

# Comparative study of 2-ethylthiophene and 2-ethylfuran

Victor Antón<sup>a</sup>, Beatriz Giner<sup>b</sup>, Héctor Artigas<sup>a</sup>, Ignacio Gascón<sup>a</sup>, Carlos Lafuente<sup>a,\*</sup>

<sup>a</sup>Departamento de Química Física, Facultad de Ciencias, Universidad de Zaragoza,  
50009, Zaragoza, Spain

<sup>b</sup>Facultad de Ciencias de la Salud, Universidad San Jorge, Villanueva de Gállego,  
50830, Zaragoza, Spain

\*Carlos Lafuente. E-mail. celadi@unizar.es Phone: +34 976762295

**ABSTRACT:** In this contribution, we report different thermophysical properties for two derivatives of heterocyclic compounds (2-ethylthiophene and 2-ethylfuran): density, speed of sound, surface tension, kinematic viscosity, and static permittivity at atmospheric pressure ( $p = 0.1$  MPa) from  $T = 278.15$  K to  $338.15$  K. Furthermore, refractive index has been analysed in the temperature range from  $T = 283.15$  K to  $338.15$  K. Additionally, density values have been obtained at pressures up to 65 MPa in the temperature range (283.15 - 338.15) K. Moreover, vapor pressures have been determined. Different derivative properties, such as isobaric expansibility, isentropic and isothermal compressibility, molar refraction, dynamic viscosity, enthalpy and entropy of surface formation per unit surface area, dipolar moment and enthalpy of vaporization have been calculated from experimental results. Finally, these properties have been analysed and compared with previous data published in the literature for the same and related compounds.

**Keywords:** 2-ethylfuran, 2-ethylthiophene, thermophysical properties

## INTRODUCTION

Nowadays, air contamination due to the emission of pollutant gases into the atmosphere, especially  $\text{SO}_x$  produced by combustion for gasoline and other kinds of fossil fuels, is an increasing global concern. In this sense, governments for numerous countries in the world have approved air quality laws to limit or eliminate sulphur emissions<sup>1</sup>. The main source of sulphur air pollution are compounds present in fossil fuels, such as thiophene and its derivatives being with an alkyl chain attached to the thiophene ring, for example 2-ethylthiophene<sup>2</sup>. In order to limit sulphur emissions, different strategies have been proposed to reduce the amount of sulphur present in these fuels. Hydrodesulphurization is the most relevant process to remove sulphur from natural gas and petroleum<sup>3</sup>. Other used methods are: photodegradation<sup>4</sup>, solvent extraction<sup>5</sup>, supercritical reaction<sup>6</sup>, or oxidative processes<sup>5-7</sup>. Also biological methods that make use of microorganisms that need sulphur for living have been investigated<sup>8</sup>. A complete thermophysical characterization of sulphurated compounds in different conditions of pressure and temperature would be very useful for the development of these methodologies and to improve their efficiency.

A different alternative for pollution reduction is the use of less contaminant biofuels obtained from renewable sources such as furan and its derivatives, like 2-ethylfuran. The last one is present in different aliments: coffee, baked products, canned foods, sauces, beverages<sup>9</sup>, or guava juice<sup>10</sup> and it is investigated as a component of the next generation of biofuels because its characteristics are similar to 2-methylfuran and 2,5-dimethylfuran<sup>11</sup>.

Here we present a thermophysical comparative study of 2-ethylthiophene and 2-ethylfuran, this work involves several properties at different temperatures and in the case of densities also at different pressures. The results obtained for both compounds

have been compared with each other and also with other members of their respective families.

A complete bibliographic survey about thermophysical properties of 2-ethylfuran and 2-ethylthiophene published in the scientific literature revealed that densities, refractive indices, dynamic viscosities, surface tensions and vapor pressures have been already reported for 2-ethylthiophene. Levi and Nicholls<sup>12</sup> presented values of density and refractive index at  $T = 293.15$  K. Jeffery et al.<sup>13</sup> reported data of density and surface tension from  $T = 293.15$  K to  $333.15$  K and refractive index at  $T = 293.15$  K. Yur'ev and Khmel'nitskii<sup>14</sup> obtained values of density and refractive index at  $T = 293.15$  K. Xiaoqin et al.<sup>15</sup> published one value of dynamic viscosity at  $T = 293.15$  K. In the contribution of Conary et al.<sup>16</sup>, density at  $T = 293.15$  K was reported. Finally, vapor-liquid equilibrium has been studied in several publications: Levi and Nicholls<sup>12</sup>, Wender et al.<sup>17</sup>, and Wang and Li<sup>18</sup> have reported data of boiling points; while Eon et al.<sup>19</sup> measured vapor pressures from  $T = 333.15$  K to  $373.15$  K. Also, Giles and Wilson<sup>20</sup> reported two values of vapor pressure.

In the case of 2-ethylfuran, previous studies are scarce. Shuikin et al.<sup>21</sup> published values of density and refractive index at  $T = 293.15$  K, and the normal boiling point. On the other hand, Paul<sup>22</sup> gave experimental data at  $T = 286.15$  K of density and refractive index. Levi and Nicholls<sup>12</sup> reported the normal boiling point and values of refractive index and density at  $T = 293.15$  K. Finally, refractive index at  $T = 294.15$  K and boiling point was presented by Scharf and Wolters<sup>23</sup>.

## **MATERIALS AND METHODS**

The chemical structure of the two studied compounds has been represented in Figure 1, while the commercial source, purity, and water content for 2-ethylthiophene

and 2-ethylfuran have been collected in Table 1. The water content of the samples can affect significantly to the obtained results in the analysis of thermophysical properties, consequently, it is very important to quantify it. To carry out this operation, we have used an automatic titrator Crison KF 1S-2B.

All the properties reported in this contribution, except refractive indices and vapor pressures, have been investigated in the range of temperature from  $T = 278.15$  K to  $338.15$  K with intervals of  $2.5$  K and at  $p = 0.1$  MPa. Refractive index at atmospheric pressure and densities at high pressures (up to  $65$  MPa), has been analysed from  $T = 283.15$  K to  $338.15$  K while vapor pressures have been determined between  $T = 285$  K and  $415$  K (depending on the compound studied).

Density,  $\rho$ , and speed of sound,  $u$ , have been determined with an Anton Paar DSA 5000 internally thermostated at  $\pm 0.005$  K. This instrument can measure both properties simultaneously; the work frequency of sound analyser is  $3$  MHz. The apparatus has been calibrated using ultra-pure water and dry air. After proper calibration, the uncertainty of density and speed of sound are  $0.05 \text{ kg}\cdot\text{m}^{-3}$  and  $0.5 \text{ m}\cdot\text{s}^{-1}$  respectively.

An Anton Paar DMA HP cell connected to an Anton Paar DMA 5000 evaluation unit has been employed to study the  $p\rho T$  behavior of the liquids. The temperature is maintained constant at  $\pm 0.01$  K. Furthermore, high pressure values are achieved thanks to a hand pump 750.1100 from Sitec. A pressure transducer US181, from Measuring Specialties is used to determine the pressure, whose uncertainty has been estimated in  $0.005$  MPa. The uncertainty of density measurements is  $0.1 \text{ kg}\cdot\text{m}^{-3}$ . Procedure and calibration details can be found in a previous paper.<sup>24</sup>

A refractometer Abbemat-HP from Dr. Kernchen has been utilised to measure refractive index,  $n_D$ , at  $589.3$  nm, sodium D wavelength. The temperature is maintained

constant at  $\pm 0.01$  K with two Peltier thermostats. The uncertainty for values of refractive index is estimated in  $5 \cdot 10^{-5}$ .

Surface tension,  $\sigma$ , has been analysed using a drop volume tensiometer Lauda TVT-2. The temperature has been maintained within  $\pm 0.01$  K by a Lauda E-200 thermostat. The estimated uncertainty for values of surface tension is  $0.2 \text{ mN} \cdot \text{m}^{-1}$ .

Kinematic viscosities,  $\nu$ , have been determined using an Ubbelohde capillary viscometer and a measuring unit Schott-Geräte AVS-440. The temperature is controlled between  $\pm 0.01$  K with a CT52 Schott-Geräte thermostat. The uncertainty, expressed as percentage of the measured values, is 1 %. Ultra-pure water was used to calibrate the device. Dynamic viscosities,  $\eta = \rho \cdot \nu$ , were obtained from experimental kinematic viscosities and densities. The estimated uncertainty for the last property is 1 %.

Static permittivities,  $\epsilon$ , were determined at the frequency of 2 MHz with an Agilent 4263BA LCR meter bridged to a four terminal Agilent 16452A test fixture. The temperature is maintained constant at  $\pm 0.01$  K, by a CT52 Schott-Geräte thermostat. The uncertainty is estimated to be 1 %.

Vapor pressures,  $p_v$ , have been determined using a dynamic recirculating still from Fischer-Labodest. An Automatic Systems Laboratories F25 thermometer has been used to measure the equilibrium temperature. For the pressure control a Paroscientific Digiquartz 735-215A-102 pressure transducer has been employed. The uncertainty in temperature and pressure is 0.01 K and 0.05 kPa, respectively.

All these devices are previously checked by measuring standard reference fluids.<sup>24</sup>

## RESULTS

Density values as a function of pressure and temperature are collected in Table 2, while experimental values of the thermophysical properties at atmospheric pressure as a function of temperature together with some derivate properties are reported in Table 3. Finally, the experimental vapour pressures as a function of temperature can be found in Table 4. On the other hand, isobaric expansibilities,  $\alpha_p$ , and isothermal compressibilities,  $\kappa_T$ , as a function of pressure and temperature calculated from  $p\rho T$  data have been included in Tables S1-S2 of the Supplementary Material.

The three-dimensional  $p\rho T$  correlating model TRIDEN<sup>25</sup> has been used to correlate the experimental values of density with pressure and temperature. This model combines the Tait equation<sup>26</sup>, used for temperature and pressure dependence, and modified Rackett equation<sup>27,28</sup> for liquid saturation densities:

$$\rho_0 = \frac{A_R}{B_R \left[ 1 + (1 - T/C_R)^{D_R} \right]} \quad (1)$$

$$\rho = \frac{\rho_0}{1 - C_T \ln \left( \frac{B_T + p}{B_T + p_0} \right)} \quad (2)$$

$$B_T = b_0 + b_1 \left( \frac{T}{E_T} \right) + b_2 \left( \frac{T}{E_T} \right)^2 + b_3 \left( \frac{T}{E_T} \right)^3 \quad (3)$$

where  $A_R$ ,  $B_R$ ,  $C_R$ , and  $D_R$  are fitting parameters and,  $T$  is absolute temperature, in Rackett equation (equation 1). These four parameters have been correlated with temperature at fixed pressure, in this case at  $p_0 = 0.1$  MPa. Meanwhile, in Tait equation, equations 2-3,  $T$  and  $p$ , are temperature, in Kelvin, and pressure, in MPa. Furthermore,  $b_0$ ,  $b_1$ ,  $b_2$ ,  $b_3$  and  $E_T$  are fitting parameters. In equation 2, the parameter  $C_T$  is

independent of temperature. The relative root mean-square deviations,  $RMSDr$  (%), between experimental and correlated data of densities have been used as statistical values for TRIDEN fits:

$$RMSD_r / \% = 100 \left( \frac{1}{n} \sum_{i=1}^n \left( \frac{\rho_{i,exp} - \rho_{i,corr}}{\rho_{i,exp}} \right)^2 \right)^{1/2} \quad (4)$$

where  $n$  is the number of experimental data. Parameters and deviations for the studied compounds have been grouped in Table 5.

The dependence of density with temperature and pressure can be analysed using isobaric expansibility,  $\alpha_p$  ( $\pm 0.012 \text{ kK}^{-1}$ ), and isothermal compressibility,  $\kappa_T$  ( $\pm 33 \text{ TPa}^{-1}$ ), respectively. These properties are given by the following thermodynamic relations:

$$\alpha_p = \frac{1}{V} \left( \frac{\partial V}{\partial T} \right)_p = -\frac{1}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_p \quad (5)$$

$$\kappa_T = -\frac{1}{V} \left( \frac{\partial V}{\partial p} \right)_T = \frac{1}{\rho} \left( \frac{\partial \rho}{\partial p} \right)_T \quad (6)$$

where temperature and pressure partial derivatives of density needed to calculate these properties have been calculated numerically.

Experimental values of densities at atmospheric pressure and at high pressures as a function of temperature along with calculated isobaric expansibilities, and isothermal compressibilities have been represented in Figures 2 and 3.

The following properties: speed of sound, refractive index, surface tension, and static permittivity had a linear dependence with temperature. The equation used to correlate the experimental data with temperature was:

$$Y = AT + B \quad (7)$$

where  $Y$  is the studied property and  $A$  and  $B$  are the fitting parameters. The best fitting parameters with the corresponding relative root-mean square deviations between experimental and correlated values have been shown in Table 6 and the correlation equations have been plotted together with experimental values in the figures indicated below.

Speeds of sound have been plotted in Figure 4. Isentropic compressibility,  $\kappa_s = 1/(\rho u^2)$  can be calculated, if the ultrasonic absorption is negligible, from experimental density and speed of sound values using Newton-Laplace equation<sup>29</sup>. The values for isentropic compressibility for the studied compounds have been plotted in Figure 5.

In Figures 6 and 7, we have presented experimental values of refractive index and molar refraction, respectively. The last property has been calculated using Lorentz-Lorenz relation, using the empirical data of density and refractive index.

$$R_m = \frac{n_D^2 - 1}{n_D^2 + 2} V_m \quad (8)$$

Surface tension values have been plotted in Figure 8. Two derived properties from surface tension were also obtained in this study: entropy,  $\Delta S_\sigma = -(\partial\sigma/\partial T)_p$ , and enthalpy,  $\Delta H_\sigma = \sigma - T(\partial\sigma/\partial T)_p$ , of surface formation per unit surface area.

The Vogel-Fulcher-Tamman equation<sup>30-32</sup> has been employed to fit the experimental values of dynamic viscosity with temperature:



$$\eta = \eta_0 \cdot \exp[B/(T - T_0)] \quad (9)$$

where  $T_0$ ,  $B$  and  $\eta_0$  are adjustable parameters. These parameters and the relative root-mean square deviations are collected in Table 6. We have represented in Figure 9 experimental data of dynamic viscosity and their correlation for 2-ethylthiophene and 2-ethylfuran.

Static permittivities have been plotted in Figure 10. The dipolar moment for both compounds was estimated with the Onsager equation<sup>33</sup>, using the experimental data of density, refractive index, and static permittivity:

$$\mu^2 = \frac{9\kappa TM}{4\pi N_A \rho} \frac{(\varepsilon - n_D^2)(2\varepsilon + n_D^2)}{\varepsilon(n_D^2 + 2)^2} \quad (10)$$

in the last expression,  $N_A$  is the Avogadro constant,  $M$  is the molecular mass and  $\kappa$  is the Boltzmann constant.

Finally, vapor pressures for 2-ethylfuran and 2-ethylthiophene have been correlated with temperature using Antoine equation.

$$\log p = A - \frac{B}{C + t} \quad (11)$$

being  $A$ ,  $B$ , and  $C$  fitting parameters,  $p$ , vapor pressure in kPa, and  $t$ , temperature in Celsius degrees. These values have been collected in Table 6, along with the corresponding relative root mean square deviations. The graphical representation of experimental results versus temperature was shown in Figure 11. From variation of vapour pressure with temperature, the enthalpy of vaporization can be obtained.

## DISCUSSION

In this section, the properties studied are discussed taking into consideration the structure and intermolecular interactions of the compounds analysed. Moreover, the properties reported have been compared with experimental information published previously in the literature<sup>12-23,34,35</sup>.

Experimental and correlated values of density at atmospheric pressure and high pressure for 2-ethylthiophene and 2-ethylfuran are shown in Figures 2 and 3, respectively. It is possible to see that density decreases when temperature increases at atmospheric pressure for both compounds. Additionally, in all the range of temperatures analysed, density for 2-ethylthiophene is higher than density for 2-ethylfuran. This difference is mainly due to the higher mass of the sulphurated compound compared to the oxygenated compound, since the molar volume of both species is quite similar. When temperature and pressure are considered simultaneously it can be observed that density increases with pressure and decreases with temperature, as it could be expected. Density decreases with temperature because of the thermal expansion and weakening of intermolecular interactions. Comparing with other related compounds, it can be established that, at atmospheric pressure, the sequence for density values in the thiophene family<sup>34</sup> is: thiophene > 2-methylthiophene > 2-ethylthiophene > 2,5-dimethylthiophene. Thiophene does not have any alkyl chain attached to the heterocycle and presents the more compact. When the number of carbon atoms attached to the heterocycle increases, density decreases. Comparing 2-ethylthiophene and 2,5-dimethylthiophene (same number of carbon atoms) it can be deduced that 2,5-dimethylthiophene presents a bigger steric hindrance than 2-ethylthiophene, consequently, density of 2,5-dimethylthiophene is smaller than density of

2-ethylthiophene. In the case of furan family<sup>35</sup>, the sequence is the same: furan > 2-methylfuran > 2-ethylfuran > 2,5-dimethylfuran.

Density data at atmospheric pressure obtained in this contribution for 2-ethylfuran are in good agreement with the value reported by Shuikin et al.<sup>21</sup>, the absolute deviation between both dataset is  $0.0029 \text{ g}\cdot\text{cm}^{-3}$ . Nevertheless, the comparison with the data obtained by Levi and Nicholls<sup>12</sup> presents a deviation of  $0.0074 \text{ g}\cdot\text{cm}^{-3}$ . For 2-ethylthiophene, experimental density at atmospheric pressure is in good agreement with reported values in the literature. The absolute deviation is  $0.0014 \text{ g}\cdot\text{cm}^{-3}$  with the data by Levi and Nicholls<sup>12</sup> and Conary et al.<sup>16</sup>,  $0.0013 \text{ g}\cdot\text{cm}^{-3}$  by Jeffery et al.<sup>13</sup> at  $T = 293.15 \text{ K}$ , and  $0.0006 \text{ g}\cdot\text{cm}^{-3}$  by Yur'ev and Khmel'nitskii<sup>14</sup>.

It is known that the stronger are molecular interactions, the lower is the expansibility of a liquid<sup>36</sup>. The values of isobaric expansibility for 2-ethylfuran are higher than  $\alpha_p$  values for 2-ethylthiophene. This suggests that the interactions between molecules of 2-ethylthiophene are stronger than interactions between 2-ethylfuran molecules. Furthermore, the values for this property increase with temperature and decrease with pressure in both liquids.

The isothermal compressibility follows the same trend than the isobaric expansibility:  $\kappa_T$  values are higher for 2-ethylfuran than for 2-ethylthiophene. This seems to indicate that molecules of 2-ethylthiophene present a more compact packing than molecules of 2-ethylfuran. In this case, isothermal compressibility decreases when pressure increases and temperature decreases.

As it could be expected, speed of sound for both liquids decreases with temperature. In this case, the values for 2-ethylthiophene are higher than the values for 2-ethylfuran. The trend followed by the thiophene family<sup>34</sup> depends on the temperature, except for 2-ethylthiophene. This compound shows always the highest values in all

range of temperatures. At low temperatures, for the rest of liquids, the trend is: thiophene > 2-methylthiophene > 2,5-dimethylthiophene. Against, at high temperatures, the sequence is: 2-methylthiophene  $\approx$  2,5-dimethylthiophene > thiophene. In the case of furan family<sup>35</sup>, the sequence for speed of sound is: 2,5-dimethylfuran  $\geq$  2-ethylfuran > 2-methylfuran > furan.

In the whole temperature range, isentropic compressibility values for 2-ethylthiophene are smaller than for 2-ethylfuran. This is in good agreement with previous observations that suggest a more compact packing for 2-ethylthiophene molecules. Comparing with thiophene and its derivatives<sup>34</sup>, the sequence for this property is: 2,5-dimethylthiophene > 2-ethylthiophene > 2-methylthiophene > thiophene, confirming the previous conclusion obtained in the density study.

Refraction index gives the relation between the speed of light in the vacuum and the speed of light in the medium under study and is a reflect of the molecular packing. The more compact is the molecular packing, the lower is the speed of light in the medium. In consequence, 2-ethylthiophene shows higher values for this property than 2-ethylfuran in all the range of analysed temperatures, probably due the larger polarizability of sulphur atom<sup>37</sup>. Considering the thiophene family<sup>34</sup>, it can be observed that thiophene presents the higher values of this property and 2-ethylthiophene and 2,5-dimethylthiophene the lower values. However, in the case of the furan family<sup>35</sup>, the sequence is: 2,5-dimethylfuran > 2-ethylfuran > 2-methylfuran > furan. This behavior suggests that the polarizability of the derivatives of furan increases when the number of methyl groups attached to the heterocycle increases, and consequently the refractive index values are also bigger for the 2,5-dimethyl and 2-ethyl derivatives.

Furthermore, we have compared our experimental data with those provided in the literature. In the case of 2-ethylfuran, experimental values are in good agreement

with the data reported by Levi and Nicholls<sup>12</sup> and Shuikin et al.<sup>21</sup>, absolute deviation are 0.0022 and 0.0006, respectively. For 2-ethylthiophene, our values are in excellent agreement with the values reported by Levi and Nicholls<sup>12</sup>, Jeffery et al.<sup>13</sup> and Yur'ev and Khmel'nitskii<sup>14</sup>, being the absolute deviations 0.0012, 0.0005 and 0.0010, respectively.

Molar refraction for both compounds decreases linearly with temperature. Moreover, molar refraction for 2-ethylfuran is smaller than for 2-ethylthiophene in the whole temperature range. Molar refraction represents the hard core volume of a mole of molecules<sup>38</sup>. The free molar volume can be calculated easily through the previous property. At  $T = 298.15$  K, 2-ethylthiophene and 2-ethylfuran present the following values for the free volume:  $79.57 \text{ cm}^3 \cdot \text{mol}^{-1}$ , and  $78.9 \text{ cm}^3 \cdot \text{mol}^{-1}$ , respectively.

Surface tension, dynamic viscosity and vapor pressure are directly related with molecular interactions in the liquid phase. As expected, the values of surface tension decrease when the temperature increases for both compounds. Moreover, surface tension is higher for 2-ethylthiophene than for 2-ethylfuran in all the range of temperatures, confirming that 2-ethylthiophene presents stronger interactions than 2-ethylfuran. Due to the linear dependence of the surface tension with temperature for both compounds the corresponding entropies of surface formation per unit surface area were constant in the temperature range considered. On the other hand, the enthalpy of surface formation is also higher for 2-ethylthiophene than for 2-ethylfuran,  $\Delta H_\sigma$  values at  $T = 298.15$  K are  $64.42 \text{ mN} \cdot \text{m}^{-1}$  and  $60.89 \text{ mN} \cdot \text{m}^{-1}$  for 2-ethylthiophene and 2-ethylfuran, respectively. Comparing the values obtained for 2-ethylthiophene with other compounds of the same family<sup>34</sup>, we found the expected sequence: thiophene > 2-methylthiophene > 2-ethylthiophene > 2,5-dimethylthiophene. In the furan family<sup>35</sup>, the sequence is: 2,5-dimethylfuran > 2-ethylfuran > 2-methylfuran > furan. This indicates

that 2,5-dimethylfuran presents the highest cohesive interactions in this family. For 2-ethylthiophene, the absolute deviation is not so good between experimental value and the value reported by Jeffery et al.<sup>13</sup> at  $T = 293.15$  K, being the difference  $0.61 \text{ mN}\cdot\text{m}^{-1}$ .

Similarly to surface tension, dynamic viscosity decreases with temperature because intermolecular forces become weaker when temperature rises and viscosity values are higher for 2-ethylthiophene than for 2-ethylfuran throughout the temperature range. In the furan family<sup>35</sup>, the sequence is the same observed for surface tension, confirming that 2,5-dimethylfuran presents the strongest intermolecular interactions. However, in the thiophene family<sup>34</sup>, it changes: 2,5-dimethylthiophene > 2-ethylthiophene > 2-methylthiophene > thiophene. For this property, we have found only one value for 2-ethylthiophene at  $T = 293.15$  K, reported by Xiaoquin<sup>15</sup>, and the difference between both values is  $0.062 \text{ mPa}\cdot\text{s}$ .

It can be observed that, in all the temperature range, static permittivities are bigger for 2-ethylthiophene than for 2-ethylfuran. While dipole moments calculated are very similar for both compounds, although is slightly higher for 2-ethylfuran; at  $T = 298.15$  K, the dipole moment obtained for 2-ethylthiophene is  $0.72 \text{ D}$ , and  $0.76 \text{ D}$  for 2-ethylfuran.

As it could be expected, at a given temperature, the vapor pressure for 2-ethylfuran is higher than vapor pressure for 2-ethylthiophene, as can be observed in Figure 11. This behavior is in good agreement with previously discussed values of surface tension and dynamic viscosities that reveal strong molecular interactions in 2-ethylthiophene. The trend for thiophene family<sup>34</sup> is: thiophene > 2-methylthiophene > 2-ethylthiophene  $\geq$  2,5-dimethylthiophene. On the other hand, in the furan family<sup>35</sup>, the sequence is the same. The enthalpies of vaporization at  $T = 298.15$  K are  $40.8 \text{ kJ}\cdot\text{mol}^{-1}$  and  $35.4 \text{ kJ}\cdot\text{mol}^{-1}$  for 2-ethylthiophene and 2-ethylfuran, respectively; that is,  $\Delta H_{\text{vap}}$  is

higher for 2-ethylthiophene as it could be expected. In the case of 2-ethylthiophene the normal boiling points that can be found in the literature<sup>12,17,18</sup> ranges from 406.15 K to 407.15 K, our experimental value (410.46 K) is clearly higher, on the other hand our experimental vapour pressures are lower than those of Eon et al.<sup>19</sup> Regarding to 2-ethylfuran our experimental normal boiling point (364.61 K) is close to the values reported by Levi and Nicholls<sup>12</sup> (365.25 K) and Shuikin et al.<sup>21</sup> (364.12 K), but the difference with the value given by Scharf and Wolters<sup>23</sup> (365.63 K) is around 1 K.

## CONCLUSIONS

In this contribution, the thermophysical behavior of two derivatives of heterocyclic compounds with an ethyl group linked to the central ring (2-ethylthiophene and 2-ethylfuran) has been investigated. The following properties have been studied in a wide range of temperatures: refractive index, density, speed of sound, surface tension, kinematic viscosity, static permittivity, and vapor pressure. Furthermore, densities have been obtained at pressures up to 65 MPa and the following derivative properties: isobaric expansibility, isothermal compressibility, molar refraction, isentropic compressibility, entropy and enthalpy of surface formation, and dipole moment, have been obtained from experimental values.

The results obtained have been discussed taking into consideration previously reported data for the same compounds and other structurally similar. A complete revision of the experimental values allow concluding that properties mainly related with molecular structure, like refractive index, density, or compressibility, show that 2-ethylthiophene present a more compact packing than 2-ethylfuran. On the other hand, properties such as dynamic viscosity, surface tension, or vapor pressures are more

related with intermolecular forces and reveal that 2-ethylthiophene also show the strongest cohesive forces.

## **Funding**

PLATON research group acknowledges financial support from Gobierno de Aragón.



## References

- (1) Marcilly, C. Evolution of Refining and Petrochemicals: What is the Place of Zeolites. *Oil Gas Sci. Technol.* **2001**, 56, 499-514.
- (2) Albro, T. G.; Dreifuss, P. A.; Wormsbecher, R. F. Quantitative-Determination of Sulfur-Compounds in FCC Gasolines by AED. A Study of the Effect of Catalyst Type and Catalytic Conditions on Sulfur Distribution. *HRC-J. High Resolut. Chromatogr.* **1993**, 16, 13-17.
- (3) Mohebali, G.; Ball, A. S. Biodesulfurization of Diesel Fuels. Past, Present and Future Perspectives. *Int. Biodeterior. Biodegrad.* **2016**, 110, 163-180.
- (4) Aazam, E.S. Visible Light Photocatalytic Degradation of Thiophene using Ag-TiO<sub>2</sub>/Multi-Walled Carbon Nanotubes Nanocomposite. *Ceram. Int.* **2014**, 40, 6705-6711.
- (5) Zannikos, F.; Lois, E.; Stournas, S. Desulfurization of Petroleum Fractions by Oxidation and Solvent Extraction. *Fuel Process. Technol.* **1995**, 42, 35-45.
- (6) Li, W.; Guo, S. C. The Variation of Sulfur Forms in Supercritical Desulfurization of Coal with Ethanol. *Fuel Sci. Technol. Int.* **1996**, 14, 651-667.
- (7) Bhutto, A.W.; Abro, R.; Gao, S. R.; Abbas, T.; Chen, X.C.; Yu, G. R. Oxidative Desulfurization of Fuel Oils Using Ionic Liquids: A review. *J. Taiwan Inst. Chem. Eng.* **2016**, 62, 84-97.
- (8) Soleimani, M.; Bassi, A.; Margaritis, A. Biodesulfurization of Refractory Organic Sulfur Compounds in Fossil Fuels. *Biotechnol. Adv.* **2007**, 25, 570-596.
- (9) Maga, J. A. Furans in Food. *CRC Crit. Rev. Food Sci. Nutr.* **1979**, 11, 355-400.
- (10) Yen, G. C.; Lin, H. T. Changes in Volatile Flavor Components of Guava Juice with High-Pressure Treatment and Heat Processing and During Storage. *J. Agric. Food. Chem.* **1999**, 47, 2082-2087.

- (11) Smith, A. R.; Meloni, G. Absolute Photoionization Cross Sections of Furanic Fuels: 2-Ethylfuran, 2-Acetylfuran and Furfural. *J. Mass. Spectrom.* **2015**, 50, 1206-1213.
- (12) Levi, L.; Nicholls, R.V.V. Formation of Styrenes. *Ind. Eng. Chem.* **1958**, 50, 1005-1008.
- (13) Jeffery, G. H.; Parker, R.; Vogel, A. I. 113. Physical Properties and Chemical Constitution. Part XXXII. Thiophen Compounds. *J. Chem Soc.* **1961**, 570-575.
- (14) Khmel'nitskii, L. I.; Yur'ev, Y. K. Preparation of Thiophene and its Homologs from Alcohols. *Zhur. Obshchei.* **1953**, 23, 1725-1730.
- (15) Zou, X.; Goupil, J.-M.; Thomas, S. B.; Zhang, F.; Zhu, G.; Valtchev, V.; Mintova, S. Detection of Harmful Gases by Copper-Containing Metal-Organic Framework Films. *J. Phys. Chem. C.* **2012**, 116, 16593-16600.
- (16) Conary, R. E.; Devaney, L. W.; Ruidisch, L. E.; McCleary, R. F.; Kreuz, K. L. Thiophene from Hydrocarbons and Sulfur Dioxide. *Ind. Eng. Chem.* **1950**, 42, 467-471.
- (17) Wender, I.; Greenfield, H.; Orchin, M. Chemistry of the Oxo and Related Reactions. 4. Reductions in the Aromatic Series. *J. Am. Chem. Soc.* **1951**, 73, 2656-2658.
- (18) Wang, X.; Li, Y. H. Isobaric Vapor-Liquid Equilibrium for Binary System of 2-Ethylthiophene plus n-Octane at 101.33 kPa. *Fluid Phase Equilib.* **2014**, 378, 113-117.
- (19) Eon, C.; Pommier, C.; Guiochon, G. Vapor Pressures and Second Virial Coefficients of some 5-Membered Heterocyclic Derivatives. *J. Chem. Eng. Data.* **1971**, 16, 408-410.
- (20) Giles, N. F.; Wilson, G. M. Phase Equilibria on Four Binary Systems: 1,2-Dichloroethane plus trans-1,2-Dichloroethylene, 1-Octene plus 2-Methyl thiophene, 2-

Ethyl thiophene plus 2,2,4-Trimethylpentane, and Cyclopropanecarbonitrile plus Water. *J. Chem. Eng. Data.* **2006**, 51, 1973-1981.

(21) Shuikin, N. I.; Karakhanov, R. A.; Ibrakhimov, I. Conversion of Tetrahydrofuran Homologs on Palladized Carbon. *Bull. Acad. Sci. USSR Div. Chem. Sci.* **1965**, 14, 147-148.

(22) Paul, R. Methods of Preparation of the alpha-Alkylfurans. *Bull. Soc. Chim. Fr.* **1935**, 2, 2227-2234.

(23) Scharf, H. D.; Wolters, E. New Synthesis Principle for Furane Derivatives. 2. Fragmentation and Recyclizing Condensation of 1,3-Dioxolane-4-ylumions. *Chem. Ber. -Recl.* **1978**, 111, 639-660.

(24) Antón, V.; Giner, B.; Artigas, H.; Gascón, I.; Lafuente, C. Thermophysical Study of 2-Acetylthiophene: Experimental and Modelled Results. *Fluid Phase Equilib.* **2017**, 433, 126-134.

(25) Ihmels, E. C.; Gmehling, J. Densities of Toluene, Carbon Dioxide, Carbonyl Sulfide, and Hydrogen Sulfide over a Wide Temperature and Pressure Range in the sub- and supercritical State. *Ind. Eng. Chem. Res.* **2001**, 40, 4470-4477.

(26) Dymond, J. H.; Malhotra, R. The Tait Equation-100 Years on. *Int. J. Thermophys.* **1988**, 9, 941-951.

(27) Rackett, H. G. Equation of State for Saturated Liquids. *J. Chem. Eng. Data.* **1970**, 15, 514-517.

(28) Spencer, C. F.; Danner, R. P. Improved Equation for Prediction of Saturated Liquid Density. *J. Chem. Eng. Data.* **1972**, 17, 236-241.

(29) Douheret, G.; Davis, M. I. Measurement, Analysis, and Utility of Excess Molar  $-(\partial V/\partial p)_S$ . *Chem. Soc. Rev.* **1993**, 22, 43-50.

- (30) Vogel, H. Das temperaturabhängigkeitsgesetz der viskosität von flüssigkeiten. *Z. Phys.* **1921**, 22,645-646.
- (31) Fulcher, G.S. Analysis of Recent Measurements of the Viscosity of Glasses. *J. Am. Ceram. Soc.* **1925**, 8, 339-355.
- (32) Tammann, G.; Hesse, W. Die abhängigkeit der viskosität von der temperatur bie unterkühlten flüssigkeiten. *Z. Anorg. Allg. Chem.* **1926**, 156,254-257.
- (33) Onsager, L. Electric Moments of Molecules in Liquids. *J. Am. Chem. Soc.* **1936**, 58, 1486-1493.
- (34) Antón, V.; Artigas, H.; Lomba, L.; Giner, B.; Lafuente, C. Thermophysical Properties of the Thiophene Family. *J. Therm. Anal. Calorim.* **2016**, 125, 509-518.
- (35) Lomba, L.; Aznar, I.; Gascón, I.; Lafuente, C.; Giner, B. Thermophysical Study of the Furan Family. *Thermochim. Acta.* **2015**, 617, 54-64.
- (36) Davila, M. J.; Alcalde, R.; Atilhan, M.; Aparicio, S. PrhoT Measurements and Derived Properties of Liquid 1-Alkanols. *J. Chem. Thermodyn.* **2012**, 47, 241-259.
- (37) Holland, R. S.; Smyth, C. P. Microwave Adsorption and Molecular Structure in Liquids. 10. The Relaxation Times of Nine Heterocyclic Molecules. *J. Phys. Chem.* 1955, 59, 1088-1092.
- (38) Brocos, P.; Piñeiro, A.; Bravo, R.; Amigo, A. Refractive Indices, Molar Volumes and Molar Refractions of Binary Liquid Mixtures: Concepts and Correlations. *Phys. Chem. Chem. Phys.* **2003**, 5, 550-557.

**Table 1.** Sample Table

Chemical Name	Formula	CAS Number	Source	Mass Fraction Purity	Method	Water content / ppm	Method
2-Ethylthiophene	C <sub>4</sub> H <sub>8</sub> S	87255-9	Alfa Aesar	0.990	GC	451	KF
2-Ethylfuran	C <sub>4</sub> H <sub>8</sub> O	3208-16-0	Sigma-Aldrich	0.995	GC	405	KF

**Table 2.** Experimental Densities,  $\rho$ , as a Function of Temperature,  $T$ , and Pressure,  $p$ .<sup>a</sup>

$T / \text{K}$	$\rho / \text{kg}\cdot\text{m}^{-3}$ at $p / \text{MPa}$															
	0.1	2.0	5.0	7.0	10.0	15.0	20.0	25.0	30.0	35.0	40.0	45.0	50.0	55.0	60.0	65.0
2-Ethylthiophene																
283.15	1003.44	1004.84	1007.00	1008.42	1010.51	1013.90	1017.18	1020.37	1023.45	1026.45	1029.36	1032.20	1034.96	1037.65	1040.28	1042.84
288.15	998.47	999.91	1002.13	1003.59	1005.73	1009.20	1012.57	1015.82	1018.97	1022.04	1025.03	1027.90	1030.72	1033.47	1036.14	1038.73
293.15	993.45	994.92	997.20	998.70	1000.90	1004.46	1007.92	1011.25	1014.49	1017.62	1020.67	1023.61	1026.49	1029.29	1032.01	1034.65
298.15	988.39	989.91	992.26	993.80	996.05	999.70	1003.24	1006.67	1009.97	1013.18	1016.30	1019.31	1022.24	1025.10	1027.87	1030.59
303.15	983.42	984.97	987.39	988.98	991.30	995.04	998.67	1002.17	1005.54	1008.81	1012.00	1015.07	1018.07	1020.99	1023.81	1026.56
308.15	978.38	979.99	982.48	984.11	986.49	990.33	994.05	997.63	1001.09	1004.45	1007.68	1010.84	1013.88	1016.86	1019.74	1022.56
313.15	973.34	975.00	977.54	979.22	981.68	985.61	989.42	993.09	996.63	1000.06	1003.38	1006.60	1009.71	1012.75	1015.69	1018.54
318.15	968.32	970.02	972.64	974.36	976.86	980.93	984.83	988.58	992.22	995.71	999.11	1002.39	1005.57	1008.66	1011.66	1014.56
323.15	963.21	964.97	967.69	969.44	972.03	976.20	980.22	984.06	987.78	991.35	994.81	998.17	1001.41	1004.56	1007.62	1010.59
328.15	958.12	959.94	962.71	964.53	967.18	971.45	975.56	979.50	983.31	986.98	990.51	993.94	997.24	1000.47	1003.58	1006.60
333.15	952.99	954.85	957.72	959.58	962.31	966.72	970.93	974.97	978.86	982.61	986.22	989.73	993.09	996.39	999.56	1002.62
338.15	947.86	949.78	952.72	954.65	957.46	961.97	966.32	970.44	974.41	978.26	981.96	985.53	988.98	992.31	995.56	998.71
2-Ethylfuran																
283.15	915.50	917.27	919.69	921.41	923.87	927.84	931.59	935.19	938.66	942.04	945.33	948.50	951.53	954.61	957.60	960.38
288.15	910.08	911.89	914.37	916.19	918.68	922.70	926.63	930.32	933.89	937.37	940.66	943.92	947.13	950.18	953.28	956.10
293.15	904.65	906.44	909.05	910.93	913.50	917.66	921.69	925.54	929.07	932.70	936.06	939.48	942.66	945.78	948.91	951.86
298.15	899.11	901.01	903.73	905.65	908.34	912.57	916.67	920.61	924.30	928.03	931.52	934.92	938.29	941.41	944.69	947.70
303.15	893.58	895.61	898.41	900.35	903.06	907.56	911.72	915.80	919.58	923.37	927.00	930.47	933.84	937.10	940.35	943.48
308.15	888.06	890.15	893.04	895.02	897.93	902.45	906.80	910.98	914.84	918.68	922.47	925.95	929.45	932.76	936.18	939.24
313.15	882.49	884.62	887.63	889.75	892.61	897.40	901.80	906.18	910.18	914.06	917.85	921.58	925.04	928.50	931.93	935.06
318.15	876.88	879.13	882.20	884.37	887.44	892.29	896.91	901.27	905.42	909.50	913.40	917.10	920.67	924.18	927.71	930.91
323.15	871.23	873.56	876.77	878.96	882.17	887.15	891.93	896.47	900.65	904.80	908.80	912.67	916.35	919.97	923.48	926.81
328.15	865.59	867.92	871.27	873.57	876.84	882.03	886.97	891.57	895.96	900.23	904.35	908.24	912.04	915.63	919.32	922.64
333.15	859.90	862.30	865.81	868.20	871.58	876.87	881.93	886.74	891.26	895.59	899.79	903.78	907.66	911.34	915.07	918.60
338.15	854.07	856.63	860.21	862.69	866.19	871.73	876.98	881.86	886.43	890.92	895.20	899.36	903.34	907.07	910.92	914.41

<sup>a</sup>Standard uncertainties  $u$  are  $u(T) = 0.01 \text{ K}$ ,  $u(p) = 0.005 \text{ MPa}$ , and the combined expanded uncertainties  $U_c$  are  $U_c(\rho) = 0.1 \text{ kg}\cdot\text{m}^{-3}$  with 0.95 level of confidence ( $k=2$ ).

**Table 3.** Experimental and Calculated Physicochemical Properties at  $p = 0.1$  MPa as a Function of Temperature.<sup>a</sup>

$T / \text{K}$	$\rho / \text{kg}\cdot\text{m}^{-3}$	$u / \text{m}\cdot\text{s}^{-1}$	$\kappa_{\text{S}} / \text{TPa}^{-1}$	$n_{\text{D}}$	$R_{\text{m}} / \text{cm}^3\cdot\text{mol}^{-1}$	$\sigma / \text{mN}\cdot\text{m}^{-1}$	$\nu / \text{mm}^2\cdot\text{s}^{-1}$	$\eta / \text{mPa}\cdot\text{s}$	$\varepsilon$
2-Ethylthiophene									
278.15	1008.35	1373.23	525.90			32.36	0.9347	0.9425	2.968
280.65	1005.86	1363.39	534.84			32.11	0.9050	0.9103	2.959
283.15	1003.37	1354.15	543.51	1.518405	33.7154	31.80	0.8766	0.8796	2.946
285.65	1000.87	1344.69	552.56	1.516990	33.6388	31.55	0.8498	0.8505	2.936
288.15	998.38	1334.12	562.75	1.515570	33.5619	31.24	0.8244	0.8231	2.929
290.65	995.88	1324.95	572.00	1.514170	33.4859	30.98	0.8003	0.7970	2.916
293.15	993.38	1315.31	581.88	1.512720	33.4071	30.66	0.7772	0.7721	2.911
295.65	990.88	1305.79	591.88	1.511250	33.3272	30.44	0.7554	0.7485	2.900
298.15	988.37	1295.82	602.55	1.509810	33.2487	30.10	0.7345	0.7260	2.887
300.65	985.87	1285.41	613.90	1.508410	33.1724	29.86	0.7148	0.7047	2.878
303.15	983.36	1276.52	624.07	1.506980	33.0944	29.54	0.6960	0.6844	2.871
305.65	980.85	1266.68	635.43	1.505560	33.0168	29.30	0.6780	0.6650	2.858
308.15	978.33	1256.84	647.07	1.504130	32.9386	28.96	0.6606	0.6463	2.848
310.65	975.82	1246.47	659.58	1.502690	32.8598	28.73	0.6442	0.6286	2.838
313.15	973.30	1237.68	670.72	1.501250	32.7808	28.41	0.6282	0.6114	2.833
315.65	970.77	1227.74	683.39	1.499810	32.7018	28.16	0.6130	0.5951	2.820
318.15	968.24	1218.03	696.14	1.498360	32.6221	27.84	0.5981	0.5791	2.810
320.65	965.71	1208.32	709.23	1.496950	32.5446	27.54	0.5840	0.5640	2.799
323.15	963.18	1197.98	723.43	1.495500	32.4647	27.27	0.5702	0.5492	2.792
325.65	960.64	1188.26	737.25	1.494050	32.3848	26.93	0.5566	0.5347	2.782
328.15	958.10	1179.09	750.75	1.492610	32.3053	26.69	0.5437	0.5209	2.775
330.65	955.55	1168.66	766.25	1.491160	32.2252	26.36	0.5313	0.5077	2.766
333.15	953.00	1159.13	780.98	1.489730	32.1461	26.03	0.5190	0.4946	2.753
335.65	950.44	1149.87	795.75	1.488270	32.0653	25.74	0.5072	0.4821	2.745
338.15	947.89	1140.32	811.32	1.486840	31.9860	25.45	0.4965	0.4706	2.734

**Table 3.** Continuation.

$T / \text{K}$	$\rho / \text{kg}\cdot\text{m}^{-3}$	$u / \text{m}\cdot\text{s}^{-1}$	$\kappa_{\text{S}} / \text{TPa}^{-1}$	$n_{\text{D}}$	$R_{\text{m}} / \text{cm}^3\cdot\text{mol}^{-1}$	$\sigma / \text{mN}\cdot\text{m}^{-1}$	$\nu / \text{mm}^2\cdot\text{s}^{-1}$	$\eta / \text{mPa}\cdot\text{s}$	$\varepsilon$
2-Ethylfuran									
278.15	920.97	1281.05	661.64			27.22	0.6870	0.6327	2.837
280.65	918.26	1270.84	674.30			26.91	0.6671	0.6126	2.823
283.15	915.55	1259.43	688.61	1.445331	25.3568	26.59	0.6481	0.5934	2.813
285.65	912.83	1248.72	702.56	1.443898	25.2868	26.31	0.6280	0.5733	2.798
288.15	910.10	1238.51	716.33	1.442451	25.2159	26.01	0.6109	0.5560	2.784
290.65	907.37	1227.58	731.33	1.441015	25.1455	25.62	0.5945	0.5394	2.766
293.15	904.64	1216.74	746.67	1.439560	25.0741	25.32	0.5764	0.5214	2.756
295.65	901.90	1205.19	763.37	1.438171	25.0059	25.09	0.5612	0.5061	2.739
298.15	899.15	1194.88	778.97	1.436723	24.9347	24.78	0.5468	0.4917	2.725
300.65	896.40	1184.06	795.71	1.435305	24.8649	24.43	0.5326	0.4774	2.709
303.15	893.64	1172.45	814.05	1.433874	24.7944	24.12	0.5189	0.4637	2.699
305.65	890.87	1161.84	831.56	1.432441	24.7237	23.81	0.5051	0.4500	2.682
308.15	888.10	1151.48	849.24	1.431001	24.6526	23.51	0.4923	0.4372	2.668
310.65	885.31	1140.56	868.30	1.429579	24.5823	23.22	0.4810	0.4258	2.657
313.15	882.52	1129.20	888.65	1.428144	24.5113	22.91	0.4701	0.4149	2.643
315.65	879.73	1118.12	909.23	1.426712	24.4404	22.66	0.4603	0.4049	2.626
318.15	876.92	1107.36	929.96	1.425280	24.3694	22.30	0.4518	0.3962	2.611
320.65	874.11	1096.53	951.47	1.423850	24.2984	22.07	0.4445	0.3885	2.601
323.15	871.29	1085.58	973.90	1.422415	24.2271	21.77	0.4354	0.3794	2.583
325.65	868.46	1074.76	996.85	1.420974	24.1554	21.40	0.4267	0.3706	2.573
328.15	865.62	1063.82	1020.79	1.419534	24.0837	21.08	0.4181	0.3619	2.559
330.65	862.76	1053.69	1043.96	1.418099	24.0121	20.87	0.4098	0.3536	2.544
333.15	859.90	1042.15	1070.76	1.416687	23.9417	20.50	0.4018	0.3455	2.527
335.65	857.02	1032.11	1095.36	1.415231	23.8689	20.28	0.3935	0.3372	2.516
338.15	854.13	1020.45	1124.33	1.413795	23.7971	19.95	0.3864	0.3300	2.503

<sup>a</sup>Standard uncertainties  $u$  are  $u(T) = 0.005$  K for densities and speeds of sound and  $u(T) = 0.01$  K for the rest of properties,  $u(p) = 0.003$  MPa, and the combined expanded uncertainties  $U_c$  are  $U_c(\rho) = 0.05$   $\text{kg}\cdot\text{m}^{-3}$ ,  $U_c(u) = 0.5$   $\text{m}\cdot\text{s}^{-1}$ ,  $U_c(n_{\text{D}}) = 5\cdot 10^{-5}$ ,  $U_c(\sigma) = 0.2$   $\text{mN}\cdot\text{m}^{-1}$ ,  $U_c(\varepsilon) = 1$  %,  $U_c(\nu) = 1\%$ ,  $U_c(\eta) = 1\%$  with 0.95 level of confidence ( $k=2$ )



**Table 4.** Experimental Vapor Pressures as a Function of Temperature.<sup>a</sup>

2-Ethylthiophene				2-Ethylfuran			
<i>T</i> / K	<i>p<sub>v</sub></i> / kPa	<i>T</i> / K	<i>p<sub>v</sub></i> / kPa	<i>T</i> / K	<i>p<sub>v</sub></i> / kPa	<i>T</i> / K	<i>p<sub>v</sub></i> / kPa
292.41	0.800	370.40	30.075	289.96	4.960	334.73	36.940
293.45	0.840	374.16	34.190	292.18	5.570	336.84	39.925
296.81	1.030	379.56	40.885	293.77	6.050	338.83	42.915
298.04	1.145	382.77	45.275	295.94	6.770	340.30	45.250
299.11	1.230	387.16	51.935	297.39	7.290	342.60	49.130
302.95	1.520	390.75	57.930	299.52	8.105	344.85	53.180
308.07	2.005	394.79	65.355	301.86	9.080	347.05	57.395
312.28	2.550	397.67	71.066	304.58	10.350	348.94	61.215
315.55	3.010	401.74	79.785	306.32	11.270	350.71	64.980
321.73	4.095	404.64	86.501	308.82	12.640	352.90	69.885
326.03	5.050	406.64	91.350	312.73	15.060	354.83	74.510
330.78	6.285	409.15	97.800	317.62	18.645	356.80	79.340
336.67	8.170	410.46	101.325	320.45	20.980	358.65	84.170
342.00	10.225			322.48	22.795	360.61	89.595
346.57	12.340			324.89	25.185	361.79	92.935
351.71	15.145			327.06	27.465	362.46	94.875
356.68	18.345			329.80	30.600	363.67	98.450
360.83	21.475			331.39	32.495	364.18	100.075
365.10	24.990			333.19	34.850	364.61	101.325

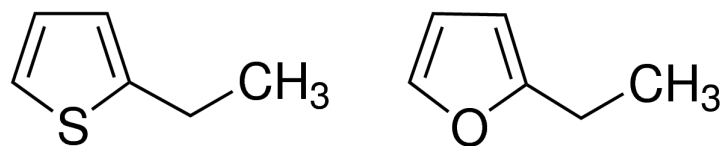
<sup>a</sup> Standard uncertainties *u* are  $u(T) = 0.01$  K,  $u(p_v) = 0.05$  kPa

**Table 5.** Parameters of the TRIDEN Equation and Relative Root Mean Square Deviations, *RMSDr*.

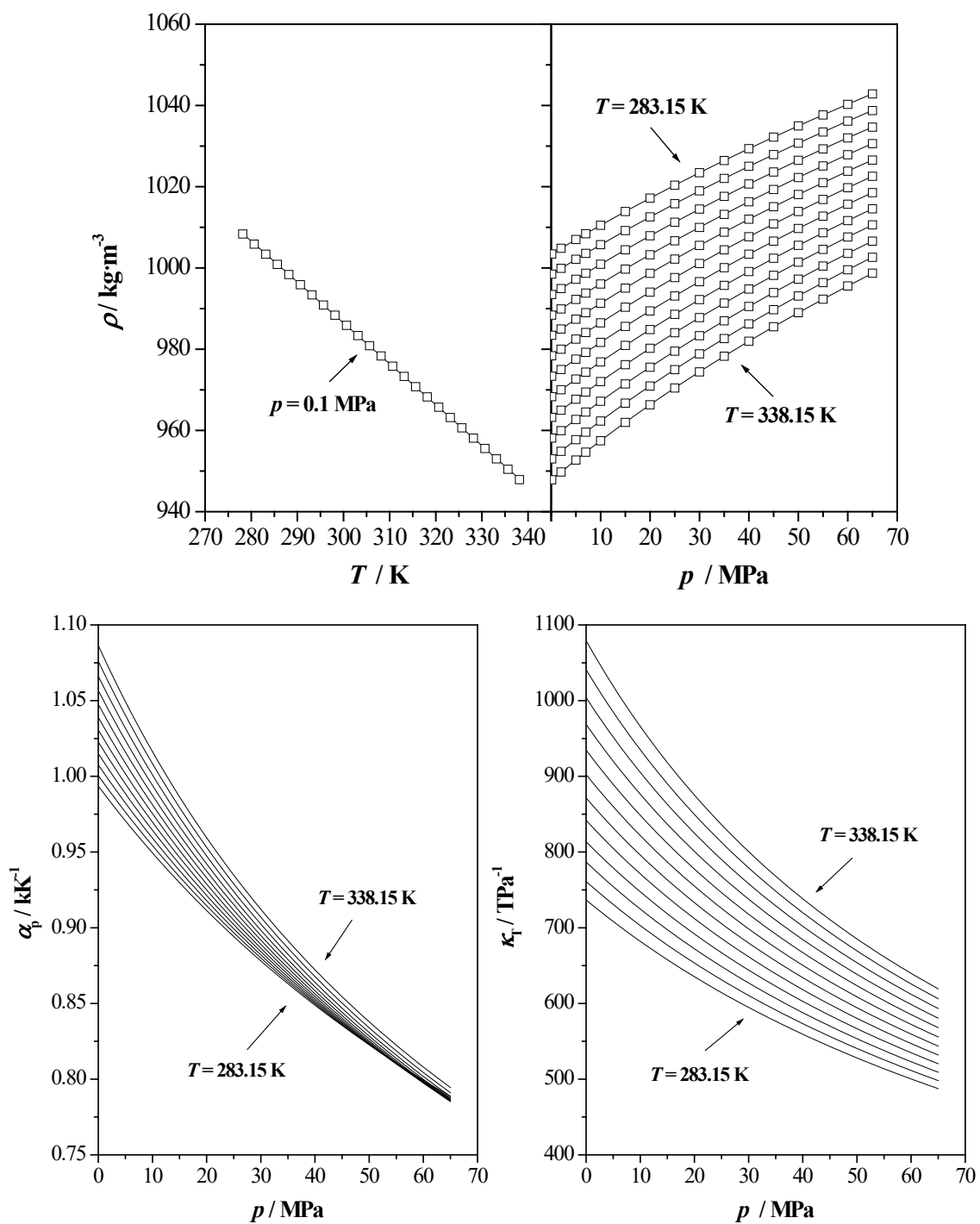
	2-Ethylthiophene	2-Ethylfuran
$A_R / \text{kg}\cdot\text{m}^{-3}$	488.80	422.73
$B_R$	0.6170	0.5901
$C_R / \text{K}$	463.0365	431.1074
$D_R$	0.75602	0.71583
$C_T$	0.08390	0.08694
$b_0 / \text{MPa}$	314.14	311.67
$b_1 / \text{MPa}$	-38.806	-118.348
$b_2 / \text{MPa}$	-42.249	-97.991
$b_3 / \text{MPa}$	8.973	43.305
$E_T / \text{K}$	125.08	222.10
$RMSD_r / \%$	0.00	0.01

**Table 6.** Fitting Parameters and Relative Root Mean Square Deviations, *RMSDr*, for the Studied Properties

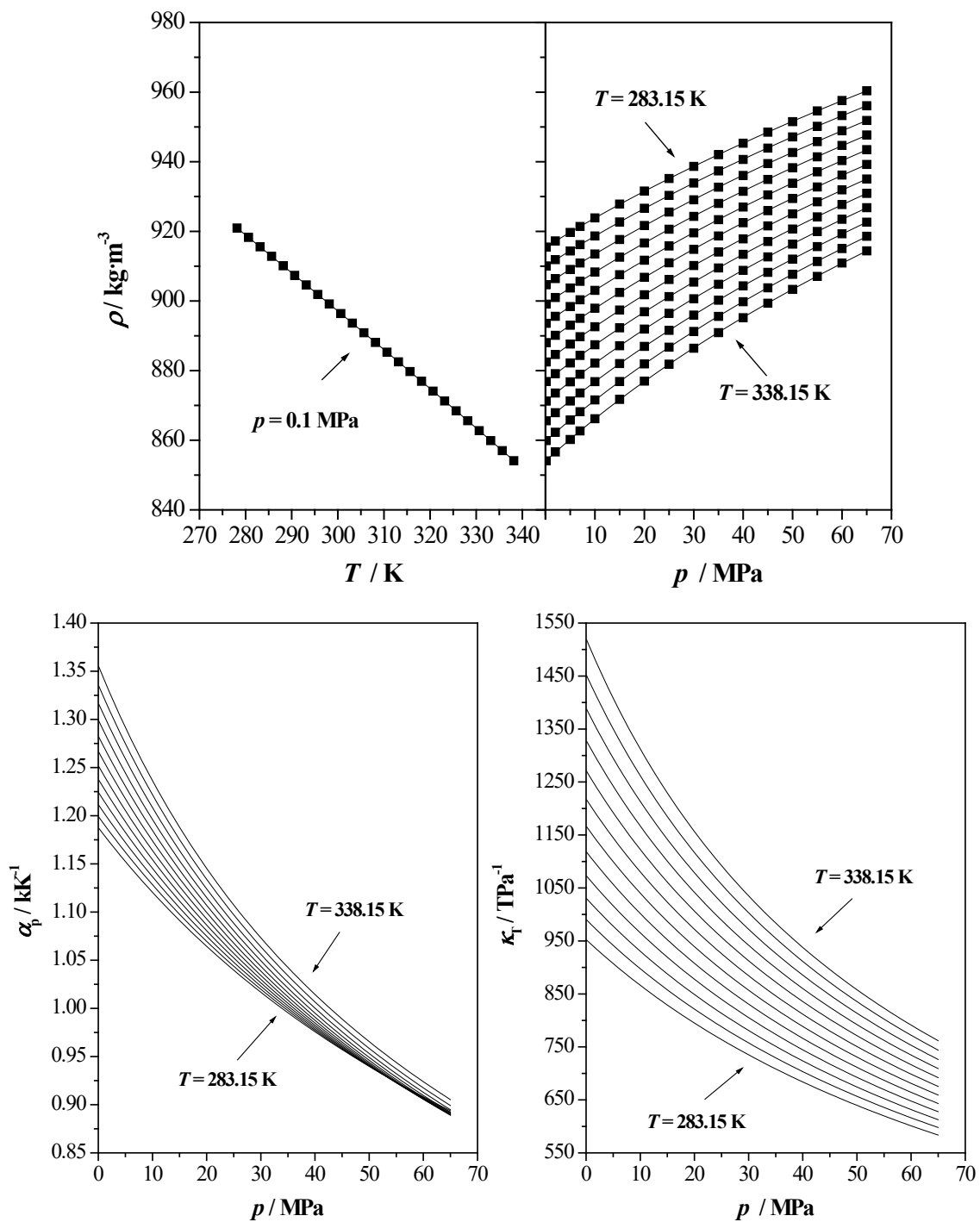
property	equation	compound	<i>A</i>	<i>B</i>	<i>C</i>	<i>RMSDr</i> / %
<i>u</i> / (m·s <sup>-1</sup> )	7	2-Ethylthiophene	-3.8919	2456.02		0.02
		2-Ethylfuran	-4.3491	2491.25		0.03
<i>n<sub>D</sub></i>	7	2-Ethylthiophene	-5.742 · 10 <sup>-4</sup>	1.681028		0.00
		2-Ethylfuran	-5.730 · 10 <sup>-4</sup>	1.607559		0.00
<i>σ'</i> (mN·m <sup>-1</sup> )	7	2-Ethylthiophene	-0.1151	64.42		0.11
		2-Ethylfuran	-0.1211	60.87		0.15
<i>η</i> / (mPa·s)	9	2-Ethylthiophene	0.01433	1269.927	-25.296	0.10
		2-Ethylfuran	0.03745	567.832	77.508	0.23
<i>ε</i>	7	2-Ethylthiophene	-0.00387	4.044		0.06
		2-Ethylfuran	-0.00562	4.400		0.07
<i>p<sub>v</sub></i> / kPa	11	2-Ethylthiophene	5.9346	1330.745	201.397	0.39
		2-Ethylfuran	6.0426	1230.203	213.289	0.09



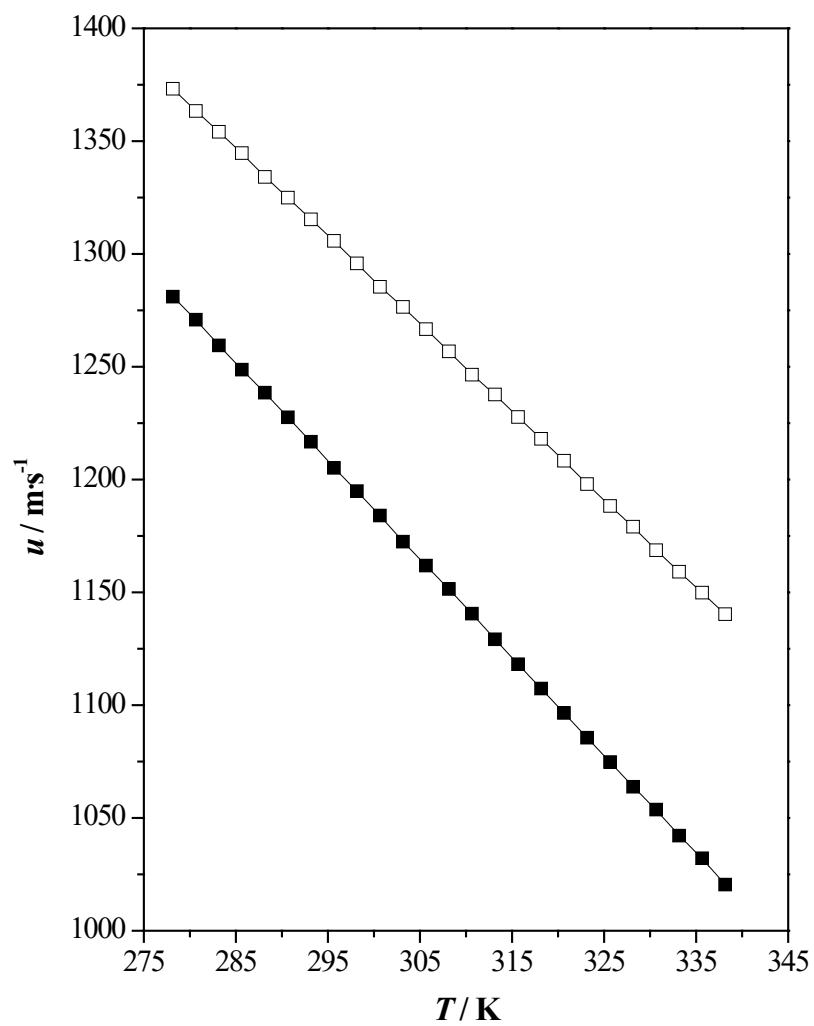
**Figure 1.** Chemical structure for 2-ethylthiophene (left) and 2-ethylfuran (right).



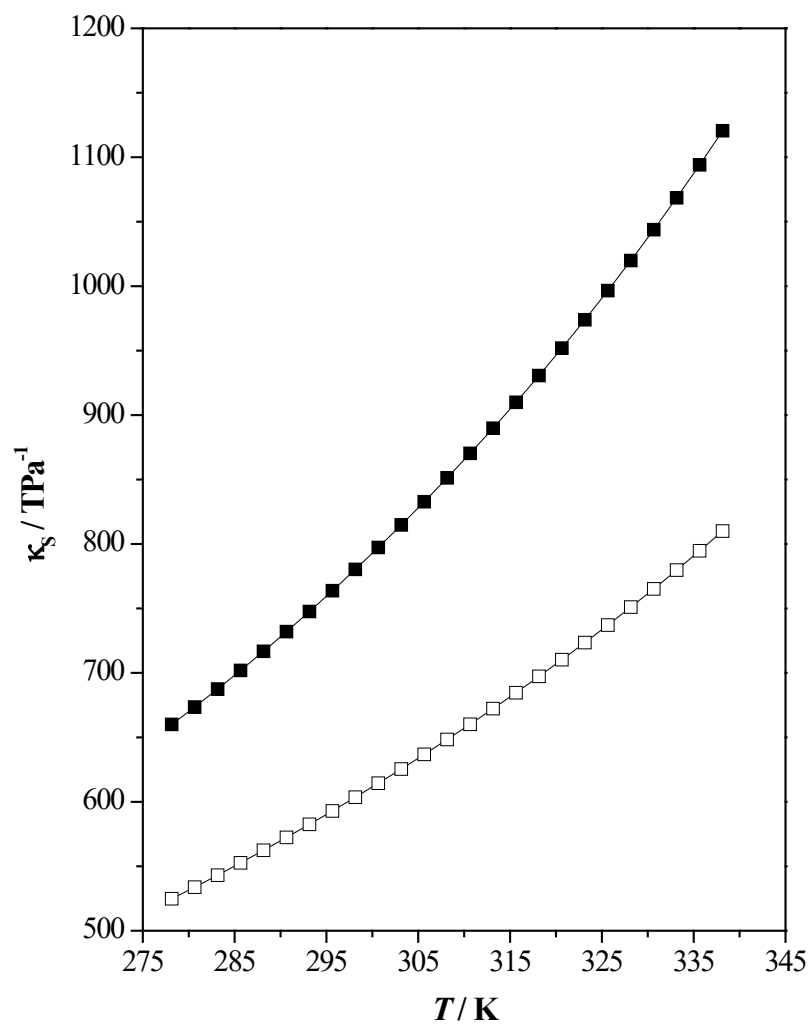
**Figure 2.** Density,  $\rho$ , isobaric expansibility,  $\alpha_p$ , and isothermal compressibility,  $\kappa_T$ , as a function of temperature and pressure for 2-ethylthiophene: ( $\square$ ), experimental densities; (—), values calculated with the TRIDEN equation.



**Figure 3.** Density,  $\rho$ , isobaric expansibility,  $\alpha_p$ , and isothermal compressibility,  $\kappa_T$ , as a function of temperature and pressure for 2-ethylfuran: (●), experimental densities; (—), values calculated with the TRIDEN equation.

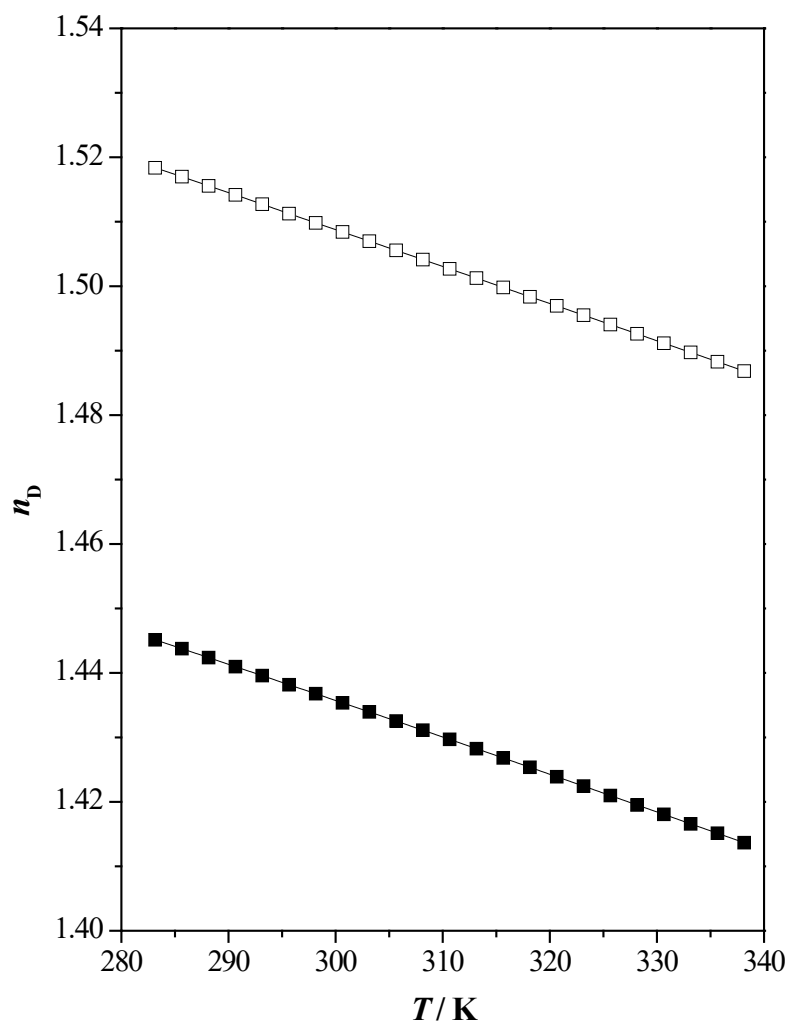


**Figure 4.** Speed of sound,  $u$ , as a function of temperature for the studied compounds:  
( $\square$ ) 2-ethylthiophene, ( $\blacksquare$ ) 2-ethylfuran.



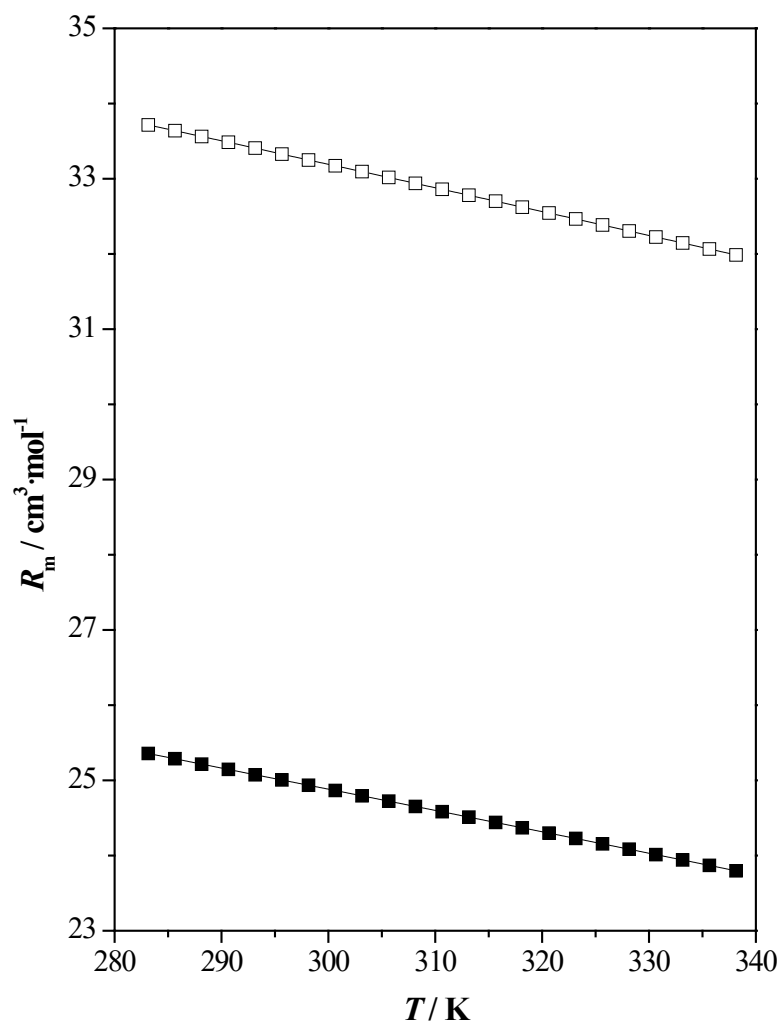
**Figure 5.** Isentropic compressibility,  $\kappa_s$ , as a function of temperature for the studied compounds: (  $\square$  ) 2-ethylthiophene, (  $\blacksquare$  ) 2-ethylfuran.





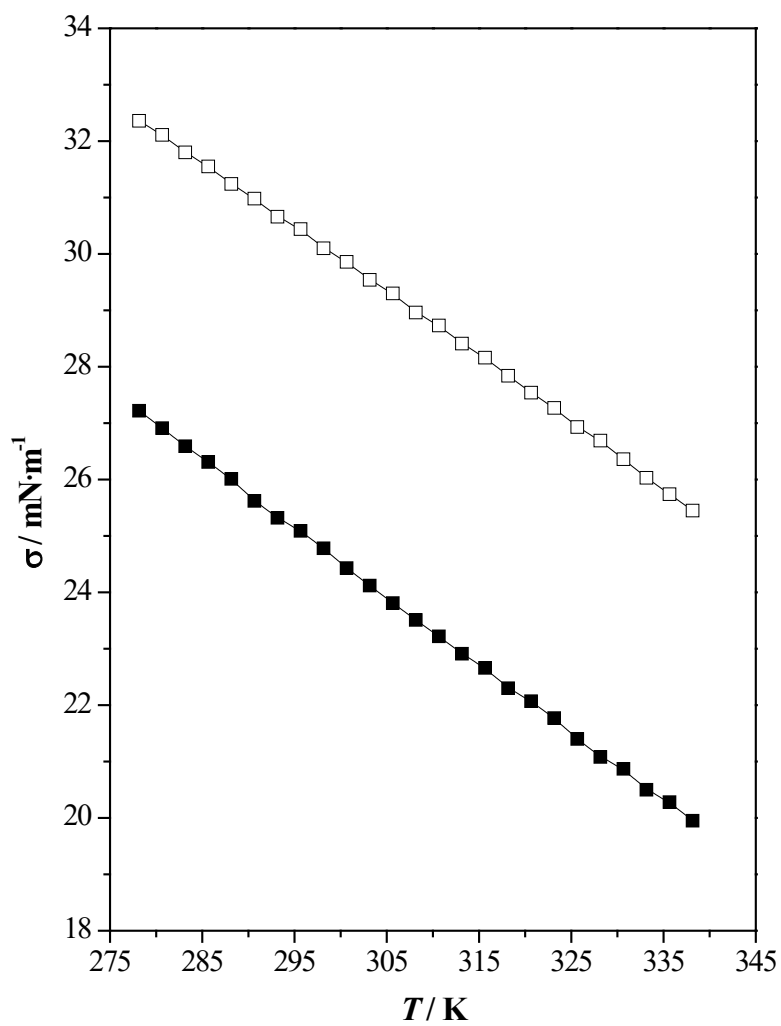
**Figure 6.** Refractive index,  $n_D$ , as a function of temperature for the studied compounds:

( $\square$ ) 2-ethylthiophene, ( $\blacksquare$ ) 2-ethylfuran.



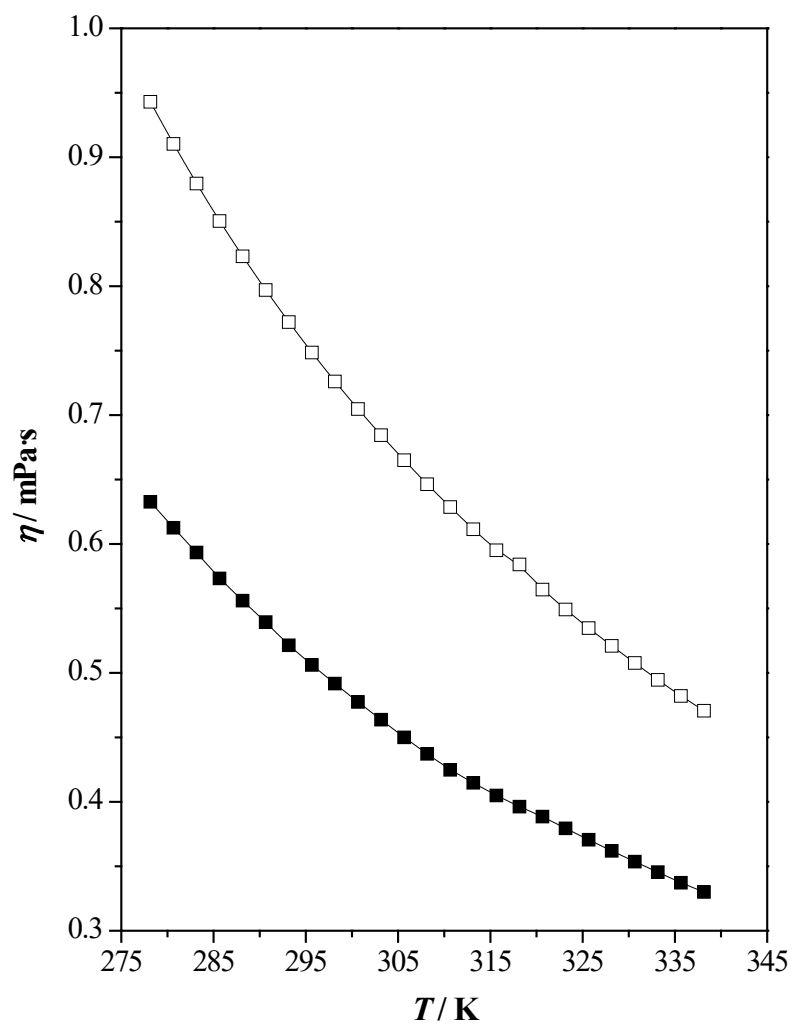
**Figure 7.** Molar refraction,  $R_m$ , as a function of temperature for the studied compounds:

( $\square$ ) 2-ethylthiophene, ( $\blacksquare$ ) 2-ethylfuran.

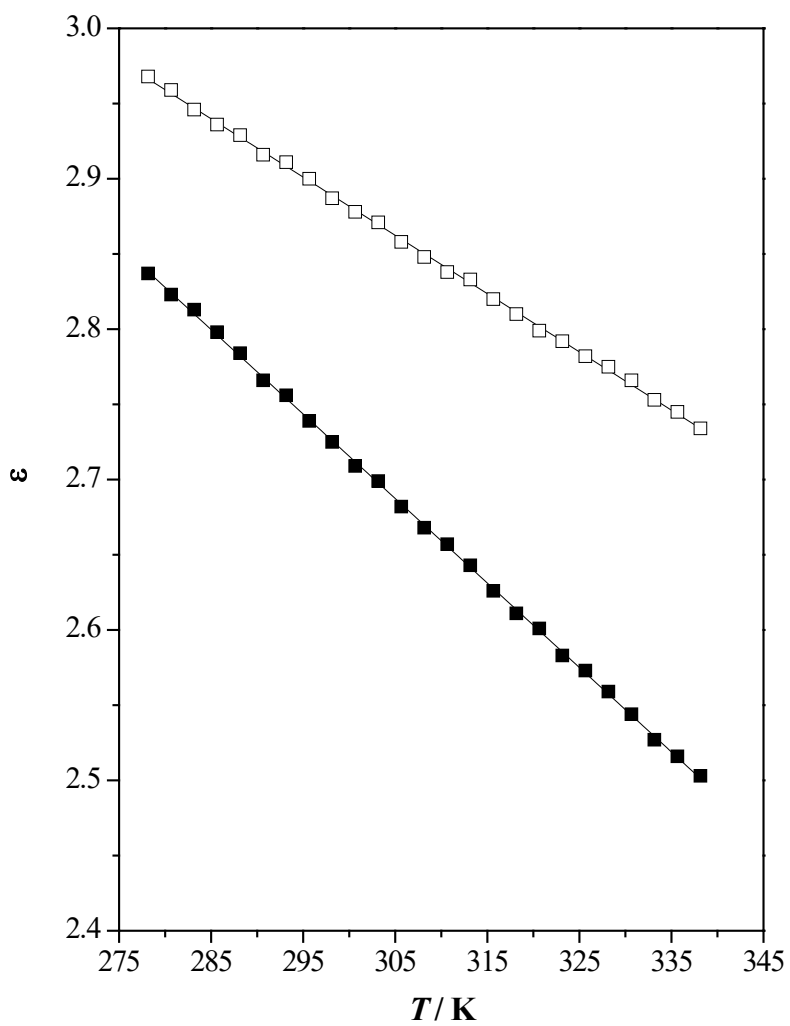


**Figure 8.** Surface tension,  $\sigma$ , as a function of temperature for the studied compounds:

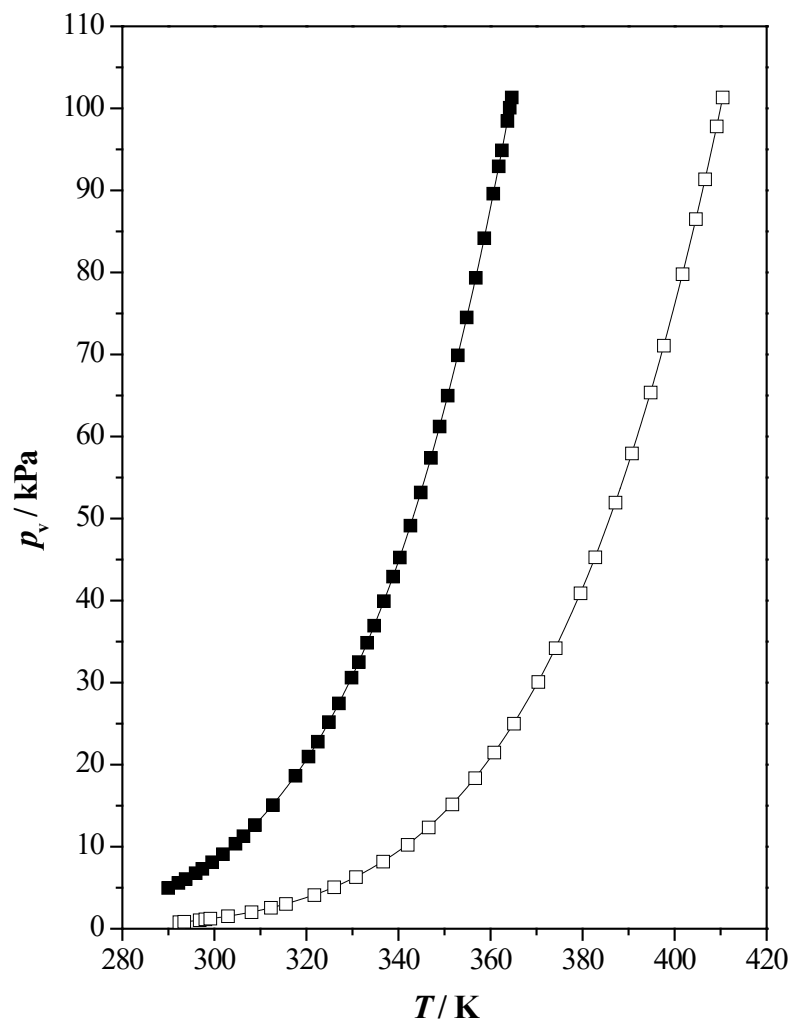
( $\square$ ) 2-ethylthiophene, ( $\blacksquare$ ) 2-ethylfuran.



**Figure 9.** Dynamic viscosity,  $\eta$ , as a function of temperature for the studied compounds: (  $\square$  ) 2-ethylthiophene, (  $\blacksquare$  ) 2-ethylfuran.



**Figure 10.** Static permittivity,  $\epsilon$ , as a function of temperature for the studied compounds: (  $\square$  ) 2-ethylthiophene, (  $\blacksquare$  ) 2-ethylfuran.



**Figure 11.** Vapor pressure,  $p_v$ , as a function of temperature for the studied compounds:  
( $\square$ ) 2-ethylthiophene, ( $\blacksquare$ ) 2-ethylfuran.

# TOC FIGURE

