}^{-3}$ ) and Molar Excess Volumes,  $V_{123}^E$ , in ( $\text{cm}^3\cdot\text{mol}^{-1}$ ), for the Ternary System 1,4-Dioxane (1) + 2-Propanol (2) + 1,1,2,2-Tetrachloroethane (3), at Pressure  $P = 101.3$  kPa and Temperature  $T = (288.15 \text{ to } 318.15)$  K. <sup>a</sup>**

$x_1$	$x_2$	$\rho$	$V_{123}^E$	$\rho$	$V_{123}^E$	$\rho$	$V_{123}^E$	$\rho$	$V_{123}^E$
		$T/\text{K} = 288.15$		$T/\text{K} = 298.15$		$T/\text{K} = 308.15$		$T/\text{K} = 318.15$	
0.250	0.750	0.85523	0.185	0.84583	0.197	0.83622	0.228	0.82638	0.284
0.237	0.712	0.90588	0.039	0.89606	0.042	0.88601	0.067	0.87572	0.115
0.236	0.708	0.91147	0.016	0.90160	0.018	0.89151	0.041	0.88116	0.089
0.211	0.632	1.00869	-0.154	0.99795	-0.155	0.98697	-0.136	0.97573	-0.094
0.187	0.562	1.09048	-0.254	1.07897	-0.254	1.06723	-0.235	1.05522	-0.193
0.167	0.500	1.16079	-0.334	1.14861	-0.330	1.13622	-0.310	1.12359	-0.270
0.135	0.450	1.22303	-0.356	1.21024	-0.346	1.19726	-0.322	1.18406	-0.280
0.137	0.412	1.25150	-0.334	1.23849	-0.326	1.22529	-0.303	1.21189	-0.265
0.125	0.375	1.28819	-0.308	1.27487	-0.299	1.26136	-0.276	1.24767	-0.238
0.113	0.338	1.32359	-0.267	1.30995	-0.256	1.29616	-0.233	1.28220	-0.197
0.088	0.263	1.39137	-0.185	1.37720	-0.174	1.36290	-0.152	1.34846	-0.121
0.062	0.187	1.45543	-0.081	1.44080	-0.071	1.42607	-0.054	1.41125	-0.029
0.041	0.123	1.50781	-0.036	1.49284	-0.029	1.47780	-0.017	1.46268	0.000
0.038	0.113	1.51602	-0.026	1.50100	-0.020	1.48591	-0.009	1.47077	0.006
0.013	0.038	1.57401	0.022	1.55868	0.021	1.54331	0.022	1.52789	0.026
0.012	0.037	1.57425	0.023	1.55892	0.021	1.54355	0.022	1.52814	0.026
0.500	0.500	0.91821	0.258	0.90804	0.278	0.89773	0.312	0.88725	0.362
0.475	0.475	0.96325	0.137	0.95278	0.145	0.94215	0.167	0.93135	0.205
0.425	0.425	1.04882	-0.030	1.03776	-0.039	1.02652	-0.034	1.01509	-0.013
0.375	0.375	1.12922	-0.137	1.11755	-0.155	1.10571	-0.160	1.09366	-0.148
0.325	0.325	1.20438	-0.212	1.19211	-0.234	1.17966	-0.242	1.16703	-0.236
0.325	0.325	1.20500	-0.218	1.19272	-0.239	1.18027	-0.248	1.16763	-0.242
0.275	0.275	1.27614	-0.245	1.26327	-0.265	1.25023	-0.274	1.23702	-0.270
0.250	0.250	1.30991	-0.248	1.29675	-0.267	1.28344	-0.275	1.26997	-0.272
0.225	0.225	1.34294	-0.239	1.32949	-0.256	1.31590	-0.263	1.30218	-0.260





**Table 6. Continued**

$x_1$	$x_2$	$\rho$	$V_{123}^E$	$\rho$	$V_{123}^E$	$\rho$	$V_{123}^E$	$\rho$	$V_{123}^E$
		$T/K = 288.15$		$T/K = 298.15$		$T/K = 308.15$		$T/K = 318.15$	
0.179	0.179	1.40147	-0.197	1.38753	-0.210	1.37348	-0.215	1.35930	-0.212
0.175	0.175	1.40607	-0.194	1.39209	-0.207	1.37800	-0.212	1.36379	-0.209
0.125	0.125	1.46563	-0.128	1.45118	-0.138	1.43663	-0.142	1.42200	-0.140
0.075	0.075	1.52230	-0.060	1.50741	-0.068	1.49246	-0.072	1.47744	-0.072
0.032	0.032	1.56941	-0.011	1.55417	-0.017	1.53888	-0.020	1.52356	-0.021
0.023	0.023	1.57880	-0.005	1.56349	-0.011	1.54814	-0.014	1.53274	-0.015
0.750	0.250	0.97912	0.211	0.96837	0.223	0.95754	0.243	0.94660	0.274
0.712	0.237	1.01917	0.132	1.00820	0.131	0.99713	0.139	0.98595	0.157
0.711	0.237	1.02040	0.119	1.00943	0.118	0.99835	0.125	0.98716	0.143
0.638	0.213	1.09488	0.021	1.08346	0.002	1.07193	-0.009	1.06028	-0.011
0.562	0.187	1.16828	-0.094	1.15643	-0.128	1.14444	-0.154	1.13233	-0.171
0.488	0.163	1.23565	-0.156	1.22335	-0.198	1.21090	-0.231	1.19833	-0.255
0.413	0.138	1.30064	-0.209	1.28785	-0.253	1.27493	-0.289	1.26188	-0.317
0.375	0.125	1.33210	-0.227	1.31906	-0.270	1.30589	-0.306	1.29260	-0.334
0.339	0.113	1.36143	-0.243	1.34814	-0.285	1.33474	-0.320	1.32122	-0.348
0.262	0.088	1.42110	-0.234	1.40730	-0.271	1.39339	-0.301	1.37939	-0.326
0.188	0.063	1.47604	-0.174	1.46174	-0.203	1.44736	-0.227	1.43291	-0.247
0.113	0.038	1.52831	-0.105	1.51354	-0.126	1.49870	-0.142	1.48381	-0.156
0.052	0.017	1.56904	-0.049	1.55387	-0.062	1.53866	-0.071	1.52341	-0.078
0.038	0.013	1.57839	-0.034	1.56313	-0.044	1.54783	-0.052	1.53249	-0.057
0.000	0.000	1.60277	0.000	1.58720	0.000	1.57163	0.000	1.55607	0.000

<sup>a</sup> Standard uncertainties  $u$  are  $u(T) = 0.01$  K.  $u(p) = 5$  kPa.  $u(x_1) = 0.001$ .  $u_r(\rho) = 0.0005$  and  $u(V_{123}^E) = 0.004$  cm<sup>3</sup> mol<sup>-1</sup>

**Table 7. Parameters  $B_i$  of Equation 11 and Standard Deviations  $\sigma$  in ( $\text{cm}^3 \cdot \text{mol}^{-1}$ ), for the Ternary System 1,4-Dioxane (1) + 2-Propanol (2) + 1,1,2,2-Tetrachloroethane (3), at  $T = (288.15 \text{ to } 318.15) \text{ K}$ .**

$T/\text{K}$	$B_0$	$B_1$	$B_2$	$\sigma$
288.15	-7.162	7.633	1.984	0.017
298.15	-7.941	-6.136	5.485	0.015
308.15	-8.274	-6.378	4.649	0.013
318.15	-8.563	-6.540	3.368	0.012

**Table 8. Values of the Physical Constants of Pure Liquid Components, at the Temperature  $T = 298.15$  K, used for the Prigogine-Flory-Patterson Model Calculations of Excess Molar Volume,  $V^E$ , Molar Volume,  $V_i^0$ , Coefficient of Thermal Expansion,  $\alpha_i$ , Isothermal Compressibility,  $\kappa_{Ti}$ , and Reduction Parameters of Volume,  $V_i^*$ , and Pressure,  $P_i^*$**

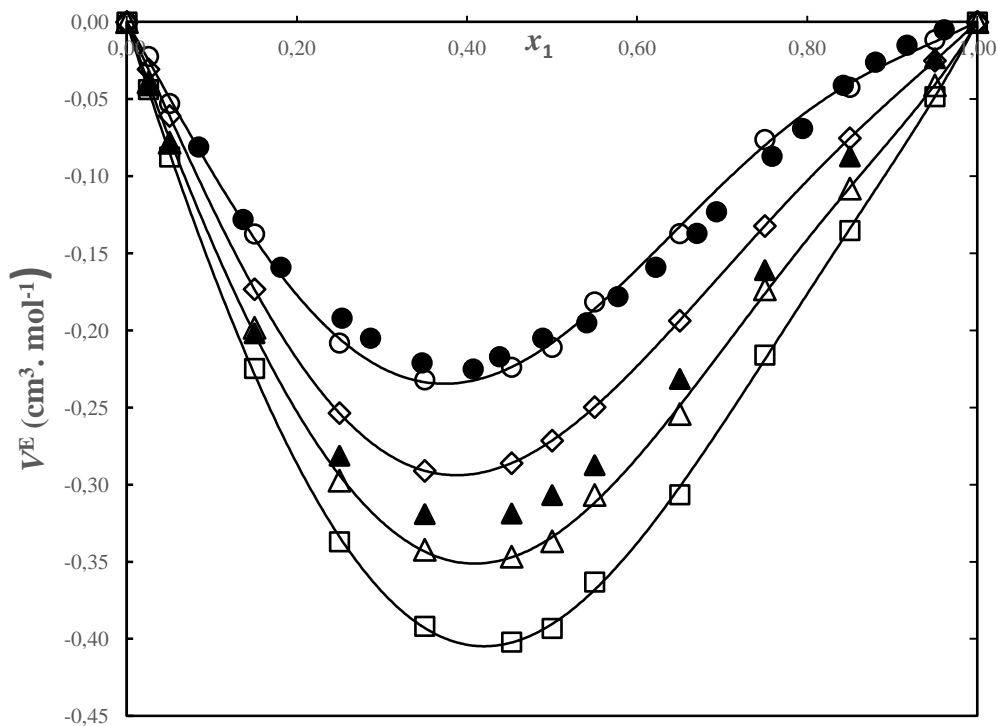
Compound	$V_i^0$	$10^3 \cdot \alpha$	$10^{12} \cdot \kappa_{Ti}$	$V_i^*$	$P_i^*$
	( $\text{cm}^3 \cdot \text{mol}^{-1}$ )	( $\text{K}^{-1}$ )	( $\text{Pa}^{-1}$ )	( $\text{cm}^3 \cdot \text{mol}^{-1}$ )	(MPa)
1.4-Dioxane	85.72 <sup>a</sup>	1.097 <sup>a</sup>	741.35 <sup>b</sup>	67.64 <sup>b</sup>	708.79 <sup>b</sup>
2-Propanol	76.94 <sup>a</sup>	1.101 <sup>a</sup>	1163.72 <sup>b</sup>	60.68 <sup>b</sup>	453.65 <sup>b</sup>
1.1.2.2-TCE	105.75 <sup>a</sup>	0.981 <sup>a</sup>	659.02 <sup>b</sup>	85.02 <sup>b</sup>	686.52 <sup>b</sup>

<sup>a</sup>This work. <sup>b</sup>Calculated using experimental  $\rho$  data along with  $C_p$  and  $u$  literature values.<sup>9,12,18,22,38-52</sup>

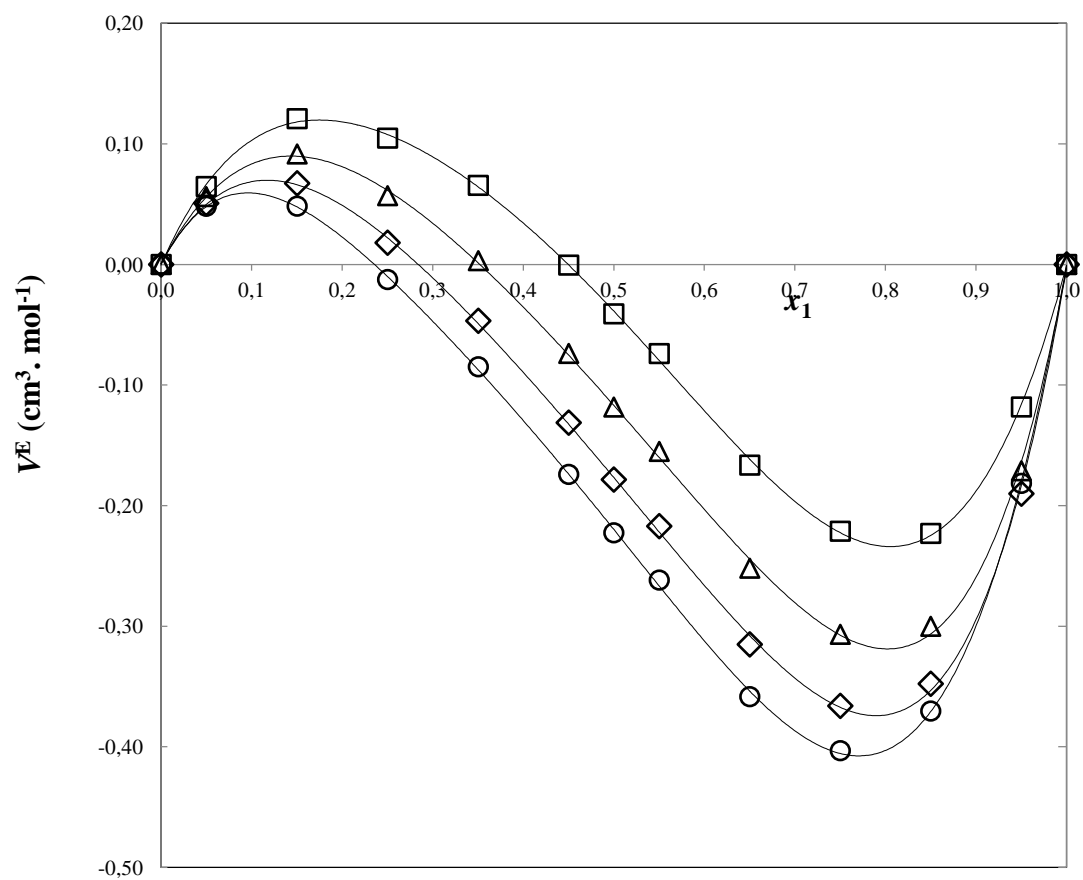
**Table 9. Values of  $X_{12}$  Interaction Parameter and Calculated Contributions to the  $V^E$  ( $x_1=0.5$ ), for the Binary Systems 1,4-Dioxane (1) + 2-Propanol or 1,1,2,2-Tetrachloroethane (2) and 2-Propanol (1) + 1,1,2,2-Tetrachloroethane (2), at Temperature  $T = (288.15 \text{ to } 318.15) \text{ K}$ .**

mixture	$\chi_{12}/ \text{J}\cdot\text{cm}^{-3}$	$V^E (x_1 = 0.5)/ \text{cm}^3\cdot\text{mol}^{-1}$		Calculated contributions to $V^E (x_1 = 0.5)/ \text{cm}^3\cdot\text{mol}^{-1}$		
		exptl	calcd	interactional	free volume	P* effect
1,4-Dioxane + 1,1,2,2-tetrachloroethane	-25.74	-0.276	-0.261	-0.260	0.016	0.014
2-Propanol + 1,1,2,2-tetrachloroethane	-3.34	-0.178	-0.220	-0.036	0.014	-0.170

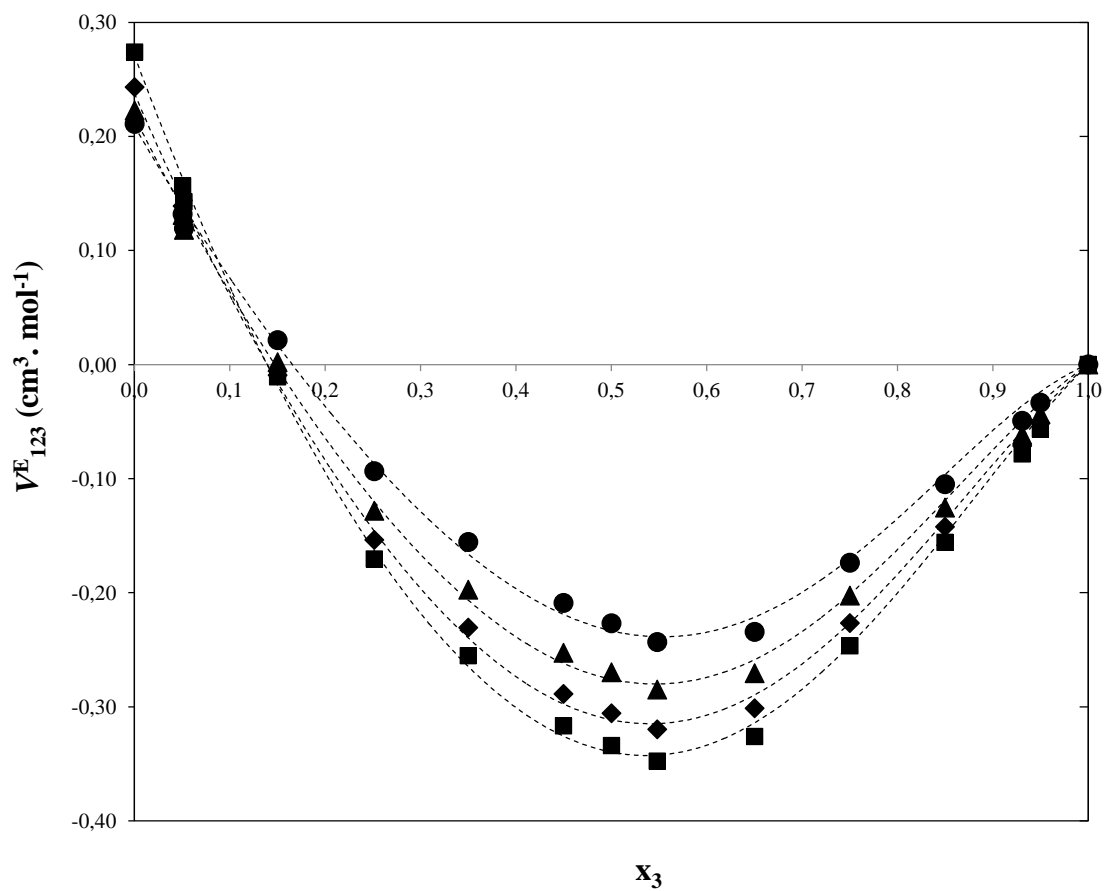
*List of figures:*



**Figure 1.** Excess molar volume,  $V^E$ , for 1,4-dioxane (1) + 1,1,2,2-tetrachloroethane (2) mixture. at several temperatures. Symbols: Experimental values [( $\circ$ ),  $T=288.15$  K; ( $\bullet^{13}$ ),  $T=293.15$  K; ( $\triangle$ ),  $T=298.15$  K; ( $\blacktriangle^{12}$ ),  $T=303.15$  K; ( $\diamond$ ),  $T=308.15$  K; ( $\square$ ),  $T=318.15$  K]; Solid lines: calculated values using eq 2.

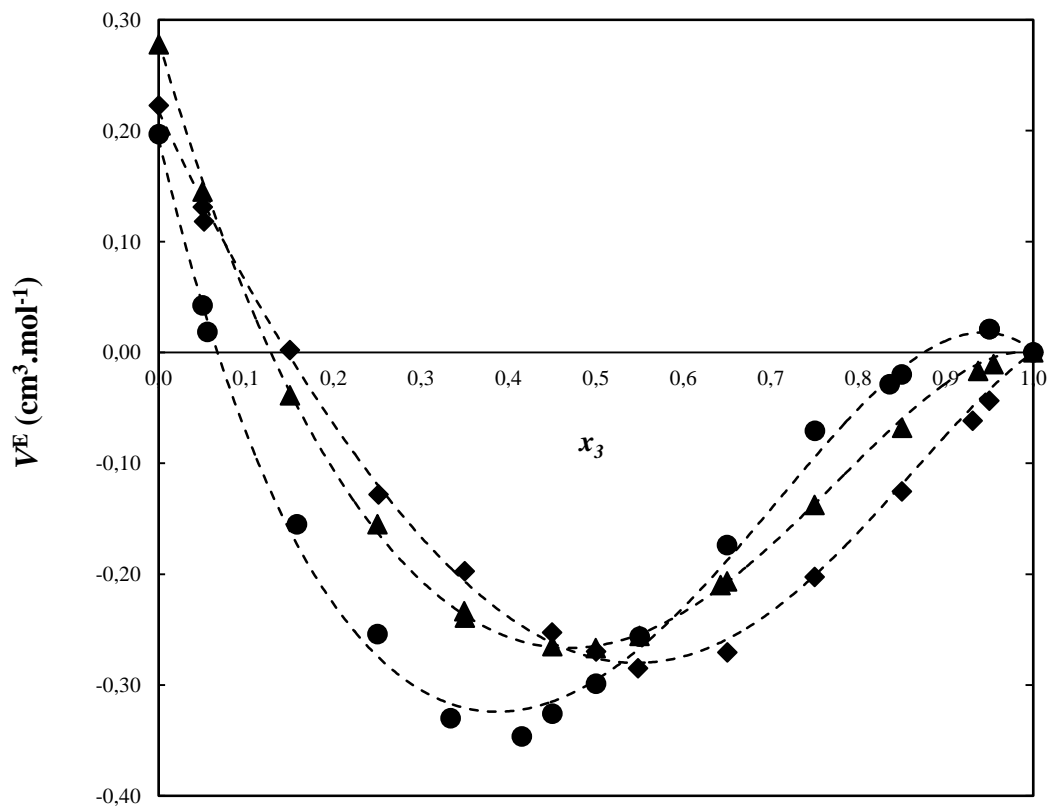


**Figure 2.** Excess molar volume,  $V^E$ , for 2-propanol (1) + 1,1,2,2-tetrachloroethane (2) system, at different temperatures. Symbols: experimental values. [( $\circ$ ),  $T=288.15$  K; ( $\triangle$ ),  $T=298.15$  K; ( $\diamond$ ),  $T=308.15$ ; ( $\square$ ),  $T=318.15$ ] K. Solid lines: calculated values using eq 2.

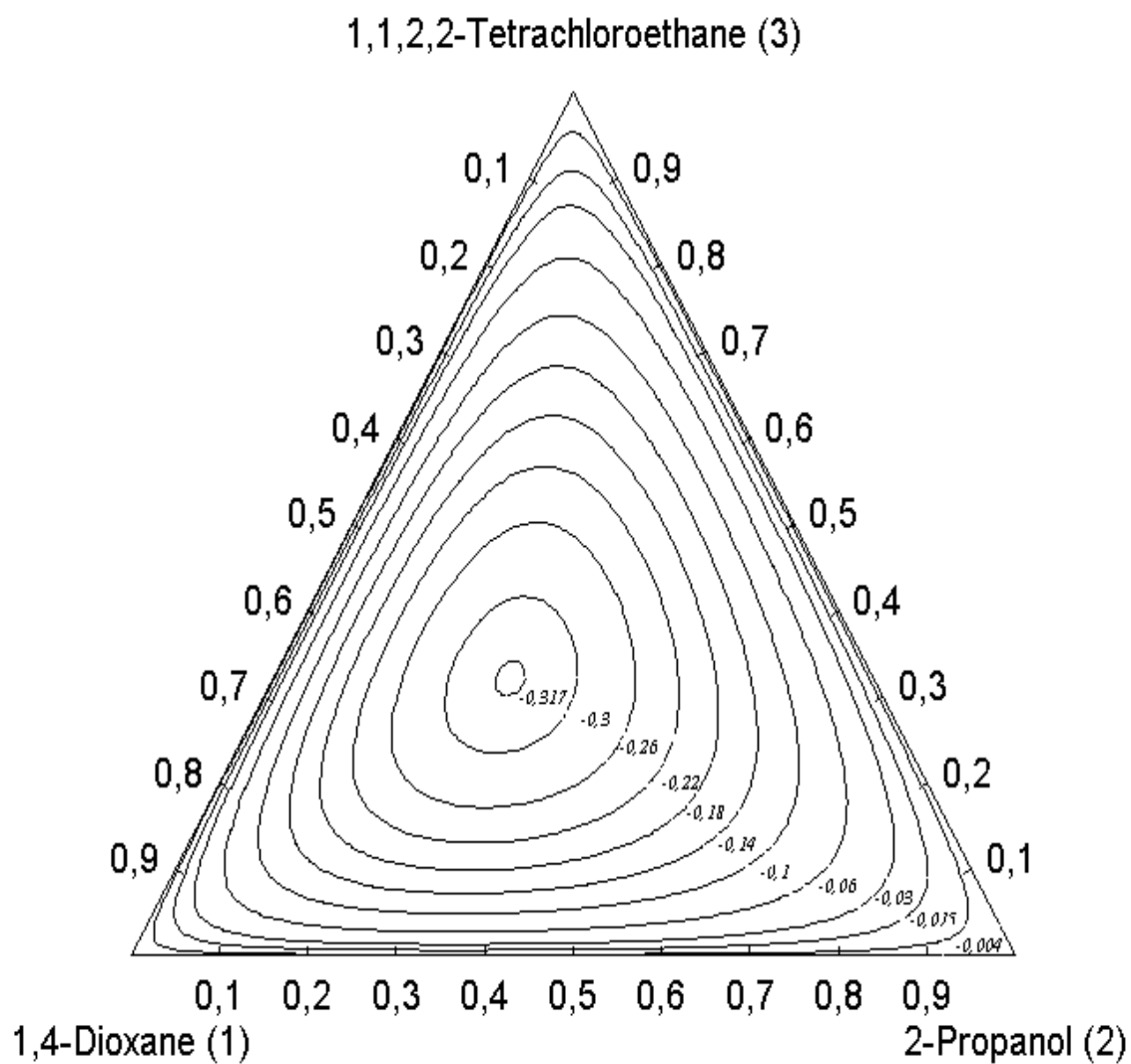


**Figure 3.** Excess molar volume,  $V_{123}^E$ , for the 1,4-dioxane (1) + 2-propanol (2) + 1,1,2,2-tetrachloroethane (3) ternary system, for the fixed mole ratio  $(x_1/x_2) = 3$ . Symbols: experimental data [ (●),  $T = 288.15 \text{ K}$ ; (▲),  $T = 298.15 \text{ K}$ ; (◆),  $T = 308.15 \text{ K}$ ; (■),  $T = 318.15 \text{ K}$ ]. Dashed lines: calculated values with eq 11.

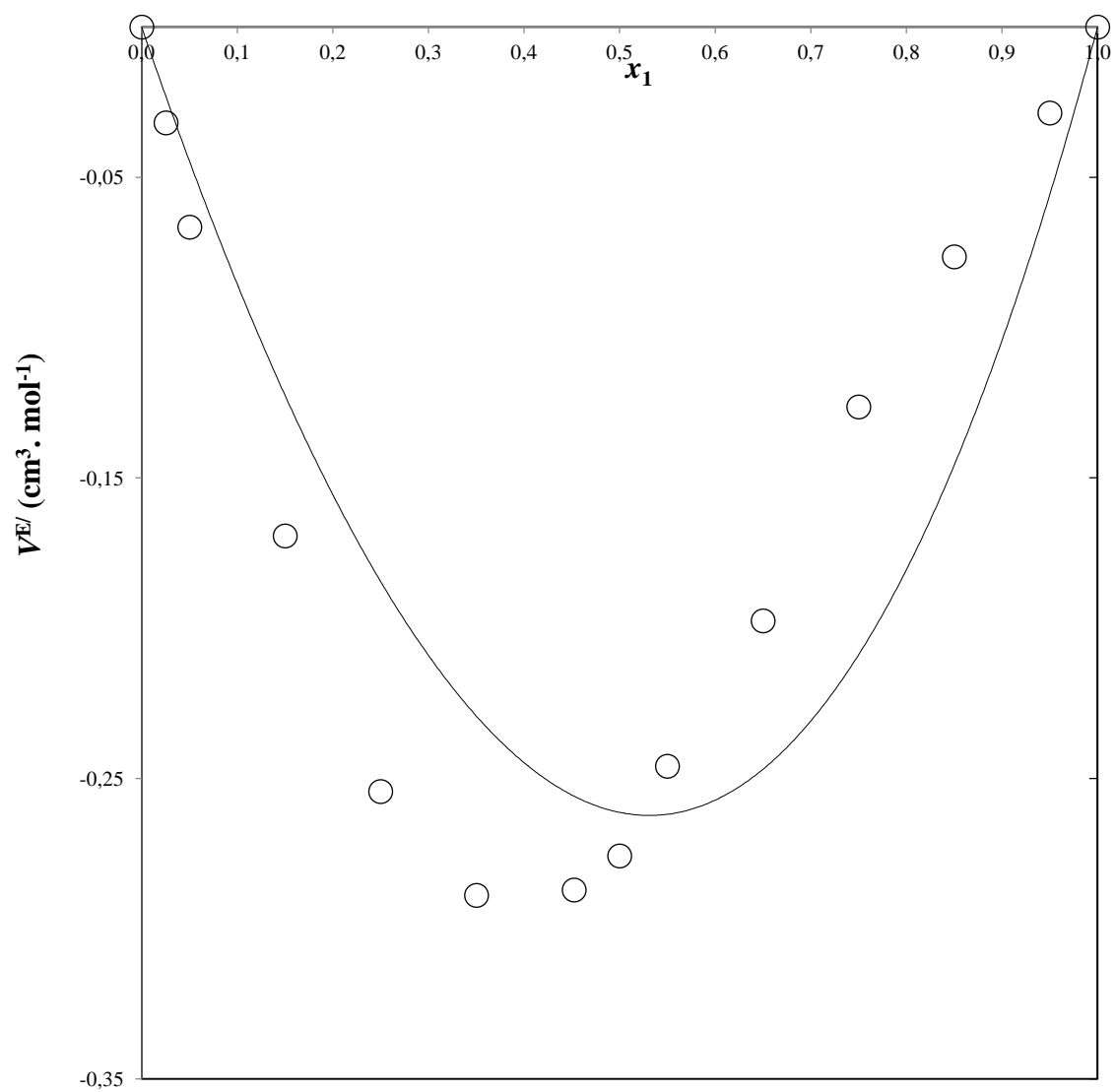




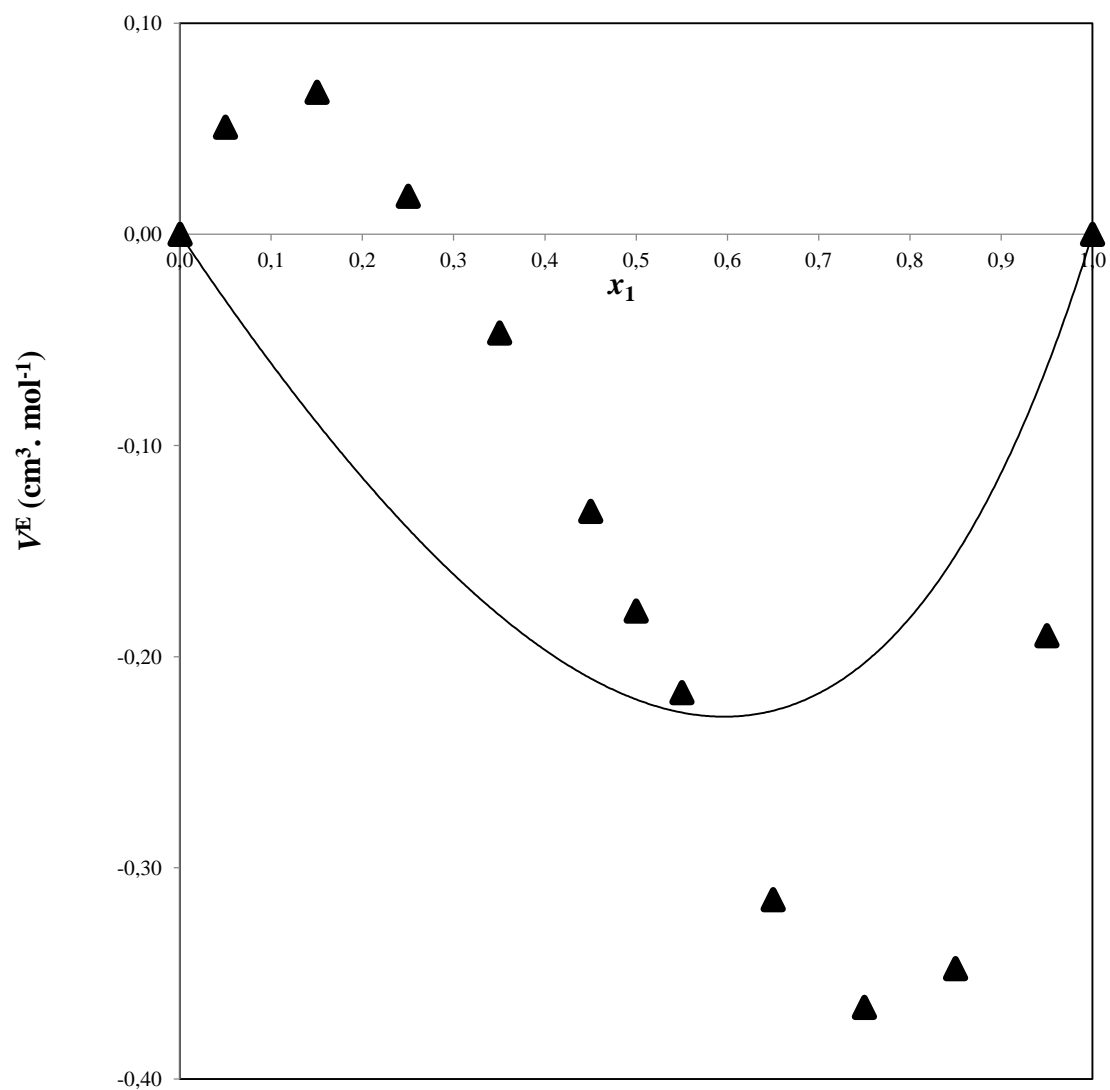
**Figure 4.** Excess molar volume,  $V_{123}^E$ , for the ternary mixture 1,4-dioxane (1) + 2-propanol (2) + 1,1,2,2-tetrachloroethane (3), at  $T = 298.15$  K. Symbols: experimental data [(●),  $x_1/x_2 = 1/3$ ; (▲),  $x_1/x_2 = 1$ ; (◆),  $x_1/x_2 = 3$ . for three values of the fixed mole ratio  $x_1/x_2$ . Dashed lines: calculated values with eq 11.



**Figure 5.** Curves of constant “ternary contribution”,  $(V_{123}^E - V_{bin}^E) / \text{cm}^3 \text{ mol}^{-1}$ , at  $T = 298.15 \text{ K}$ .  
for the ternary system 1,4-dioxane (1) + 2-propanol (2) + 1,1,2,2-tetrachloroethane (3).



**Figure 6.** Excess molar volumes,  $V^E$ , for 1,4-dioxane (1) + 1,1,2,2-tetrachloroethane (2) mixture, at 298.15 K. Symbols: experimental values. Lines: PFP calculations.



**Figure 7.** Excess molar volumes,  $V^E$ , for 2-propanol (1) + 1,1,2,2-tetrachloroethane (2) mixture, at 298.15 K. Symbols: experimental values. Lines: PFP calculations.

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