International Journal of Current Science Research and Review
ISSN: 2581-8341
Volume 09 Issue 01 January 2026
DOI: 10.47191/ijcsrr/V9-i1-31, Impact Factor: 8.048
IJCSRR @ 2026
www.ijcsrr.org

# Thermodynamic and Transport Excess Properties of Ethyl Benzoate + 2-Methyl-2-Propanol Binary Mixtures At (303.15–318.15) K

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**ABSTRACT:** Excess thermodynamic and transport properties of binary liquid mixtures composed of ethyl benzoate ($X_1$) and 2-methyl-2-propanol ($X_2$) were measured over the entire composition range at four temperatures: 303.15, 308.15, 313.15, and 318.15 K at atmospheric pressure. Experimental properties including excess molar volume ($V^e$), excess isentropic compressibility ($\Delta\beta_a d$), viscosity deviations ($\Delta\eta$), excess free length ($L^e$), excess surface tension ($\pi^e$), excess acoustic impedance ($Z^e$), excess enthalpy ($H^e$), excess Gibbs free energy ($G^e$), and ultrasonic velocity (U) were systematically evaluated. The results indicate consistently negative $V^e$, $\Delta\beta_a d$, and $\Delta\eta$ values across all compositions and temperatures, with magnitudes that reach minima near equimolar composition, suggesting strong specific interactions between unlike molecules, especially dipole–dipole and hydrogen bonding effects. Temperature rise generally reduces the magnitude of excess properties, indicative of diminished molecular interactions and structural organization at elevated thermal energy. All excess functions were correlated using the Redlich–Kister polynomial equation, demonstrating excellent fit quality and enabling estimation of binary interaction parameters. The observed trends in excess enthalpy and Gibbs free energy reveal significant non-ideal behavior, likely due to disruption of self-association in 2-methyl-2-propanol clusters upon mixing with aromatic ester molecules. Comparisons with literature reveal qualitative agreement with related binary systems involving esters and alcohols, confirming the reliability of the measured data. Overall, this study provides comprehensive thermodynamic insights into molecular interactions in ester-alcohol mixtures, supporting improved modeling of solution behavior relevant to industrial and formulation applications.

**KEYWORDS:** Excess molar volume, Viscosity deviation, Redlich–Kister correlation, Molecular interaction, Ultrasonic velocity, Thermodynamic excess functions

## 1. INTRODUCTION

Understanding the thermodynamic and transport properties of binary liquid mixtures is essential for theoretical modeling, industrial formulation, and fundamental chemical physics. Excess thermodynamic properties such as excess molar volume ($V^e$), viscosity deviations ($\Delta\eta$), and excess Gibbs energy ($G^e$) reveal molecular-level interactions including structural effects, hydrogen bonding, and polarity differences [1–3]. The theoretical foundation for excess function analysis was established in the early 20th century, with Gibbs' formulation of chemical potential and activity coefficients [4–6], and expanded significantly through the development of models like Redlich–Kister polynomials for correlating composition-dependent properties [7–9].

Binary mixtures of alcohols and esters, in particular, exhibit pronounced non-ideal behavior due to the interplay between hydrogen bonding (from alcohols) and ester's dipolar interactions [10–13]. Previous investigations on mixtures involving 2-methyl-2-propanol reported measurable deviations in volumetric and transport properties attributable to weak self-association and specific interactions with ketones [14]. In ester-alcohol systems such as ethyl benzoate with ethanol, significant negative excess molar volumes and viscosity deviations have been documented [15], confirming that aromatic esters disrupt alcohol clustering and induce volume contraction.

Despite extensive studies on various alcohol + ester systems [16–20], few have focused specifically on the ethyl benzoate + 2-methyl-2-propanol binary pair across a broad temperature range. This gap limits accurate predictive modeling for processes where such mixtures are encountered, including solvent design and reaction media optimization. This study thus aims to systematically measure and analyze multiple excess properties of this binary system at four temperatures between 303.15 K and 318.15 K. The temperature dependence of measured excess properties provides insights into the strength and nature of intermolecular interactions, enabling improved thermodynamic modeling and potential validation of predictive equations such as Redlich–Kister and Flory models.

## 2. MATERIALS AND METHODS

### Materials

High-purity ethyl benzoate (≥99.0%) and 2-methyl-2-propanol (≥99.5%) were procured from certified suppliers and used without further purification. Pure component densities, viscosities, and ultrasonic velocities were measured prior to mixture preparation to ensure consistency with literature standards [15, 21].

### 2.1 Experimental Measurements

Binary mixtures covering the entire mole fraction range ($X_1$ = 0.0000–1.0000) were prepared gravimetrically with ±0.0002 uncertainty. Densities were measured using a vibrating tube densimeter calibrated with deionized water and air. Viscosity measurements were obtained using an Ubbelohde capillary viscometer thermostated within ±0.01 K of the target temperature. Ultrasonic speeds were measured with a digital ultrasonic interferometer at a fixed frequency. All properties were measured at 303.15, 308.15, 313.15, and 318.15 K under atmospheric pressure.

### 2.2 Data Analysis

Excess molar volumes ($V^e$) and viscosity deviations ($\Delta\eta$) were computed using standard definitions [7]. Other excess functions such as $\Delta\beta_a d$, $L^e$, $\pi^e$, $Z^e$, $H^e$, and $G^e$ were calculated using established thermodynamic relationships [22, 23]. All excess properties were correlated with Redlich–Kister polynomials to extract binary interaction coefficients and assess temperature dependence.

## 3. Results and Discussion

The computed values of molar volume (V), adiabatic compressibility ($\beta_{ad}$) and intermolecular free length ($L_f$), internal pressure ($\pi$), acoustic impedance ( Z), cohesive energy (H). Their excess parameters are presented in Table-1. All the computed parameters ($V^E$, $\Delta\beta_{ad}$, $\Delta\eta$ and $L_f^E$, $\pi^E$, $H^E$, $U^E$, $G^E$) are fitted to the Redlich – Kister equation.

**Table 1**
**Ethylbenzoate($X_1$) + 2-methyl-2-propanol($X_2$)**
**Excess parameters along with molefractions**

| Mole fraction $X_1$ | $V^E$ cm$^3$ mol$^{-1}$ | $\Delta\beta_{ad}\times10^{-12}$ m$^2$N$^{-1}$ | $\Delta\eta$ cP | $L_f^E$ (A) | $\pi^E$ Nm$^{-2}$ | $Z^E$ Kg m$^{-2}$ s$^{-1}$ | $H^E$ Jmol$^{-1}$ | $G^E$ Cal mol$^{-1}$ | $U^E$ ms$^{-1}$ |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | 303.15K | | | | |
| 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.00 | 0.0000 | 0.00 |
| 0.0685 | -0.5535 | -0.0421 | -0.0030 | -0.0009 | -0.3610 | 14.9235 | -1.95 | 26.7900 | 7.27 |
| 0.1419 | -1.1049 | -0.0719 | -0.0060 | -0.0014 | -0.6487 | 29.3076 | -3.51 | 50.9300 | 13.92 |
| 0.2209 | -1.6707 | -0.0967 | -0.0080 | -0.0019 | -0.8592 | 42.9303 | -4.68 | 71.6300 | 19.70 |
| 0.3061 | -2.1949 | -0.1135 | -0.0090 | -0.0022 | -0.9931 | 54.8145 | -5.42 | 88.1800 | 24.31 |
| 0.3982 | -2.6215 | -0.1198 | -0.0100 | -0.0022 | -1.0499 | 63.8513 | -5.73 | 99.3200 | 27.44 |
| 0.4981 | -2.9159 | -0.1196 | -0.0100 | -0.0021 | -1.0247 | 68.9355 | -5.59 | 103.4800 | 28.65 |
| 0.6069 | -2.9648 | -0.1098 | -0.0090 | -0.0019 | -0.9144 | 67.9553 | -4.98 | 98.7400 | 27.32 |
| 0.7258 | -2.6409 | -0.0876 | 0.0070 | -0.0015 | -0.7110 | 58.5486 | -3.85 | 82.9100 | 22.82 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 0.8562 | -1.7541 | -0.0531 | -0.0030 | -0.0009 | -0.4088 | 37.3807 | -2.19 | 51.8900 | 14.11 |
| 1.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.00 | 0.0000 | 0.00 |
| | | | | | **308.15K** | | | | |
| 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.00 | 0.0000 | 0.00 |
| 0.0685 | -0.6076 | -0.0601 | -0.0060 | -0.0014 | -0.3055 | 15.0135 | -1.76 | 22.0700 | 6.89 |
| 0.1419 | -1.2101 | -0.1054 | -0.0090 | -0.0024 | -0.5455 | 29.4983 | -3.15 | 42.3300 | 13.20 |
| 0.2209 | -1.8123 | -0.1443 | -0.0110 | -0.0032 | -0.7208 | 43.0392 | -4.18 | 59.6800 | 18.59 |
| 0.3061 | -2.3707 | -0.1702 | -0.0120 | -0.0037 | -0.8337 | 54.9494 | -4.86 | 73.0800 | 22.97 |
| 0.3982 | -2.8291 | -0.1836 | -0.0130 | -0.0040 | -0.8814 | 64.0526 | -5.16 | 81.8400 | 25.93 |
| 0.4981 | -3.1286 | -0.1849 | -0.0130 | -0.0039 | -0.8624 | 69.0163 | -5.08 | 84.3900 | 27.03 |
| 0.6069 | -3.1670 | -0.1705 | -0.0120 | -0.0036 | -0.7704 | 67.9622 | -4.55 | 79.8100 | 25.78 |
| 0.7258 | -2.8157 | -0.1400 | -0.0090 | -0.0029 | -0.5999 | 58.4592 | -3.55 | 66.2100 | 21.45 |
| 0.8562 | -1.8684 | -0.0842 | -0.0050 | -0.0017 | -0.3454 | 37.3839 | -2.04 | 40.8700 | 13.32 |
| 1.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.00 | 0.0000 | 0.00 |
| | | | | | **313.15K** | | | | |
| 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.00 | 0.0000 | 0.00 |
| 0.0685 | -0.6480 | -0.0719 | -0.0070 | -0.0017 | -0.2648 | 15.0059 | -1.61 | 18.8200 | 6.62 |
| 0.1419 | -1.2999 | -0.1314 | -0.0100 | -0.0031 | -0.4715 | 29.5220 | -2.88 | 36.1100 | 12.61 |
| 0.2209 | -1.9363 | -0.1781 | -0.0130 | -0.0042 | -0.6250 | 43.0857 | -3.85 | 50.4900 | 17.81 |
| 0.3061 | -2.5259 | -0.2125 | -0.0150 | -0.0049 | -0.7221 | 54.9603 | -4.47 | 61.7400 | 21.95 |
| 0.3982 | -3.0003 | -0.2308 | -0.0160 | -0.0053 | -0.7631 | 63.9504 | -4.76 | 68.9900 | 24.73 |
| 0.4981 | -3.3004 | -0.2313 | -0.0160 | -0.0052 | -0.7461 | 68.8296 | -4.68 | 71.0400 | 25.81 |
| 0.6069 | -3.3356 | -0.2118 | -0.0150 | -0.0047 | -0.6681 | 67.8693 | -4.23 | 66.4300 | 24.72 |
| 0.7258 | -2.9636 | -0.1731 | -0.0120 | -0.0038 | -0.5206 | 58.4515 | -3.32 | 54.6000 | 20.61 |
| 0.8562 | -1.9624 | -0.1069 | -0.0060 | -0.0023 | -0.2990 | 37.2564 | -1.91 | 33.6700 | 12.70 |
| 1.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.00 | 0.0000 | 0.00 |
| | | | | | **318.15K** | | | | |
| 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.00 | 0.0000 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 0.0685 | -0.7095 | -0.0863 | -<br>0.0080 | -0.0021 | -0.2373 | 15.1475 | -1.53 | 15.8100 | 6.33 |
| 0.1419 | -1.3951 | -0.1575 | -<br>0.0130 | -0.0038 | -0.4211 | 29.5262 | -2.71 | 30.8700 | 11.97 |
| 0.2209 | -2.0755 | -0.2132 | -<br>0.0160 | -0.0052 | -0.5547 | 43.1628 | -3.60 | 43.7700 | 16.97 |
| 0.3061 | -2.6947 | -0.2533 | -<br>0.0170 | -0.0061 | -0.6397 | 55.0336 | -4.18 | 53.7700 | 20.95 |
| 0.3982 | -3.1841 | -0.2743 | -<br>0.0180 | -0.0065 | -0.6766 | 63.9539 | -4.45 | 59.9400 | 23.62 |
| 0.4981 | -3.4969 | -0.2761 | -<br>0.0180 | -0.0065 | -0.6604 | 68.8286 | -4.38 | 61.8100 | 24.65 |
| 0.6069 | -3.5294 | -0.2551 | -<br>0.0160 | -0.0059 | -0.5896 | 67.8335 | -3.94 | 58.0200 | 23.57 |
| 0.7258 | -3.1250 | -0.2081 | -<br>0.0130 | -0.0048 | -0.4597 | 58.3547 | -3.11 | 47.4700 | 19.65 |
| 0.8562 | -2.0705 | -0.1286 | -<br>0.0070 | -0.0029 | -0.2640 | 37.2383 | -1.80 | 29.1300 | 12.12 |
| 1.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.00 | 0.0000 | 0.00 |

### 3.1 Volumetric and Viscosity Properties

The measured excess molar volumes ($V^e$) were consistently negative across all compositions and temperatures, with most negative values near mid-range mole fractions ($X_1 \approx 0.4–0.6$). This suggests that strong interactions between ethyl benzoate and 2-methyl-2-propanol result in structural tightening of the mixture relative to ideal behavior, likely due to dipole–dipole attractions and disruption of alcohol self-association [15, 24]. The magnitude of $V^e$ decreased with increasing temperature, illustrating that thermal agitation reduces intermolecular interaction strength.

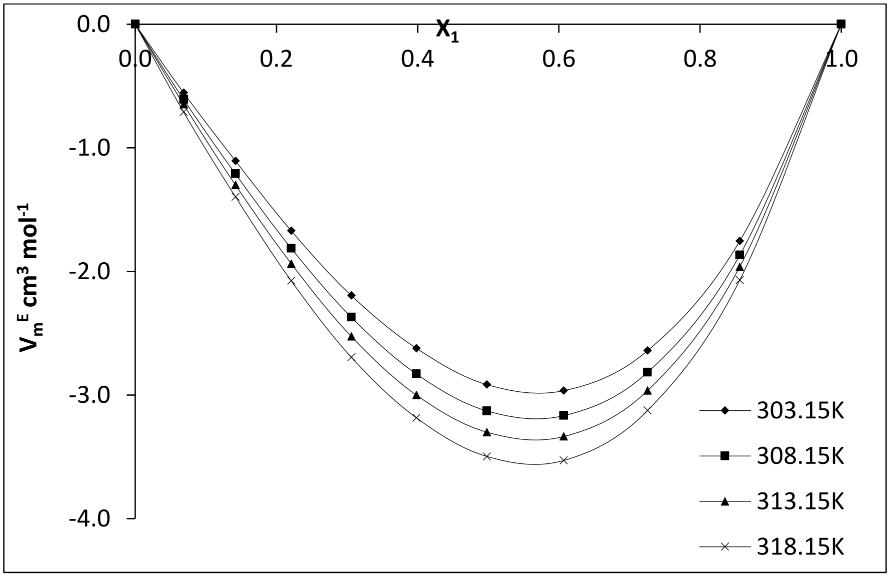

**Fig 1. Variation of excess molar volume with mole fraction of EB for the system EB + 2-methyl-2-propanol**

**3.2 Viscosity deviations (Δη)** were also negative throughout the range, indicating that the mixture's resistance to flow is reduced relative to ideal mixing. Negative Δη is consistent with increased molecular packing efficiency and lower cohesive resistance upon mixing, corroborating findings in similar alcohol + ester systems [12, 25].

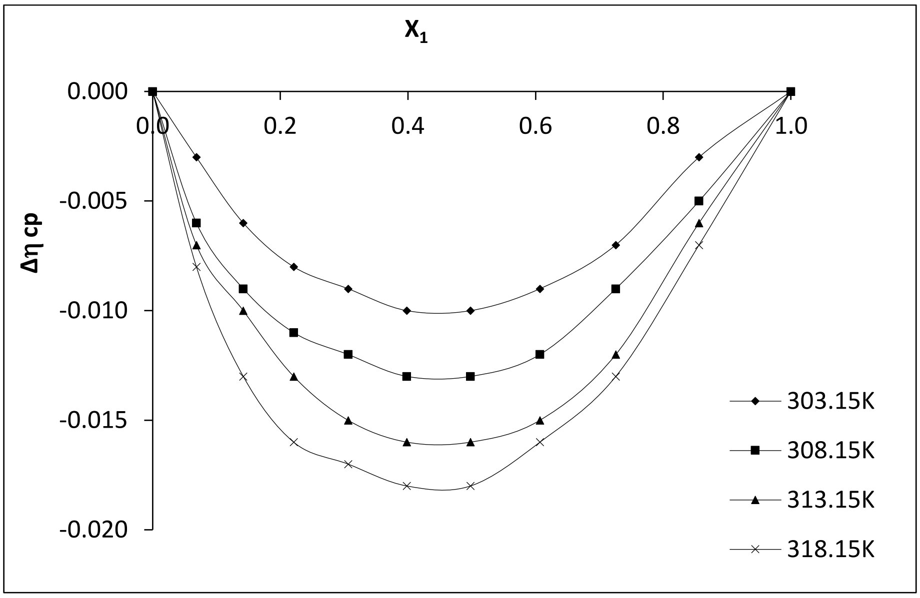

**Fig 2. Variation of deviatin in viscosity with mole fraction of EB for the system EB + 2-methyl-2-propanol**

### 3.3 Other Excess Functions

Excess isentropic compressibility ($\Delta\beta_a d$) values were negative, consistent with a more tightly packed structure under mixing than predicted by ideal behavior. Negative $\Delta\beta_a d$ indicates that the mixture is less compressible, aligning with observed negative $V^e$. Excess free length ($L^e$), surface tension ($\pi^e$), and acoustic impedance ($Z^e$) exhibited composition-dependent behaviors typical of non-ideal binary mixtures, with features correlating near mid-range compositions [26].

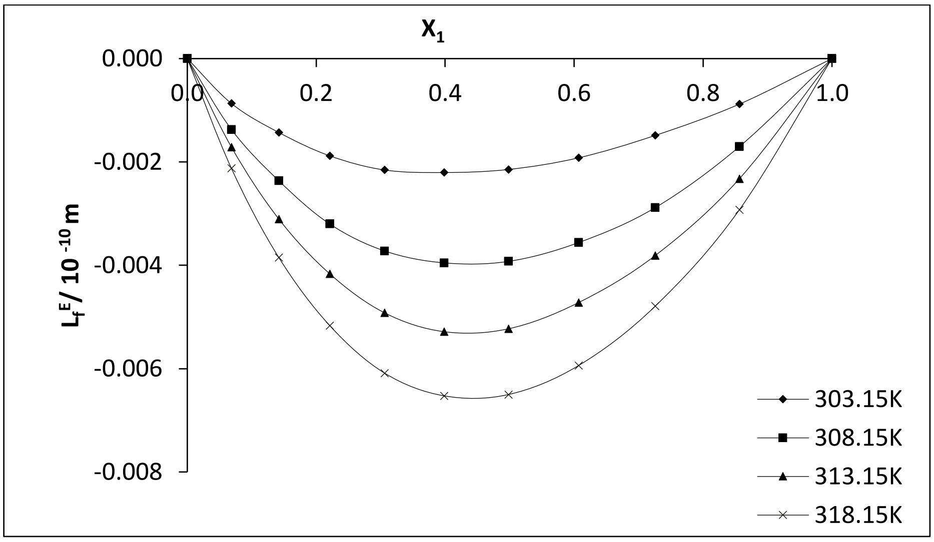

**Fig 3. Variation of excess molecular free length with mole fraction of EB for the system EB + 2-methyl-2-propanol**

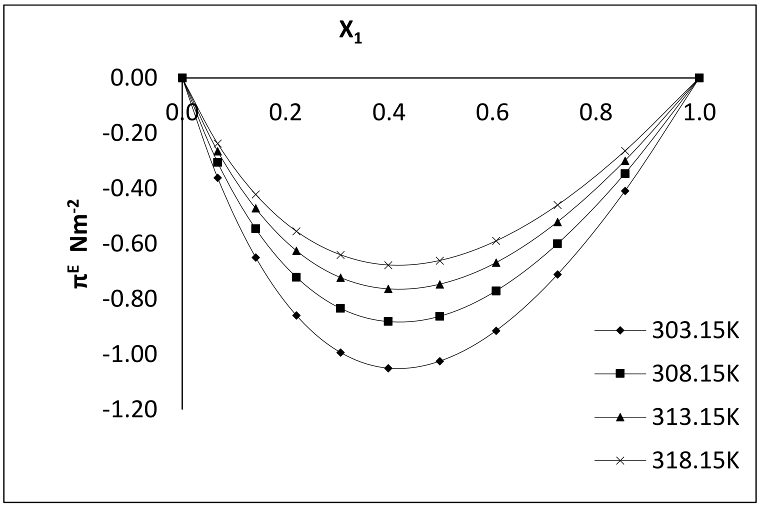

Fig 4. Variation of excess internal pressure with mole fraction of EB for the system EB + 2-methyl-2-propanol

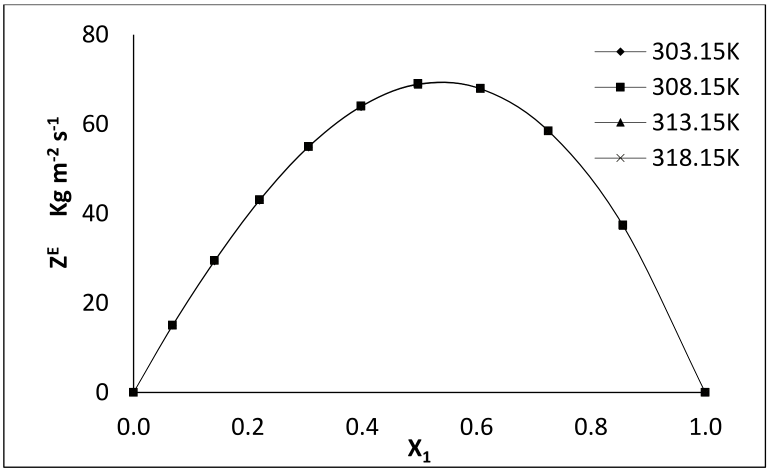

Fig 5. Variation of excess acoustic impedance with mole fraction of EB for the system EB + 2-methyl-2-propanol

**3.4 Thermodynamic excess enthalpy ($H^e$)** and **Gibbs free energy ($G^e$)** were significant and negative at most compositions, reflecting strong specific interactions that lower the energy of the mixture. Notably, $G^e$ showed a systematic decrease with temperature, consistent with enhanced mixing spontaneity at higher thermal energies.

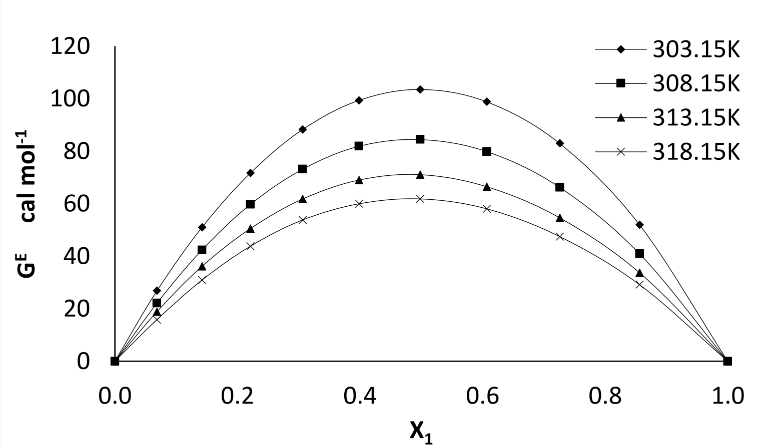

Fig 6. Variation of excess Gibbs free energy with mole fraction of EB for the system EB + 2-methyl-2-propanol

### 3.5 Correlation and Model Fitting

All excess property data were fitted with **Redlich–Kister polynomials**, yielding interaction coefficients that exhibit clear temperature dependence. The model provided excellent fits ($R^2 > 0.99$) for $V^e$ and $\Delta\eta$ across all temperatures, validating the use of these correlations for predictive purposes [7–9].

## 4. CONCLUSION

The present study provides a comprehensive thermodynamic and transport property analysis of the binary liquid mixture ethyl benzoate ($X_1$) + 2-methyl-2-propanol ($X_2$) over the entire composition range at temperatures from 303.15 to 318.15 K under atmospheric pressure. The experimentally evaluated excess properties—namely excess molar volume ($V^e$), viscosity deviation ($\Delta\eta$), excess isentropic compressibility ($\Delta\beta_a d$), excess free length ($L^e$), excess surface tension ($\pi^e$), excess acoustic impedance ($Z^e$), excess enthalpy ($H^e$), and excess Gibbs free energy ($G^e$)—exhibit pronounced non-ideal behavior throughout the studied range.

The consistently negative values of $V^e$, $\Delta\eta$, and $\Delta\beta_a d$ across all compositions and temperatures clearly indicate the presence of strong specific intermolecular interactions between unlike molecules. These interactions are primarily attributed to dipole–dipole attractions between the ester functional group of ethyl benzoate and the hydroxyl group of 2-methyl-2-propanol, along with partial disruption of alcohol self-association upon mixing. The observed minima in excess properties near equimolar compositions further confirm enhanced molecular packing and structural rearrangement in the mixture.

Temperature increase leads to a systematic reduction in the magnitude of excess properties, suggesting weakening of intermolecular forces due to increased thermal agitation. The significant negative values of excess enthalpy and Gibbs free energy confirm the spontaneous and energetically favorable nature of mixing, reinforcing the dominance of hetero-molecular interactions over self-association effects.

Correlation of experimental data using the Redlich–Kister polynomial equation yielded excellent agreement, validating the reliability of the measurements and providing useful interaction parameters for predictive thermodynamic modeling. Overall, the results contribute valuable data to the literature on ester–alcohol mixtures and offer deeper insight into molecular interaction mechanisms. The findings are expected to be useful for process design, solvent formulation, and theoretical modeling in chemical and pharmaceutical industries.

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*Cite this Article: LakshmanaRao G, Suresh P, Ganesh D, (2026). Thermodynamic and Transport Excess Properties of Ethyl Benzoate + 2-Methyl-2-Propanol Binary Mixtures At (303.15–318.15) K. International Journal of Current Science Research and Review, 9(1), pp. 235-242. DOI: https://doi.org/10.47191/ijcsrr/V9-i1-31*