Chemical Data Collections 17–18 (2018) 111–120

Contents lists available at ScienceDirect

Chemical Data Collections

journal homepage: www.elsevier.com/locate/cdc

Data Article

# Density, viscosity, excess molar volume and viscosity deviation for [chloroform (1) + di-isopropyl-ether(2) + 1-propanol (3)] ternary system at 298.15 K.

Ruth Medina Naessens[1], René Amadeo Clará, Ana C. Gómez Marigliano[2,*]

*Departamento de Física, Facultad de Ciencias Exactas y Tecnología, Universidad Nacional de Tucumán, INFINOA CONICET, Avenida Independencia 1800*

ARTICLE INFO

*Article history:*
Received 16 April 2018
Revised 31 July 2018
Accepted 3 August 2018
Available online 4 August 2018

*Keywords:*
Ternary system
Excess molar volume
Viscosity deviations
Nagata-tamura equation
Radojkovi'c equation

ABSTRACT

Densities $\rho$ and viscosity $\eta$ of the [chloroform (1) + di-isopropyl ether (DIPE) (2) + 1-propanol (3)] ternary system have been measured at 298.15 K and pressure of 960 hPa using an Anton Paar DMA 500 stavigmeter. Excess molar volumes $\boldsymbol{V^E}$ and viscosity deviation $\Delta\eta$ were calculated. The excess molar volume $\boldsymbol{V^E}$ and viscosity deviation $\boldsymbol{\Delta\eta}$ for binary and ternary systems were correlated by a Redlich-Kister and Nagata and Tamura type equation. Also, the ternary excess molar volume and viscosity deviation $Y^E_{123}$ were predicted using the Radojković equation. From the macroscopic behavior inferences were made about the molecular interactions in the ternary mixture.



| | |
|---|---|
| Subject area | *Physical chemistry* |
| Compounds | Chloroform; di-isopropyl ether (DIPE); 1-propanol |
| Data category | *Physicochemical* |
| Data acquisition format | *Physical properties* |
| Data type | *Raw, analyzed, and calculated* |
| Procedure | *Determination:* |
| | *density with vibrating tube densimeter* |
| | *viscosity with concentric cylinder viscometer, Hall effect* |
| | *Excess molar volume and viscosity deviation are calculated with the general expressions* |
| Data accessibility | *In this article* |

## 1. Rationale

The importance of experimental data of binary and ternary systems is well known, both from the viewpoint of chemical engineering applications and the possibility of drawing conclusions about the interactions between the components of the mixture [1–4].

* Corresponding author.
*E-mail address:* agomezmarigliano@herrera.unt.edu.ar (A.C.G. Marigliano).
[1] Fellow CONICET.
[2] Member of the Carrera de Investigador Científico CONICET, Argentina.

https://doi.org/10.1016/j.cdc.2018.08.005
2405-8300/

The information available in the open literature of the thermophysical properties of the binary systems studied is very scarce, particularly in the systems where DIPE is present. The ternary system presented here was not studied, according to exhaustive search carried out. Thus, these data are very useful for the scientific and technological community, mainly if the fact that both alkanols and ethers are used as fuel additives is taken into account.

In this paper we report density and viscosity data at $T = 298.15$ K and 960hPa of three pure chemicals (chloroform, DIPE and 1-propanol), as well as for the [chloroform (1) + 1-propanol (3)] binary system and the [chloroform (1) + DIPE (2) + 1-propanol(3)] ternary liquid mixture over the whole composition range. Empiric equations for the excess molar volumes $\boldsymbol{V^E}$ and viscosity deviation $\boldsymbol{\Delta\eta}$ of the binary system as well as for the ternary system as a function of composition were developed using Origin Pro 8.5. These equations were fitted using least squares with all points equally weigthed. The appropriate number of constants and significant digits are obtained by comparing with the experimental errors.

The binary systems [chloroform (1) + DIPE (2)] and [DIPE (2) + 1-propanol (3)], were already studied and published by our research group [5,6].

The excess molar volume $\boldsymbol{V^E}$ and viscosity deviation $\boldsymbol{\Delta\eta}$ for binary system were fitted to a Redlich-Kister [7] type equation. The ternary excess molar volumes $\boldsymbol{V^E}$ and viscosity deviation $\boldsymbol{\Delta\eta}$ were correlated by a Redlich-Kister [7] type equation and Nagata and Tamura [8] type equation using least squares in order to obtain their respective dependency on concentration. The parameters calculated with the Redlich-Kister equation [7] for the binary systems [DIPE (2) + 1-propanol (3)] and [chloroform (1) + 1-propanol (3)], reported in previous works [5,6], were used in the terms for the binary contribution of Nagata and Tamura [8] type equation. Also, the ternary excess molar volume and viscosity deviation $Y^E_{123}$ were predicted using the Radojković [9] equation. In all cases Origin Pro 8.5 was used.

We found papers on density [10] and two on viscosity [10,11] data of the binary system [chloroform 1) + 1-propanol ((3)] and experimental values of these reagents. To our knowledge no data density and viscosity, or excess molar volume values and viscosity deviation of [chloroform (1) + di-isopropyl ether (DIPE) (2) + 1-propanol (3)] ternary system have been published.

## 2. Procedure

### 2.1. Reagents

Chloroform (p.a.) and 1-propanol (p.a.) were supplied by Dorwill, while DIPE (p.a.) was supplied by MERK (Germany). The purity of the reagents used was controlled by chromatography and IR spectroscopy which guarantees its purity, and the instruments used are certified by the manufacturer and monitored regularly, each time a series of measurements starts.The purity of the reagents, determined by gas chromatography was 99.8%.

### 2.2. Measurements

Liquid mixtures were prepared by mass in airtight-stoppered bottles. The same techniques described in previous publication [12] were used for the preparation of samples. The same instruments described in previous publications [13] were used. Density and viscosity were simultaneously measured with an Anton Paar Stabinger viscometer (SVM 30 0 0/G2). Total uncertainties in this work are $\pm 0.0\ 0\ 01$ mPa.s of for viscosity value, $\pm 0.1$ kg/m$^3$ for density, and $\pm 0.01$ K for temperature. The uncertainty in the mole fractions for these mixtures is estimated to be around than $\pm 1 \times 10^{-4}$.

Ternary mixtures were prepared from binary mixtures of constant molar fraction ratio $\boldsymbol{\gamma_k = x_{1k}/\ x_{2k}}$ and adding known volumes of the third component. Each set of ternary mixtures with a constant molar fraction ratio $\boldsymbol{\gamma_k = x_{1k}/\ x_{2k}}$ is called series and k the number of serie. In this case, the starting binary system was [chloroform (1) + DIPE (2)].

At least three measurements were made for each solution or pure component.

### 2.3. Excess molar volumes and viscosity deviation

The excess molar volume $V^E$ and viscosity deviation $\Delta\eta$ for the binary and ternary systems were calculated from the following equations:

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

$$\Delta\eta = \eta - \left(\sum_{i=1}^{n} \eta_i x_i\right) \tag{2}$$

Where n is the number of components, $x_i$ the mole fraction of component i in the mixture, $M_i$ its molecular weight, $\rho$, $\eta$, are the density and viscosity of the mixture and $\eta_i$, $\rho_i$ are the measured densities and viscosities of the pure component, respectively.

Excess molar volume $V^E$ and viscosity deviation $\Delta\eta$ of the binary systems were fitted using the Redlich-Kister [7] polynomial equation of the type:

$$Y_{ij} = x_i x_j \sum_{p=0}^{k} a_p (1 - 2x_i)^p \tag{3}$$

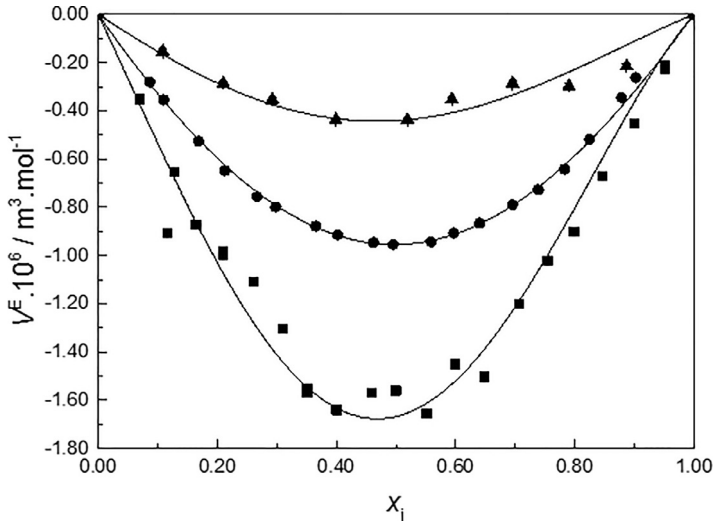


**Fig. 1.** Experimental values of $V^E$ against $x_i$ $(i=1,2)$ for binary systems:(■): [chloroform (1) + dipe (2)]; (•):[chloroform (1) + 1-propanol (3)] and (▲) :[dipe (2) + 1-propanol (3)] at (298.15 ± 0.01) K.

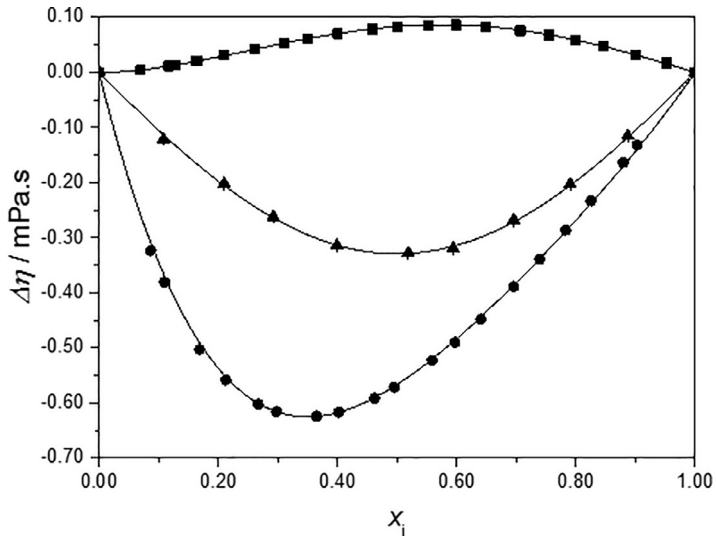


**Fig. 2.** Experimental values of $\Delta\eta$ against $x_i$ $(i=1,2)$ for binary systems:[(■): chloroform (1) + *dipe* (2)]; (•): [chloroform (1) + 1-propanol (3)] and (▲) :[dipe (2) + 1-propanol (3)] at (298.15 ± 0.01) K.

$Y_{ij}$ is the excess property of the *ij* binary system and $a_p$ are adjustable parameters. These equations were fitted using least squares [14] with all points equally weighed. The appropriate number of constants and significant digits are obtained by comparison with the experimental errors mentioned above.

A series of equations was proposed that adjust the excess properties and the deviations of the ideality of the ternary systems. Some of these equations adjust the excess properties from those of the binary systems [15–17]. There are several articles in the literature [17–20] that use these proposals. Also in some ternary systems the applicability of associated solution models was evaluated [21].

In this paper, the ternary excess molar volumes and viscosity deviation $Y^E_{123}$ were predicted using the Radjković equation [9]:

$$Y^E_{123} = Y^E_{12} + Y^E_{13} + Y^E_{23} \tag{4}$$

Where $Y^E_{12}, Y^E_{13}, Y^E_{23}$ are the excess molar volume or viscosity deviation for the three binary systems.

Also, the ternary excess molar volumes $V^E$ and viscosity deviation $\Delta\eta$ were correlated by Nagata and Tamura equation type [8]:

$$Y^E_{123} = Y^E_{12} + Y^E_{13} + Y^E_{23} + x_1x_2x_3 \times R \times T \times \left(B_0 - B_1x_1 - B_2x_3 - B_3x_1^2 - B_4x_2^2 - B_5x_1x_2 - B_6x_1^3 - B_7x_2^3 - B_8x_1^2x_2\right) \tag{5}$$

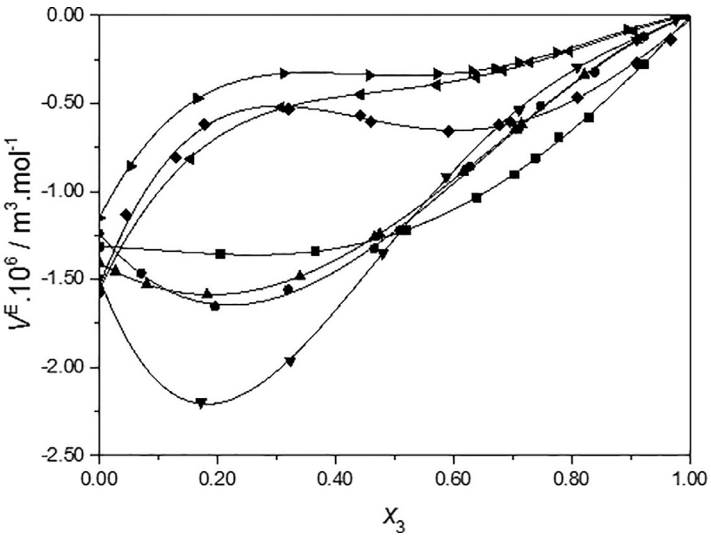


**Fig. 3.** Experimental values of $V^E$ against $X_3$ for series ■ : $S_1$ , ● : $S_2$ , ▲: $S_3$ , ▼: $S_4$ , ♦ : $S_5$ , ◄ : $S_6$ and ► : $S_7$ at (298.15 ± 0.01) K.

**Table 1**
Densities and viscosities of the pure components at (298.15 ± 0.01) K.

| Reagent | $\rho$ / kg.m$^{-3}$ | | $\eta$ / mPa.s | |
|---|---|---|---|---|
| | Experimental | Literature | Experimental | Literature |
| Chloroform | 1478.4 | 1478.82 [11] | 0.5357 | 0.556 [11] |
| | | 1479.70 [22] | | 0.5357 [22] |
| | | 1478.8 [13] | | 0.556 [13] |
| Dipe | 718.2 | 718.54 [22] | 0.3791 | 0.379 [22] |
| 1-propanol | 799.8 | 786.30 [11] | 1.8343 | 1.8468 [11] |
| | | 799.60 [23] | | 1.9430 [23] |

Experimental uncertainties u: u(T) = 0.01 K, u($\rho$) = 0.1 kg•m$^{-3}$, u($\eta$) = 0.0001 mPa.s.

and the Redlich-Kister equation type [7]:

$$Y^E_{123} = Y^E_{12} + Y^E_{13} + Y^E_{23} + x_1x_2x_3.[B_0 + B_1.(x_1 - x_2) + B_2.(x_2 - x_3) + B_3.(x_1 - x_3) + B_4.(x_1 - x_2)^2 + B_5.(x_2 - x_3)^2 + B_6.(x_1 - x_3)^2 + \cdots] \quad (6)$$

Where $B_n$ are the adjustable parameters obtained from fitting the $V^E$ and $\Delta\eta$ data (calculated from experimental data). In this work a modified version of the Nagata –Tamura equation is proposed.

$$Y^E_{123} = x_1x_2x_3 \times R \times T \times \left(B_0 - B_1x_1 - B_2x_3 - B_3x_1^2 - B_4x_2^2 - B_5x_1x_2 - B_6x_1^3 - B_7x_2^3 - B_8x_1^2x_2\right) \quad (7)$$

In all cases we calculate de standard deviations using the equation:

$$\sigma = \sqrt{\left(\frac{\sum_{i=1}^{N}\left(Y^E_{exp} - Y^E_{calc}\right)^2}{N - p}\right)} \quad (8)$$

Figs. 1 and 2 show excess molar volume and viscosity deviation plotted against the mole fraction of chloroform for the systems: [chloroform (1) + DIPE (2)] and [chloroform (1) + 1-propanol (3)] and against the mole fraction of DIPE for the system [DIPE (2) + 1-propanol (3)] at 298.15 K.

Figs. 3 and 4 show the behavior of the excess molar volume and viscosity deviation plotted against the mole fraction of 1-propanol (3) for the different series studied in this work at 298.15 K.

Figs. 5 and 6 show surface of the excess molar volume and viscosity deviation against molar fractions of DIPE (2) and 1-propanol (3).

Figs. 7 and 8 show contour lines of excess molar volume and viscosity deviation for the [chloroform (1) + DIPE(2) + 1-propanol(3)] at 298.15 K, respectively.

Origin Pro 8.5 was used for all the figures.

**Table 2**
Experimental density $\rho$ and viscosity $\eta$ for the [chloroform (1)+ 1-propanol (3)] binary system at (298.15 ± 0.01) K.

| $x_1$ | $\rho$ / kg/m3 | $\eta$ / mPa.s | $V^E$ $m^3$/mol | $\Delta\eta$ / mPa.s |
|---|---|---|---|---|
| Chloroform (1)+ 1-propanol (3) | | | | |
| 0.0000 | 800.0 | 1.9732 | 0.00 | 0.00 |
| 0.1081 | 883.1 | 1.6982 | $-1.63.10^{-7}$ | −0.095 |
| 0.2102 | 955.0 | 1.4729 | $-2.86.10^{-7}$ | −0.179 |
| 0.2919 | 1010.0 | 1.2968 | $-3.54.10^{-7}$ | −0.241 |
| 0.3989 | 1089.9 | 1.0941 | $-3.92.10^{-7}$ | −0.297 |
| 0.5188 | 1170.1 | 0.9102 | $-4.11.10^{-7}$ | −0.314 |
| 0.5941 | 1220.1 | 0.8129 | $-3.84.10^{-7}$ | −0.308 |
| 0.6958 | 1279.9 | 0.7201 | $-3.35.10^{-7}$ | −0.259 |
| 0.7900 | 1340.0 | 0.6508 | $-2.67.10^{-7}$ | −0.197 |
| 0.8869 | 1403.2 | 0.6019 | $-1.84.10^{-7}$ | −0.112 |
| 1.0000 | 1470.2 | 0.5580 | 0.00 | 0.000 |

Experimental uncertainties u: u(T) = 0.01 K, u($\rho$) = 0.1 kg•$m^{-3}$, u($\eta$) = 0.0001 mPa.s

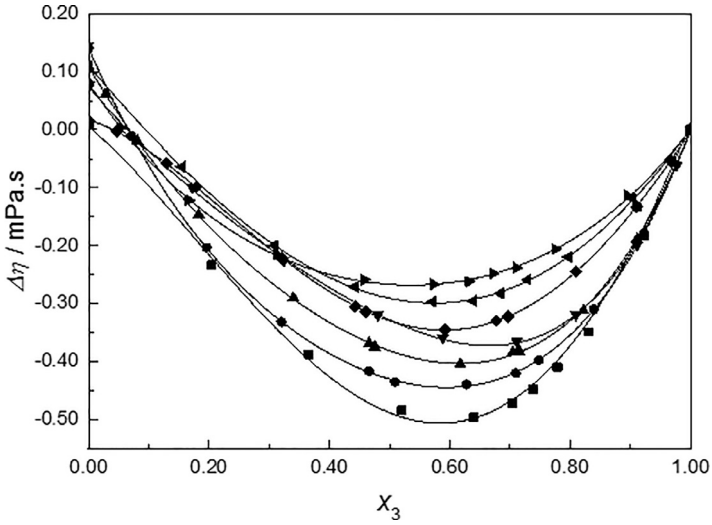


**Fig. 4.** Experimental values of $\Delta\eta$ against $X_3$ for series ■ : $S_1$ , ● : $S_2$ , ▲: $S_3$ , ▼: $S_4$ , ♦ : $S_5$ , ◄ : $S_6$ and ► : $S_7$ at (298.15 ± 0.01) K.

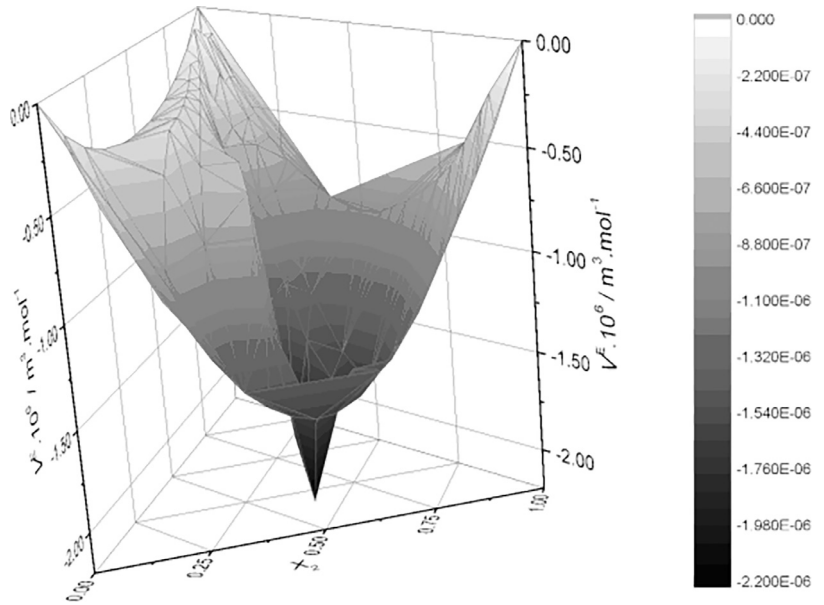


**Fig. 5.** 3D surface of excess molar volume $V^E$ against molar fractions of chloroform ($x_1$) and dipe($x_2$) + 1-propanol ($x_3$)] at (298.15 ± 0.01) K.

**Table 3**
Experimental density $\rho$ and viscosity $\eta$, excess molar volume $V^E$ and viscosity deviation $\Delta\eta$ for the [chloroform 1)+DIPE (2)+1-propanol ((3)] ternary system at (298.15 ± 0.01) K.

| $X_1$ | $X_3$ | $\rho$ / kg/m3 | $\eta$ / mPa.s | $V^E$ m$^3$/mol | $\Delta\eta$ / mPa.s |
|---|---|---|---|---|---|
| $\boldsymbol{\delta_1} = 0.28910$ | | | | | |
| 0.1984 | 0.0000 | 820.1 | 0.4183 | $-1.31.10^{-6}$ | $8.21.10^{-3}$ |
| 0.1577 | 0.2050 | 819.6 | 0.4689 | $-1.35.10^{-6}$ | $-2.33.10^{-1}$ |
| 0.1257 | 0.3664 | 818.8 | 0.5440 | $-1.34.10^{-6}$ | $-3.88.10^{-1}$ |
| 0.0952 | 0.5203 | 817.0 | 0.6666 | $-1.22.10^{-6}$ | $-4.84.10^{-1}$ |
| 0.0714 | 0.6400 | 814.6 | 0.8251 | $-1.03.10^{-6}$ | $-4.96.10^{-1}$ |
| 0.0587 | 0.7039 | 812.9 | 0.9410 | $-9.04.10^{-7}$ | $-4.71.10^{-1}$ |
| 0.0518 | 0.7389 | 811.7 | 1.0150 | $-8.09.10^{-7}$ | $-4.47.10^{-1}$ |
| 0.0439 | 0.7788 | 810.2 | 1.1098 | $-6.94.10^{-7}$ | $-4.09.10^{-1}$ |
| 0.0338 | 0.8294 | 808.5 | 1.2424 | $-5.80.10^{-7}$ | $-3.49.10^{-1}$ |
| 0.0153 | 0.9231 | 804.1 | 1.5410 | $-2.75.10^{-7}$ | $-1.83.10^{-1}$ |
| 0.0000 | 1.0000 | 799.8 | 1.8340 | 0.00 | 0.00 |
| $\boldsymbol{\delta_2} = 0.49047$ | | | | | |
| 0.2957 | 0.0000 | 873.2 | 0.5660 | $-1.24.10^{-6}$ | $1.41.10^{-1}$ |
| 0.2746 | 0.0713 | 872.2 | 0.515 | $-1.46.10^{-6}$ | $-1.08.10^{-2}$ |
| 0.2377 | 0.1959 | 868.7 | 0.4981 | $-1.65.10^{-6}$ | $-2.03.10^{-1}$ |
| 0.2009 | 0.3206 | 862.5 | 0.545 | $-1.56.10^{-6}$ | $-3.32.10^{-1}$ |
| 0.1580 | 0.4657 | 853.3 | 0.665 | $-1.33.10^{-6}$ | $-4.16.10^{-1}$ |
| 0.1451 | 0.5092 | 850.0 | 0.708 | $-1.22.10^{-6}$ | $-4.35.10^{-1}$ |
| 0.1100 | 0.6279 | 839.5 | 0.870 | $-8.58.10^{-7}$ | $-4.39.10^{-1}$ |
| 0.0859 | 0.7096 | 831.9 | 1.005 | $-6.47.10^{-7}$ | $-4.20.10^{-1}$ |
| 0.0746 | 0.7478 | 827.8 | 1.082 | $-5.14.10^{-7}$ | $-3.97.10^{-1}$ |
| 0.0475 | 0.8395 | 818.5 | 1.298 | $-3.22.10^{-7}$ | $-3.10.10^{-1}$ |
| 0.0228 | 0.9227 | 808.9 | 1.547 | $-1.21.10^{-7}$ | $-1.78.10^{-1}$ |
| 0.0000 | 1.0000 | 799.8 | 1.834 | 0.00 | 0.00 |
| $\boldsymbol{\delta_3} = 0.79141$ | | | | | |
| 0.4038 | 0.0000 | 940.6 | 0.552 | $-1.41.10^{-6}$ | $1.10.10^{-1}$ |
| 0.3927 | 0.0276 | 938.7 | 0.541 | $-1.45.10^{-6}$ | $6.03.10^{-2}$ |
| 0.3711 | 0.0811 | 934.9 | 0.535 | $-1.53.10^{-6}$ | $-1.98.10^{-2}$ |
| 0.3300 | 0.1829 | 926.5 | 0.550 | $-1.59.10^{-6}$ | $-1.47.10^{-1}$ |
| 0.2666 | 0.3398 | 910.3 | 0.625 | $-1.48.10^{-6}$ | $-2.90.10^{-1}$ |
| 0.2156 | 0.4662 | 894.4 | 0.723 | $-1.26.10^{-6}$ | $-3.68.10^{-1}$ |
| 0.2119 | 0.4753 | 893.2 | 0.729 | $-1.24.10^{-6}$ | $-3.75.10^{-1}$ |
| 0.1544 | 0.6176 | 872.0 | 0.898 | $-8.91.10^{-7}$ | $-4.04.10^{-1}$ |
| 0.1192 | 0.7049 | 857.2 | 1.040 | $-6.31.10^{-7}$ | $-3.83.10^{-1}$ |
| 0.1150 | 0.7152 | 855.5 | 1.056 | $-6.14.10^{-7}$ | $-3.82.10^{-1}$ |
| 0.0719 | 0.8219 | 836.1 | 1.278 | $-3.49.10^{-7}$ | $-3.08.10^{-1}$ |
| 0.0358 | 0.9113 | 818.3 | 1.522 | $-1.35.10^{-7}$ | $-1.89.10^{-1}$ |
| 0.0000 | 1.0000 | 799.8 | 1.834 | 0.00 | 0.00 |
| $\boldsymbol{\delta_4} = 1.08051$ | | | | | |
| 0.4804 | 0.0000 | 993.0 | 0.528 | $-1.49.10^{-6}$ | $7.37.10^{-2}$ |
| 0.3974 | 0.1728 | 978.1 | 0.593 | $-2.20.10^{-6}$ | $-9.97.10^{-2}$ |
| 0.3247 | 0.3241 | 954.9 | 0.676 | $-1.96.10^{-6}$ | $-2.26.10^{-1}$ |
| 0.2497 | 0.4804 | 924.4 | 0.798 | $-1.35.10^{-6}$ | $-3.20.10^{-1}$ |
| 0.1978 | 0.5884 | 901.1 | 0.907 | $-9.14.10^{-7}$ | $-3.59.10^{-1}$ |
| 0.1387 | 0.7113 | 873.4 | 1.070 | $-5.37.10^{-7}$ | $-3.65.10^{-1}$ |
| 0.0915 | 0.8095 | 849.8 | 1.253 | $-2.92.10^{-7}$ | $-3.19.10^{-1}$ |
| 0.0428 | 0.9109 | 824.3 | 1.512 | $-1.39.10^{-7}$ | $-1.99.10^{-1}$ |
| 0.0113 | 0.9766 | 806.3 | 1.741 | $-2.32.10^{-8}$ | $-6.10.10^{-2}$ |
| 0.0000 | 1.0000 | 799.8 | 1.834 | 0.00 | 0.00 |
| $\boldsymbol{\delta_5} = 1.64289$ | | | | | |
| 0.5844 | 0.0000 | 1071.5 | 0.4870 | $-1.58.10^{-6}$ | $1.64.10^{-2}$ |
| 0.5575 | 0.0461 | 1058.6 | 0.5310 | $-1.13.10^{-6}$ | $-2.41.10^{-3}$ |
| 0.5088 | 0.1294 | 1039.5 | 0.5890 | $-8.06.10^{-7}$ | $-5.80.10^{-2}$ |
| 0.4799 | 0.1788 | 1027.8 | 0.6160 | $-6.17.10^{-7}$ | $-9.83.10^{-2}$ |
| 0.3969 | 0.3208 | 997.1 | 0.6860 | $-5.31.10^{-7}$ | $-2.21.10^{-1}$ |
| 0.3259 | 0.4423 | 969.7 | 0.7688 | $-5.69.10^{-7}$ | $-3.05.10^{-1}$ |
| 0.3153 | 0.4604 | 965.7 | 0.7849 | $-6.02.10^{-7}$ | $-3.14.10^{-1}$ |
| 0.2382 | 0.5923 | 933.0 | 0.9333 | $-6.58.10^{-7}$ | $-3.45.10^{-1}$ |
| 0.1887 | 0.6771 | 909.5 | 1.0651 | $-6.22.10^{-7}$ | $-3.29.10^{-1}$ |
| 0.1776 | 0.6962 | 903.9 | 1.0980 | $-6.03.10^{-7}$ | $-3.22.10^{-1}$ |
| 0.1113 | 0.8095 | 868.7 | 1.3298 | $-4.67.10^{-7}$ | $-2.45.10^{-1}$ |
| 0.0522 | 0.9106 | 833.9 | 1.5790 | $-2.71.10^{-7}$ | $-1.33.10^{-1}$ |
| 0.0189 | 0.9677 | 812.8 | 1.7361 | $-1.38.10^{-7}$ | $-5.39.10^{-2}$ |
| 0.0000 | 1.0000 | 799.8 | 1.8340 | 0.00 | 0.00 |

(*continued on next page*)

**Table 3** (*continued*)

| $X_1$ | $X_3$ | $\rho$ / kg/m3 | $\eta$ / mPa.s | $V^E$ m$^3$/mol | $\Delta\eta$ / mPa.s |
|---|---|---|---|---|---|
| $\delta_6 = 2.82580$ | | | | | |
| 0.7075 | 0.0000 | 1176.6 | 0.600 | $-1.56.10^{-6}$ | $1.10.10^{-1}$ |
| 0.5982 | 0.1545 | 1123.9 | 0.634 | $-8.15.10^{-7}$ | $-6.40.10^{-2}$ |
| 0.4896 | 0.3080 | 1073.5 | 0.704 | $-5.21.10^{-7}$ | $-2.00.10^{-1}$ |
| 0.3949 | 0.4418 | 1028.6 | 0.813 | $-4.50.10^{-7}$ | $-2.71.10^{-1}$ |
| 0.3033 | 0.5713 | 982.2 | 0.961 | $-3.95.10^{-7}$ | $-2.97.10^{-1}$ |
| 0.2557 | 0.6386 | 956.6 | 1.053 | $-3.52.10^{-7}$ | $-2.95.10^{-1}$ |
| 0.2237 | 0.6839 | 938.7 | 1.127 | $-3.10.10^{-7}$ | $-2.82.10^{-1}$ |
| 0.1916 | 0.7292 | 920.3 | 1.211 | $-2.66.10^{-7}$ | $-2.59.10^{-1}$ |
| 0.1439 | 0.7965 | 892.1 | 1.341 | $-2.04.10^{-7}$ | $-2.20.10^{-1}$ |
| 0.0676 | 0.9045 | 844.4 | 1.587 | $-8.78.10^{-8}$ | $-1.19.10^{-1}$ |
| 0.0000 | 1.0000 | 799.8 | 1.834 | 0.00 | 0.00 |
| $\delta_7 = 4.47134$ | | | | | |
| 0.7928 | 0.0000 | 1254.2 | 0.585 | $-1.15.10^{-6}$ | $8.19.10^{-2}$ |
| 0.7509 | 0.0529 | 1231.3 | 0.583 | $-8.57.10^{-7}$ | $9.36.10^{-3}$ |
| 0.6610 | 0.1662 | 1184.3 | 0.613 | $-4.71.10^{-7}$ | $-1.11.10^{-1}$ |
| 0.5456 | 0.3118 | 1125.8 | 0.703 | $-3.29.10^{-7}$ | $-2.15.10^{-1}$ |
| 0.4298 | 0.4579 | 1065.5 | 0.850 | $-3.39.10^{-7}$ | $-2.63.10^{-1}$ |
| 0.3385 | 0.5731 | 1015.0 | 0.999 | $-3.31.10^{-7}$ | $-2.67.10^{-1}$ |
| 0.2921 | 0.6316 | 988.2 | 1.082 | $-3.16.10^{-7}$ | $-2.62.10^{-1}$ |
| 0.2605 | 0.6715 | 969.5 | 1.149 | $-3.02.10^{-7}$ | $-2.48.10^{-1}$ |
| 0.2293 | 0.7108 | 950.5 | 1.216 | $-2.67.10^{-7}$ | $-2.33.10^{-1}$ |
| 0.1782 | 0.7753 | 918.6 | 1.331 | $-2.10.10^{-7}$ | $-2.04.10^{-1}$ |
| 0.0830 | 0.8954 | 856.4 | 1.581 | $-7.92.10^{-8}$ | $-1.14.10^{-1}$ |
| 0.0000 | 1.0000 | 799.8 | 1.834 | 0.00 | 0.00 |

Experimental uncertainties u: u(T) = 0.01 K, u($\rho$) = 0.1 kg.m$^{-3}$, u($\eta$) = 0.0001 mPa.s.

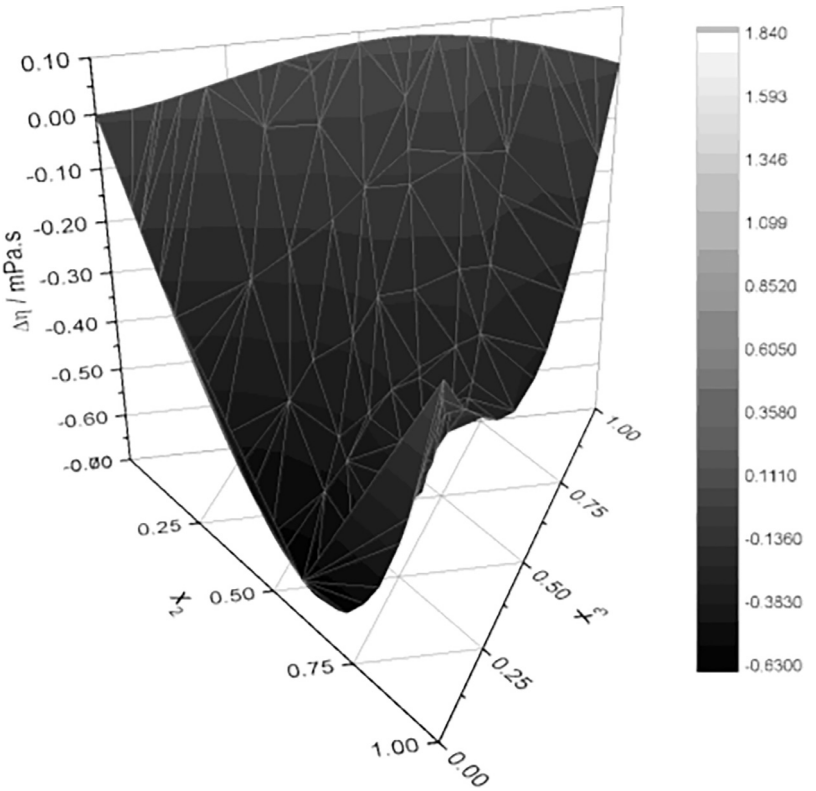


**Fig. 6.** 3D surface of viscosity deviation $\Delta\eta$ against molar fractions of chloroform ($x_1$) and dipe( $x_2$) + 1-propanol ($x_3$)] at (298.15 ± 0.01) K.

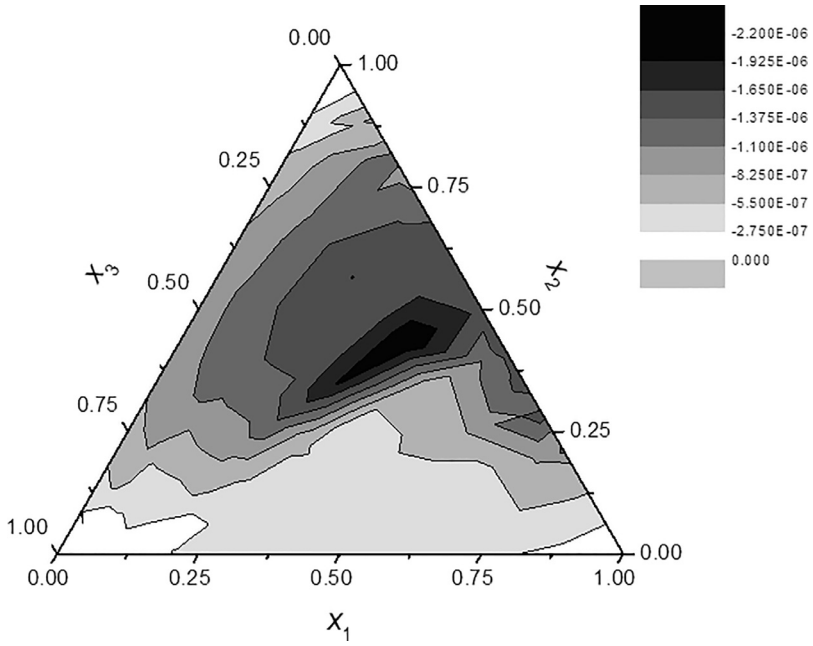


**Fig. 7.** Contourn lines of excess molar volume $V^E$ for the [chloroform (1) + dipe(2) + 1-propanol (3)] ternary system at (298.15 ± 0.01) K.

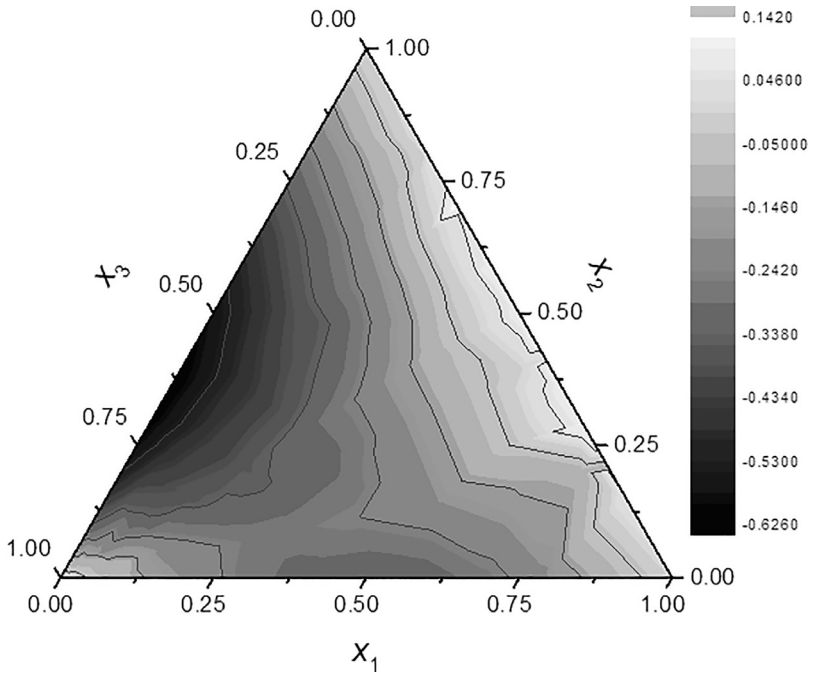


**Fig. 8.** Contourn lines of viscosity deviation $\Delta\eta$ for the [chloroform (1) + dipe(2) + 1-propanol system (3)] ternary system at (298.15 ± 0.01) K.

## 3. Data, value and validation

In Table 1 the measured and literature values of density $\rho$ and viscosity $\eta$ of the reagents at (298.15 ± 0.01) K were reported.

Scarce data on density or viscosity was found in the literature for the 1-propanol at the temperature of 298.15 K, thus, the data provided in this work is a valuable contribution. The values obtained fit well within the experimental uncertainty.

The experimental values of the density $\rho$ and viscosity $\eta$ and the values calculated of the excess molar volume $V^E$ and viscosity deviation $\Delta\eta$ for the [chloroform (1) + 1-propanol(3)] binary system at (298.15 ± 0.01) K are shown in Table 2.

**Table 4**
Parameters $a_p$ of Eq. 3 and the corresponding standard deviation for the [chloroform (1) + 1-propanol (3)] binary system.

| $a_0$ | $a_1$ | $a_2$ | $\sigma$ |
|---|---|---|---|
| Chloroform (1) + 1- propanol (3) | | | |
| $-1.62.10^{-6}$ | $-6.7.10^{-8}$ | $-1.9.10^{-7}$ | $2.10^{-9}m^3.mol^{-1}$ |
| −2.491 | −2.015 | −0.402 | $1.10^{-4}$mPa.s |

**Table 5**
Parameters $B_n$ of Eq. 5 and standard deviations $\sigma_R$, $\sigma_{N\&T}$ and $\sigma_{RCT}$ for Eqs. 4, 5 and 7 for [chloroform (1) + DIPE (2)+ 1-propanol (3)] ternary system at 298.15 K.

| *Parameter* | $V^E$ / $m^3.mol^{-1}$ | $\Delta\eta$ / *mPa.s* |
|---|---|---|
| $B_0$ | $-1.5871.10^{-8}$ | −0.03247 |
| $B_1$ | $-4.39307.10^{-8}$ | −0.1542 |
| $B_2$ | $-1.22859.10^{-7}$ | −0.06278 |
| $B_3$ | $-2.99683.10^{-8}$ | 0.32455 |
| $B_4$ | $3.09256.10^{-7}$ | 0.10224 |
| $B_5$ | $3.66017.10^{-7}$ | 0.10537 |
| $B_6$ | $1.46658.10^{-7}$ | −0.21519 |
| $B_7$ | $-3.14895.10^{-7}$ | −0.08222 |
| $B_8$ | $-6.38317.10^{-7}$ | −0.15915 |
| $\sigma_R$ | $5.10^{-7}$ | $4.10^{-1}$ |
| $\sigma_{N\&T}$ | $6.10^{-7}$ | $7.10^{-1}$ |
| $\sigma_{CT}$ | $8.10^{-7}$ | $5\ 0.10^{-2}$ |

Table 3 shows the experimental values of the density $\rho$ and the viscosity $\eta$, and the calculated values for the excess molar volume $V^E$ and viscosity deviation $\Delta\eta$ for the [chloroform (1) + DIPE (2) + 1-propanol (3)] ternary system at $(298.15 \pm 0.01)$ K.

Experimental determinations were repeated at least three times. Mixtures of any composition are also prepared and their properties are determined experimentally to obtain the total uncertainty of the proposed relationship. Additionally, residual analysis is performed in each case.

Excess thermodynamic functions and deviations of non thermodynamic ones of binary and ternary liquid mixtures are very important for the design of industrial equipment and for the interpretation of the liquid state, particularly when polar components are involved because there exists a possibility of drawing conclusions about the interactions between the components of the mixture.

Numerical values of the coefficients $a_p$ of Eq. 3 obtained from a least squares analysis of the data for the [chloroform (1) + 1-propanol (3)] binary system are listed in Table 4 with standard deviations. The parameters corresponding to the others binary systems have already been published [6,22].

Numerical values of the coefficients Bn of the Eq. 5, obtained from a least squares analysis [14] of the data for ternary systems are listed in Table 5 with standard deviations ($\sigma_{N\&T}$). Table 5 also shows the standard deviation that is obtained by applying Eq. 4 corresponding to the Radojković ($\sigma_R$) equation and modified version of the Nagata –Tamura equation ($\sigma_{CT}$), Eq. (7).

The results of the adjustment with the Redlich-Kister equation are poor for this ternary system and for this reason they were not included in the table.

## 4. Conclusions and discussion

Experimental data of density and viscosity are provided for the [chloroform (1) + 1-propanol (3)] binary system and [chloroform (1) DIPE (2) + 1-propanol (3)] ternary system at $(298.15 \pm 0.01)$ K, and adjustment equations for binary and ternary systems are provided across the range of composition.

The excess molar volume $\boldsymbol{V^E}$ and viscosity deviation $\boldsymbol{\Delta\eta}$ for binary systems correlate well within of the experimental error by a Redlich-Kister (Eq. 3) type equation. The ternary excess molar volumes $V^E$ and viscosity deviation $\Delta\eta$ correlate well within the experimental error by Nagata and Tamura (Eq. 5) type equation and poorly with the one the Redlich-Kister (Eq. 6) type equation. Also, the ternary excess molar volumes and viscosity deviation $Y^E_{123}$ were predicted using the Radojković (Eq. 4) equation.

For this ternary system, the prediction using the Radojković equation has a dispersion of the same order as the experimental error and it is less than that corresponding to those obtained with the correlation equations and with the modified version of the Nagata –Tamura equation (Eq. 7).

In the mixture of [chloroform (1) + DIPE (2)] intermolecular bonds appear and therefore the excess molar volume is negative over the full range of composition and with a minimum near to $x_1 \approx 0.5$. The viscosity deviation is positive over

the range of composition with a maximum nearest 0.5. For [chloroform (1) + 1-propanol (3)] and [DIPE (2) + 1-propanol (3)] systems, solvent effect appears which is responsible to break the self-association of 1-propanol. Both systems have a negative excess molar volume and positive viscosity deviation over the entire composition range (see Fig. 1 and Fig. 2), which corroborates the previous statement.

Figs. 3 and 6 show that the molar excess volume is negative, showing remarkable minimum at low concentrations of chloroform and 1-propanol and high of DIPE. The viscosity deviation is negative throughout the composition range, which would imply that the predominant process in this ternary system is the breakage of the self-associations in the 1-propanol.

Figs. 5 and 6 show the 3D graphs of the excess molar volume and the viscosity deviation for the [chloroform (1) + DIPE (2) + 1-propanol (3)] ternary system at (298.15 ± 0.01) K. Figs. 7 and 8 show the contours of the excess molar volume and viscosity deviation for this ternary system.

## Acknowledgment

Financial support from the Consejo de Investigaciones de la Universidad Nacional de Tucumán, Argentina (CIUNT), Grant 26E/516, is gratefully acknowledged.

## References

[1] R. Battino, Volume changes on mixing for binary mixtures of liquids, Chem. Rev. 71 (1971) 5–45.
[2] J.S. Rowlinson, Liquids and Liquid Mixtures, Butterworths, London, 1969.
[3] I. Prigogine, The Molecular Theory of Solutions, Amsterdam, North Holland, 1957.
[4] M. Rami, S Maken, Excess molar enthalpies and excess molar volumes of formamide + 1-propanol or 2-propanol and thermodynamic modeling by Prigogine-Flory-Patterson theory and Treszczanowicz Benson association model, Thermochim. Acta. 559 (2013) 98–106.
[5] R. Medina Naessens, A.C Gómez Marigliano, Density, viscosity, vapor-liquid equilibrium, excess molar enthalpy and IR spectrocopy of [chloroform + Di - isopropylether (DIPE), J. Phys. Chem.& Bioph. 3 (2015) 1–9.
[6] R. Medina Naessens, Gómez Marigliano, Densidad, viscosidad, volumen molar de exceso, desviación de la viscosidad y calor de mezcla de los sistemas Dipe + (Metanol, o Etanol, o Propanol) a 298.15 K, Investigaciones en Facultades de Ingeniería del NOA 1 (1853-7871) (2013) 1–5. ISSN(2013)http://fce.unse.edu.ar/jcyt/ .
[7] O. Redlich, A.T Kister, Algebraic representation of thermodynamic properties and the classification of solution, Ind. Eng. Chem. 40 (1948) 345–348.
[8] I. Nagata, K. Tamura, Excess molar enthalpies of {methanol or ethanol+(2-butanone+benzene)} at 298.15 K, J. Chem. Termodyn. 22 (1990) 279–283.
[9] N. Radojkovic˘, A. Tasic˘, B. Grozdanic˘, M. Malic˘, Excess volumes of acetone + benzene, acetone + cyclohexane, and acetone + benzene + cyclohexane at 298.15 K, J. Chem. Thermodyn. 9 (1977) 349–356.
[10] U.B. Kadam, A.P. Hiray, A.B. Sawant, M. Hasan, Density, viscosity, and ultrasonic velocity studies of binary mixtures of trichloromethane with methanol, ethanol, propan1-ol, and butan-1-ol al T = (298.15 and 308.25) K, J. Chem. Termodyn. 38 (2016) 1675–1683.
[11] A.M. Crabtree, J.F. OB̆rian, Excess viscosities of binary mixtures of chloroform and alcohols, J. Chem. Eng. Data 36 (1991) 140–142.
[12] R.A. Clará, A.C. Gómez Marigliano, H.N. Sólimo, Density, viscosity, vapour-liquid equilibrium, excess molar volume, viscosity deviation, and their correlations for chloroform + 2-butanone binary system, J. Chem. Eng. Data 51 (2006) 1473–1478.
[13] R.A. Clará, A.C. Gómez Marigliano, D. Morales, H.N. Sólimo, Thermodynamic, transport, and equilibrium properties for [chloroform + methyl tert-butyl ether] binary system and for its pure constituents, J. Chem. Eng. Data. 55 (2010) 5862–5867.
[14] W.H. Press, S;A Teukolsky, W.T. Vetterling, Numerical Recipes in C, 2nd ed., Cambridge University Press, 1992.
[15] F. Kohler, Estimation of the thermodynamic data for a ternary system from the corresponding binary systems, Monatsh. Chem. 91 (1960) 738–740.
[16] R.P. Rastogi, J. Nath, S.S Das, Thermodynamic properties of ternary mixtures. 2. The excess volumes of mixing of ternary mixtures of cyclohexane, aromatics, and halomethanes, J. Chem. Eng. Data. 22 (1977) 249–252.
[17] K.J. Han, I.C. Hwang, S.JU. Park, I.W. Park, Isothermal vapor-liquid equilibrium at 333.15 K. density, and refractive index at 298.15 K for the ternary mixture of di-butyl ether + ethanol + benzene and binary subsystems., J. Chem. Eng. Data. 52 (2007) 1018–1024.
[18] M.Lj. Kijevcanin, P.S. Slodoban, I.R. Radovic´, B.D. Djordjevic´, A.Z. Tasic˘, Volumetric properties of the ternary system ethanol + chloroform + benzene at temperature range (288.15-313.15) K: Experimental data, correlation and prediction by cubic EOS, Fluid Phase Equilibria 251 (2007) 78–92.
[19] P.H. Garcia, M.A Postigo, Volúmenes molares y viscosidad de exceso para sistemas binarios y ternarios formados por 1,4 dioxano, n-butanol y acetato de metilo, Información Tecnológica 8 (1997) 341–346.
[20] T.A. Salman, A.K. Shams, Thermodynamic properties of the binary and ternary systems containing n-formylmorpholine, methanol, benzene and toluene at 298.15 K, J. Al-Nahrain U. 14 (2011) 1–10.
[21] P.P. Singh, R. Malik, S. Maken, W.E. Acree Jr, Thermodynamics properties of ternary non-electrolyte solutions. Part 3. Excess molar volumes of 2-propanone-tribromomethane-alkane mixtures, Faraday Trans. 86 (1990) 2853–2857.
[22] R.N. Medina Naessens, R.A. Clará, A.C. Gómez Marigliano, Density, viscosity, excess molar volume and viscosity deviation for [chloroform (1) + methanol (3)] binary system and [chloroform (1) + di-isopropylether (2) + methanol (3)] ternary system at 298.15 K", Chem. Data Collections. 7-8 (2017) 68–79.
[23] J.A. Riddick, W.B. Bunger, T.K. Sakano, Organic Solvents.Physical Properties and Methods of Purification, 4th ed, John Wiley, New York, 1986.