



Density, Speed of Sound and Derived Properties of Binary Mixtures Propiophenone + Butoxyethanol at T = (303.15, 308.15, 313.15 and 318.15) K

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The current study reports the experimental density (ρ) and sound speed (u) values for binary mixes of liquids propiophenone + 2-butoxyethanol at atmospheric pressure (0.1 MPa) and T = (303.15, 308.15, 313.15 and 318.15) K for the full spectrum of composition. Densities and sound speed measurements from experiments have been used to estimate excess isentropic compressibility (κ_s^E), excess molar volume (V_m^E), excess molar isentropic compressibility ($K_{s,m}^E$), excess isobaric thermal expansivity (α_p^E) and excess sound speed (u^E). The Redlich-Kister polynomials were used to correlate excess parameters. Excess partial molar volume quantities ($\bar{V}_{m,1}^E$ and $\bar{V}_{m,2}^E$) at infinite dilution and their limiting values ($\bar{V}_{m,1}^{0E}$ and $\bar{V}_{m,2}^{0E}$) have been analytically determined using Redlich-Kister polynomials from the experimental density data. The results have been analyzed in light of strength and interactions among molecular entities scope and extent prevalent in these mixtures.

Keywords: Propiophenone, 2-Butoxyethanol, Sound speed, Density, Molar volume.

INTRODUCTION

Thermodynamic functions of solvent mixtures may be useful to researchers and scientists who are interested in assessing, identifying and comprehending the non-ideal behaviour of the mixtures in a variety of contexts [1-3]. The chemical, pharmaceutical, agrochemical and petrochemical sectors have all made extensive use of multicomponent solvents due to their widespread availability. Understanding the thermodynamic properties of liquids and the combinations is imperative for developing, testing and modeling the best possible industrial designs and simulations. The physico-chemical properties depend on the non-ideal solvent mixing characteristics and these are due to interaction between different molecules [4,5].

In light of the increasing necessity to decrease emissions of greenhouse gases and the related issues caused by the depletion of fossil fuels, the development of environmental friendly substitutes for transportation fuels is a significant scientific and engineering challenge. By establishing the chemical foundations of thermodynamics, biotechnology evolves into an inter-

disciplinary study that enables a comprehensive understanding of the diverse elements and attributes of biological systems. Biofuels, derived from vegetable, animal or waste oils as fatty acid methyl esters, provide sustainable and eco-friendly alternatives to traditional fuels for automobiles, reducing their dependence on fossil fuels [6-8].

Measurements of various physico-chemical and derived properties of solutions have proven helpful in understanding the packing effects of solute molecules with solvent molecules and the solute-solvent interaction [9,10]. The V_m^E , κ_s^E , $K_{s,m}^E$, u^E and α_p^E values considered in this work provide information on propiophenone + 2-butoxyethanol mixture interactions between molecules the solvent's and the solute as the mole fraction of propiophenone is increased and the efficiency of packing. The investigations objectives are to characterize the bonds between these molecules in mixtures and investigate the impact of lengthening the chain of alkyl using a common solvent.

Propiophenone is mostly found in milk as well as coffee products and also used as perfumery for its powerful, herbaceous floral effect. It is a valuable compound for synthesizing

drugs that target the nervous system and serves as a stabilizer in paints. A prospective candidate to generate inter- and intramolecules of hydrogen bonds is 2-butoxyethanol, which is a member of the class of cellosolves and compounds with amphiphilicity [11,12]. Its structure consists of partially etheric -O- and alcoholic -OH. The chemical and physical characteristics exhibited by 2-butoxyethanol emerging due to its self-relationship allows it to be positioned between solvents that are both protic and aprotic. Pure 2-butoxyethanol and their aqueous solutions are used to some extent as an aprotic solvent to dissolve electrolytes [13,14] and frequently described as a quasi-protic solvent.

The main thermodynamic characteristics of biofuels are complex and mostly involve volatile mixtures of methyl and ethyl esters of fatty acids, making experimental research on these properties extremely challenging [15,16]. From low-value biomass wastes, volatile organic acids like ethyl butyrate are created. As a result, they are classified as alternative bioenergy fuels. The shorter ignition delay of ethyl butyrate may lead to a decrease in the inlet temperature, making these esters suitable for use as transportation fuels. To be successful, these fuels may need to be mixed with other fuels or used in different combinations to control the engine. Because alkanediols are not the only oxygenated fuels that have been investigated as a replacement for fossil fuels, they are both practical and fundamentally interesting [17]. Alkanediols, for example, can be thought of as model substances with two donor and two acceptor functions. Hydrogen bonds (inter- and intramolecular) have primarily determined the structure and properties of alkanediols. Two terminal primary hydroxyl groups characterize -alkanediols. This work presents the results of an interaction study of binary mixtures of ethyl butyrate with isomeric butanediols. The goal of this study is to provide a framework for predicting the energy exchanges that occur in processes like chemical reactions and for assuring the viability or spontaneity of specific transformations.

As far as we are aware, no volumetric statistics have been reported for the systems that are being examined. This study intends to examine the potential impact of mixing butoxyethanol molecules with propiophenone on the nature and extent of additional thermodynamic properties. The binary mixtures were measured using the sound speed data, 2-butoxyethanol and pure propiophenone densities and the data at different temperatures. The change of these properties with composition reveals the ways in which the molecules interact in the quality and extent of component molecules.

EXPERIMENTAL

Standard techniques [18,19] were employed to purify the 2-butoxyethanol (Sigma Aldrich, CAS No. 111-76-2) and propiophenone (Sigma Aldrich, CAS No. 93-55-0) used in this investigation. Prior to use, all compounds were degassed at low pressure and kept over 72 h on 0.4 nm molecular sieves to eliminate any water percentage. To prevent evaporation, the combinations were prepared in bulk and stored in Amber glass bottles with airtight stops. All samples were carefully prepared within 1×10^{-5} g using a digital scale (CPA-225D, Sartorius,

Germany) right before the quantification. The mole fraction's degree of uncertainty was calculated to be contained 1×10^{-4} .

The pure liquids densities and their binary mixtures were determined using a single-capillary pycnometer with a bulb capacity of approximately 10 mL. Utilizing triple-distilled water, the calibration marks on the capillary were determined. The published data were used to determine pure water densities at the desired temperature. The repeatability of the measures of density was within 0.6 kg m^{-3} . The temperature of the mixture was maintained during the measurement procedure in $\pm 0.02 \text{ K}$ accurate electronically controlled thermostatic waterbath (Julabo). The sound speed of binary systems with pure liquids assessed using a 2 MHz Mittal Enterprises, India, single-crystal variable-path multifrequency ultrasonic interferometer model F-81. The sound speeds had a repeatability of $\pm 0.67 \text{ m/s}$. The accuracy of quantification of sound speed and density at various temperatures was established experimentally [9,10,20-29] by comparing the pure liquid experimental results with the corresponding scholarly values. The results are compiled in Table-1.

RESULTS AND DISCUSSION

The formulas that are utilized to compute different parameters are provided elsewhere [30-39]. The experimental density (ρ) and sound speed (u) measurements of the binary mixtures of propiophenone with 2-butoxyethanol at studied temperatures are provided in Table-2 and V_m^E , κ_s^E , $K_{s,m}^E$, u^E and α_p^E values of all the mixtures at various temperatures were also measured.

The magnitude and sign of the excess functions are influenced by various factors, such as the accommodation of different molecules in the interstitial spaces due to variations in free and molar volumes of each component (mostly negative impact), as well as specific interactions like strong dipole-dipole interactions, formation of H-bonds, and charge transfer complexes between the mixture's components. The positive or negative values are a result of the molecules' highly different molecular sizes fitting (favourably or unfavourably) geometrically into each other's geometries. The H-bond cleavage and structural instability between dissimilar components can be blamed for the growth of and values with an increase in temperature. Fig. 1 illustrates visually the fluctuation of V_m^E with mole percentage of propiophenone at various temperatures. The V_m^E values are negative throughout the full range of measured temperatures over the full compositional spectrum. The negative excess values of V_m^E exhibit a decreasing trend with temperature increases from 303.15 K to 318.15 K for the system. The maximum negative value was observed at $x_1 = 0.5448$ at all temperatures studied.

Due to variations in the components' size, shape and nature as well as the unrestricted volumes of the individual molecules, the magnitude and sign of V_m^E fluctuates depending on the structural characteristics of the component. These variations are the result of one component's geometry being fitted into another component's structural geometry. The molar volumes of 2-butoxyethanol ($132.36 \times 10^{-6} \text{ m}^3 \text{ mol}^{-1}$) and propiophenone ($134.34 \times 10^{-6} \text{ m}^3 \text{ mol}^{-1}$) differ significantly at 303.15 K, suggesting that halogenated molecules of hydrocarbons intercalate in the polymeric matrix units of propiophenone and break their

TABLE-1
DENSITY (ρ) AND SOUND SPEED (u) DATA AT DIFFERENT TEMPERATURES

Compounds	Temp. (K)	ρ (kg m^{-3})		u (m s^{-1})		C_p ($\text{J K}^{-1} \text{mol}^{-1}$)
		Present work	Reported value	Present work	Reported value	
Propiophenone	303.15	1003.7	1004.37 [5] 1001.41 [5]	1439.6	1440.0 [5]	246.39
	308.15	1000.8	1008.70 [5] 1000.60 [9] 996.80 [10]	1425.4	1425.0 [5] 1445.0 [9]	247.84
	313.15	997.8		1411.1		249.61
	318.15	994.9		1397.5		251.02
2-Butoxyethanol	303.15	892.8	892.35 [11] 892.03 [13] 892.40 [14]	1289.8	1290.6 [11]	271.82
	308.15	887.9	887.83 [11] 888.91 [13] 888.90 [18] 883.59 [11]	1273.2	1273.5 [11] 1285.0 [13] 1283.0 [19]	273.05
	313.15	883.5	883.40 [13] 883.40 [14]	1257.8	1257.7 [11]	274.32
	318.15	879.0		1241.6		275.6

Common unpredictability, u , are $u(u) = \pm 0.67 \text{ m s}^{-1}$; $u(\rho) = \pm 0.6 \text{ kg m}^{-3}$; $u(T) = \pm 0.02 \text{ K}$

TABLE-2
DENSITY (ρ) AND SOUND SPEED (u) DEPENDING ON THE MOLE FRACTION OF PROPIOPHENONE AT $T = (303.15\text{-}318.15) \text{ K}$

x_1	T = 303.15 K		T = 308.15 K		T = 313.15 K		T = 318.15 K	
	ρ (kg/m^3)	u (m/s)	ρ (kg/m^3)	u (m/s)	ρ (kg/m^3)	u (m/s)	ρ (kg/m^3)	u (m/s)
0.0000	892.8	1289.8	887.9	1273.2	883.5	1257.8	879.0	1241.6
0.0814	902.3	1298.6	897.5	1283.0	893.0	1268.0	888.6	1252.0
0.1663	912.1	1308.9	907.4	1295.5	903.1	1282.0	898.8	1265.9
0.2548	922.2	1321.4	917.8	1309.8	913.5	1297.5	909.4	1281.3
0.3472	932.8	1336.5	928.5	1326.5	924.4	1314.5	920.3	1298.9
0.4438	943.7	1352.4	939.6	1343.7	935.6	1332.5	931.7	1317.5
0.5448	954.9	1369.3	951.0	1361.5	947.2	1350.9	943.5	1336.2
0.6506	966.4	1387.0	962.7	1379.1	959.0	1368.3	955.5	1354.0
0.7614	978.3	1405.5	974.9	1396.7	971.4	1385.0	968.0	1370.6
0.8778	990.7	1423.4	987.5	1412.3	984.2	1399.6	981.0	1385.2
1.0000	1003.7	1439.6	1000.8	1425.4	997.8	1411.1	994.9	1397.5

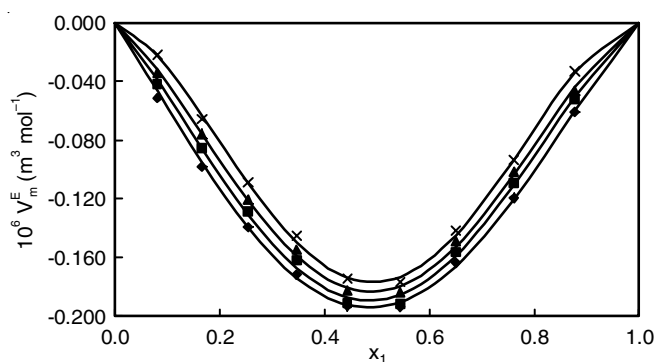


Fig. 1. Plots of excess molar volume, V_m^E against mole percentage, x_1 of propiophenone for propiophenone + 2-butoxyethanol binary mixture at \blacklozenge 303.15 K, \blacksquare 308.15 K, \blacktriangle 313.15 K; \times 318.15 K. Values derived from the Redlich-Kwong equation are represented by lines and experimental values are represented by points

H-bonding. This results in an increase in the total volume of the solution.

The two factors contributing to negative excess volume values may be arising from existence of specific interactions present in the combination of the different component by means

of dipole-dipole and presence of interactions arising in the combination of the solvent and cosolvent molecules *via* complexes of electron donors and acceptors. Fig. 2 displays the system's graphical representations of κ_s^E vs. x_1 for various temperatures.

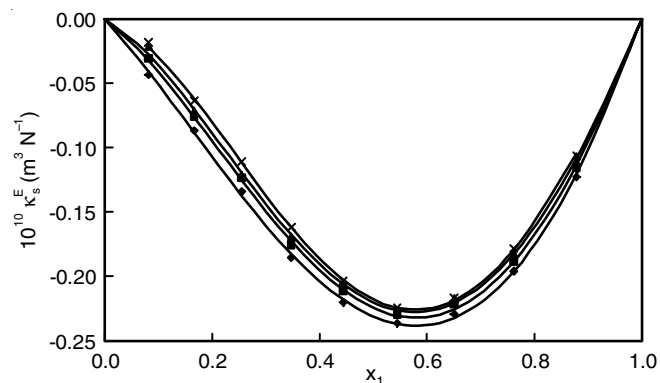


Fig. 2. Excess isentropic compressibilities (κ_s^E) against mole percentage, x_1 of propiophenone for propiophenone + 2-butoxyethanol binary mixture at \blacklozenge 303.15 K, \blacksquare 308.15 K, \blacktriangle 313.15 K; \times 318.15 K. Values derived from the Redlich-Kwong equation are represented by lines and experimental values are represented by points

Over the whole composition, the κ_s^E , it is observed that values are negative. As the temperature rises, the κ_s^E values get more favourable.

The dipole-dipole interactions of pure propiophenone are disrupted when the second component, 2-butoxyethanol, is added to the mixture. Nonetheless, the dipole-dipole interaction between dissimilar molecules arises and plays a significant impact because the second component is polar as well. Given that propiophenone and 2-butoxyethanol are both highly polar components of the current system under examination, the positive variances in κ_s^E values can be explained by two effects: (i) physical force: dispersion brought on by dipole breaking; and (ii) chemical force: complex formations of donors and acceptors, as well as connections between dipoles. The former benefit contributes to improving free-length, which causes the speed of sound to deviate negatively and isentropic compressibility to deviate positively. Conversely, the latter result in a detrimental divergence in isentropic compressibility and an increase in the sound speed. The relative strengths of the two influences determine the actual deviation's sign and magnitude. The negative sign of κ_s^E values for the system points towards the dominance of the latter effect on the former which is further strengthened by the ultrasonic velocity and the density values of the system (Table-3).

According to the results displayed in Fig. 3, for the binary mixture across the whole composition range and at every temperature that was investigated, the $\kappa_{s,m}^E$ values are negative. The existence of specific relationships, like intense interactions between dipole molecules of 2-butoxyethanol and propiophenone, which lessen the mixture's compressibility and result in negative $\kappa_{s,m}^E$ values, is indicated by the noted negative amounts of $\kappa_{s,m}^E$ for binary mixtures. For these combinations, the $\kappa_{s,m}^E$ values increases as the temperature increase. Increasing the temperature ruptures the dipolar interactions between different molecules, leading to the expansion of propiophenone and thus

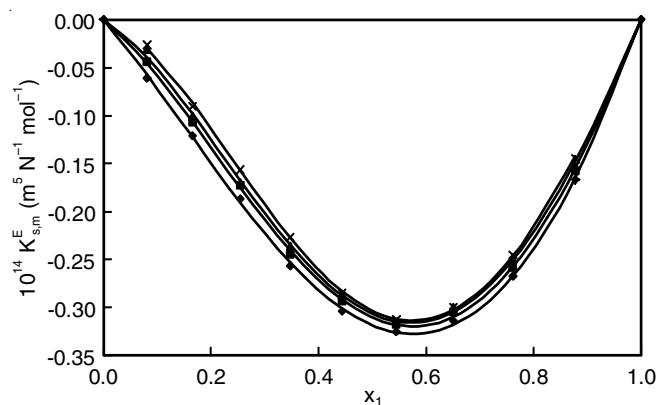


Fig. 3. Excess molar isentropic compressibilities ($\kappa_{s,m}^E$) against mole percentage, x_1 of propiophenone for propiophenone + 2-butoxyethanol binary mixture at \blacklozenge 303.15 K, \blacksquare 308.15 K, \blacktriangle 313.15 K; \times 318.15 K. Values derived from the Redlich-Kwong equation are represented by lines and experimental values are represented by points

increasing the molar compressibility of the propiophenone mixture.

For propiophenone + 2-butoxyethanol mixture throughout the full range of mole percentage at the studied temperatures, where Fig. 4 shows the positive u^E values. The dimensions, form and alignment of the individual molecules all effect the intermolecular interactions, which are described by this parameter. A mixture with strong molecular connections tends to be more densely packed, leading to a rise in internal energy (u) and positive u^E values. Eyring also suggested that during mixing, a decrease in sound speed takes place, causing the excess isentropic compressibility to decrease and the intermolecular free length to increase. The dipole-dipole and hydrogen bond formation between the molecules that the reported positive values u^E for these binary mixtures point to one important interaction make up the mixture.

TABLE-3
COEFFICIENTS A_i OF EQUATION [Ref. 16]

Parameter	Temp. (K)	A_0	A_1	A_2	σ
V_m^E ($10^6 \text{ m}^3 \text{ mol}^{-1}$)	303.15	-0.7756	0.0636	0.2945	0.0022
	308.15	-0.7564	0.0672	0.4134	0.0027
	313.15	-0.7322	0.0527	0.4949	0.0029
	318.15	-0.707	0.0420	0.6300	0.0030
κ_s^E ($10^{10} \text{ m}^2 \text{ N}^{-1}$)	303.15	-0.9250	-0.3541	0.1146	0.0024
	308.15	-0.8980	-0.3771	0.2143	0.0021
	313.15	-0.8815	-0.3779	0.2740	0.0032
	318.15	-0.8721	-0.4037	0.3524	0.0015
$\kappa_{s,m}^E$ ($10^{14} \text{ m}^5 \text{ N}^{-1} \text{ mol}^{-1}$)	303.15	-1.2745	-0.4660	0.1629	0.0032
	308.15	-1.2424	-0.4959	0.3085	0.0030
	313.15	-1.2266	-0.4997	0.4012	0.0040
	318.15	-1.2156	-0.5381	0.5125	0.0023
u^E (10^2 m s^{-1})	303.15	1.0360	0.6600	0.0370	0.0020
	308.15	0.9834	0.6613	-0.0817	0.0021
	313.15	0.9415	0.6370	-0.1474	0.0023
	318.15	0.8957	0.6390	-0.2063	0.0013
α_v^E (10^3 K^{-1})	303.15	-5.8338	-0.4535	2.2255	0.0004
	308.15	-5.6674	-0.4860	3.1147	0.0003
	313.15	-5.4619	-0.3843	3.6992	0.0004
	318.15	-5.2510	-0.3089	4.6935	0.0003

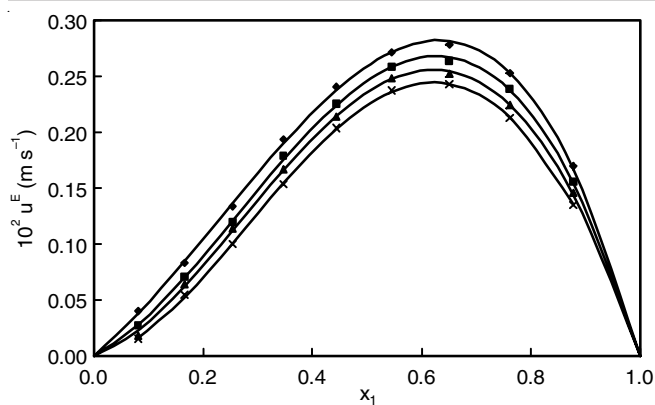


Fig. 4. Excess speed of sound (u^E) against mole percentage, x_1 of propiophenone for propiophenone + 2-butoxyethanol binary mixture at \blacklozenge 303.15 K, \blacksquare 308.15 K, \blacktriangle 313.15 K; \times 318.15 K. Values derived from the Redlich-Kwong equation are represented by lines and experimental values are represented by points

The results for α_p^E versus x_1 in Fig. 5 displays the system at various temperatures. The α_p^E throughout the entire composition range, the values are negative. Isobaric coefficients of thermal expansion with negative excess, α_p^E values may indicate strong interactions between dissimilar molecules, which results in more tightly packed molecules in the mixture. When the mixture's temperature rises, more dipolar connections between molecules that are unlike one another are created, as shown by the decreasing α_p^E values.

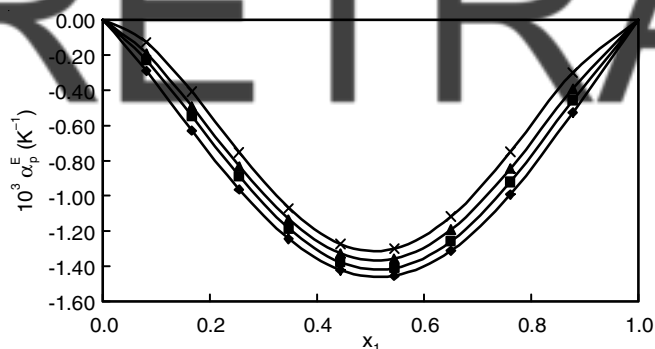


Fig. 5. Excess isobaric thermal expansivity (α_p^E) against mole percentage, x_1 of propiophenone for propiophenone + 2-butoxyethanol binary mixture at \blacklozenge 303.15 K, \blacksquare 308.15 K, \blacktriangle 313.15 K; \times 318.15 K. Values derived from the Redlich-Kwong equation are represented by lines and experimental values are represented by points

The molecular interactions in the systems being studied accurately represent the properties of partial molar volumes. The amount of electrostriction in the structural contribution and the solvent and the intrinsic volume of dipolar are a few examples of the contributions that result in the partial molar

volumes and compressibilities. The partial molar volume, $\bar{V}_{m,1}$ and $\bar{V}_{m,2}$ values and the excess partial molar volume, $\bar{V}_{m,1}^E$ and $\bar{V}_{m,2}^E$ values for the system the temperatures under study are given in Table-4, whereas the results for $\bar{V}_{m,1}^E$ and $\bar{V}_{m,2}^E$ versus x_1 are shown in Fig. 6 for the system at various temperatures.

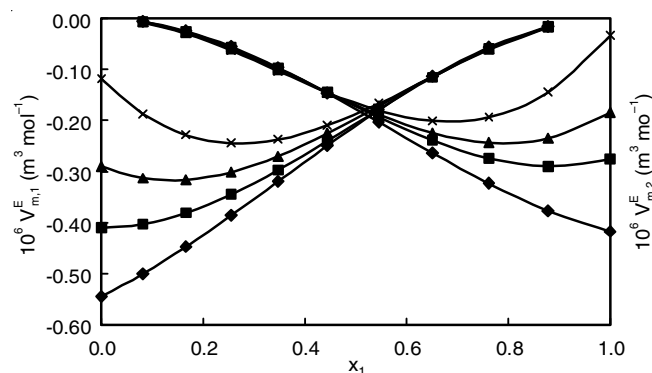


Fig. 6. Excess partial molar volume ($\bar{V}_{m,1}^E$ and $\bar{V}_{m,2}^E$) against mole percentage, x_1 of propiophenone for propiophenone + 2-butoxyethanol binary mixture at \blacklozenge 303.15 K, \blacksquare 308.15 K, \blacktriangle 313.15 K; \times 318.15 K. Values derived from the Redlich-Kwong equation are represented by lines and experimental values are represented by points

Conclusion

The densities and sound velocities of propiophenone and 2-butoxyethanol binary mixture were measured at temperatures of 303.15 K, 308.15 K, 313.15 K, and 318.15 K across the whole composition range in this study. The findings of the experiments were used to compute the different excess properties ($\bar{V}_{m,1}^E$, $\bar{V}_{m,2}^E$, K_s^E , $K_{s,m}^E$, u^E and α_p^E). Strong physical interactions between the component molecules predominate over propiophenone effect on the addition of 2-butoxyethanol, as confirmed by the excess function values and partial molar volumes for the liquid mixes in binary form of propiophenone and 2-butoxyethanol, which holds true for the whole range of compositions.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this article.

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TABLE-4
EXCESS PARAMETERS DATA OF THE COMPONENTS FOR PROPIOPHENONE + 2-BUTOXYETHANOL
BINARY MIXTURE AT T = 303.15-318.15 K FROM REDLICH-KWONG EQUATION

Temp. (K)	$10^6 \bar{V}_{m,1}^0$ ($m^3 mol^{-1}$)	$10^6 \bar{V}_{m,1}^*$	$10^6 \bar{V}_{m,1}^{0E}$	$10^6 \bar{V}_{m,2}^0$	$10^6 \bar{V}_{m,2}^*$	$10^6 \bar{V}_{m,2}^{0E}$
303.15	133.14	133.69	-0.5446	131.94	132.36	-0.4175
308.15	133.66	134.07	-0.4102	132.81	133.08	-0.2758
313.15	134.19	134.48	-0.2900	133.57	133.76	-0.1847
318.15	134.75	134.87	-0.1187	134.40	134.43	-0.0340

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