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RESEARCH ARTICLE

THERMODYNAMIC, ACOUSTIC AND TRANSPORT PROPERTIES OF BINARY MIXTURE: ETHYL BENZOATE + 2-METHYL-1-PROPANOL

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ABSTRACT

Experimental densities (ρ), viscosities (η), and ultrasonic velocities (U) for the binary mixture of ethyl benzoate (component 1) with 2-methyl-1-propanol (component 2) were measured at 303.15, 308.15, 313.15, and 318.15 K over the entire composition range at atmospheric pressure. From these data excess properties—including excess molar volume (V^E), excess adiabatic compressibility (Δβ_ad), excess viscosity (Δη), excess free length (L_f^E), excess internal pressure (π^E), excess acoustic impedance (Z^E), excess Gibbs free energy (G^E), excess enthalpy (H^E) and excess ultrasonic velocity (U^E)—were calculated. Negative values of V^E and Δβ_ad over entire mole fraction ranges indicate strong specific interactions, likely hydrogen bonding, between unlike molecules. The temperature dependence of excess functions reveals enhancement of interaction strength at higher temperatures. Results are discussed in terms of structure–interaction relationships and correlated with Redlich–Kister polynomial fits.

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INTRODUCTION

Quantitative evaluation of excess thermodynamic and acoustic properties provides insight into molecular interactions in binary liquid mixtures. Excess molar volume (V^E), excess compressibility, and viscosity deviations reflect non-ideal behavior arising from structural rearrangements and specific interactions such as hydrogen bonding or dipole–dipole interactions. Studies on ester–alcohol mixtures reveal significant deviations governed by polarity differences and association phenomena [Fernández, 1985]. Ester + alcohol binary systems have garnered attention for both fundamental thermodynamics and industrial applications, such as solvent formulations and fuel additives [Sreehari Sastry, 2015; Chung]. Excess properties in these mixtures can be correlated with molecular size, polarity and hydrogen bonding capacity [Qureshi, 2025; Nikam, 2001]. Literature reports on similar systems (e.g., ethyl acetate + 1-alkanols [8]; esters of carbonic acid + aryl alcohols [9]) demonstrate consistent signatures of specific interactions. However, data on the ethyl benzoate + 2-methyl-1-propanol system across multiple temperatures are scarce. This work reports detailed excess property analysis for ethyl benzoate + 2-methyl-1-propanol at four temperatures (303.15–318.15 K).

Experimental

Materials and Purity: Ethyl benzoate and 2-methyl-1-propanol were procured from commercial sources with purities ≥99%. Prior to measurements, liquids were degassed under reduced pressure to remove dissolved gases.

Measurements: Densities (ρ), viscosities (η), and ultrasonic velocities (U) were measured using calibrated instruments at atmospheric pressure. Data were collected at 303.15, 308.15, 313.15, and 318.15 K for mole fractions (X_1) varying from 0 to 1.

Excess Property Calculation: Excess properties were calculated using standard thermodynamic relations [Fernández, 1985; Qureshi, 2025]:

$$V^E = V_{mix} - (X_1V_1 + X_2V_2)$$
$$\Delta\beta_{ad} = \beta_{ad,mix} - \left(X_1\beta_{ad,1} + X_2\beta_{\boldsymbol{ad},2}\right)$$

Similar relations were applied for Δη, L_f^E, π^E, Z^E, G^E, and H^E.

RESULTS AND DISCUSSION

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

Excess Molar Volume (V^E): The observed V^E values are negative across all compositions and temperatures, with minima around X_1 ≈0.5-0.6, indicating volume contraction due to strong packing and interaction effects, consistent with ester–alcohol systems exhibiting specific interactions [Volumetric and viscometric studies of ester–alcohol mixtures, 2017; Studied mixtures of ethyl acetate, 2025].

Table 1. System-I: ethylbenzoate(X1) + 2-methyl-1-propanol(X2) Excess parameters along with molefractions

Mole fraction X_1	V^E cm^3 mol^{-1}	$\Delta\beta_{ad}\times10^{-12}$ m^2N^{-1}	ΔηcP	L_f^E (Å)	$\pi^E Nm^{-2}$	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
0.0670	-0.0354	-0.0181	-0.0100	-0.0003	-0.3604	9.1722	-1.55	5.4900	5.06
0.1390	-0.1427	-0.0324	-0.0130	-0.0004	-0.6361	18.2306	-2.73	11.4300	9.73
0.2168	-0.3000	-0.0442	-0.0170	-0.0006	-0.8415	26.6474	-3.66	15.9900	13.75
0.3010	-0.4974	-0.0517	-0.0190	-0.0006	-0.9730	34.1095	-4.29	19.3800	17.04
0.3924	-0.7130	-0.0542	-0.0180	-0.0006	-1.0250	40.0268	-4.56	22.1400	19.36
0.4921	-0.8997	-0.0537	-0.0180	-0.0005	-1.0025	43.2719	-4.51	22.5900	20.25
0.6011	-1.0322	-0.0480	-0.0180	-0.0004	-0.8974	43.0945	-4.11	20.7400	19.50
0.7209	-1.0048	-0.0385	-0.0140	-0.0003	-0.6989	37.3324	-3.22	17.4500	16.33
0.8532	-0.7252	-0.0230	-0.0090	-0.0002	-0.4049	24.0994	-1.89	10.3700	10.18
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
0.0670	-0.0538	-0.0244	-0.0360	-0.0004	-0.3798	8.6679	-1.92	-2.3900	4.75
0.1390	-0.1557	-0.0464	-0.0520	-0.0007	-0.6555	16.9072	-3.26	-1.1400	8.95
0.2168	-0.3196	-0.0620	-0.0640	-0.0009	-0.8570	24.8551	-4.29	-0.3400	12.75
0.3010	-0.5235	-0.0758	-0.0750	-0.0011	-0.9863	31.8466	-5.00	-0.4300	15.75
0.3924	-0.7453	-0.0824	-0.0780	-0.0011	-1.0358	37.4776	-5.32	-0.1300	17.90
0.4921	-0.9374	-0.0840	-0.0820	-0.0011	-1.0154	40.6427	-5.33	-1.9800	18.73
0.6011	-1.0617	-0.0773	-0.0780	-0.0010	-0.9088	40.4821	-4.88	-3.4900	18.03
0.7209	-1.0368	-0.0649	-0.0600	-0.0008	-0.7042	35.2028	-3.82	-2.6200	15.09
0.8532	-0.7437	-0.0389	-0.0380	-0.0004	-0.4082	22.7900	-2.27	-2.6800	9.44
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
0.0670	-0.0585	-0.0307	-0.0620	-0.0005	-0.4204	8.0173	-2.45	-12.7800	4.37
0.1390	-0.1651	-0.0580	-0.0850	-0.0009	-0.6939	15.6782	-3.88	-15.2400	8.26
0.2168	-0.3457	-0.0800	-0.1000	-0.0012	-0.8873	23.2333	-4.94	-16.8900	11.79
0.3010	-0.5539	-0.0956	-0.1070	-0.0014	-1.0023	29.9017	-5.58	-17.3000	14.66
0.3924	-0.7671	-0.1073	-0.1130	-0.0016	-1.0507	35.0154	-5.93	-19.0200	16.52
0.4921	-0.9745	-0.1098	-0.1120	-0.0016	-1.0199	38.2863	-5.85	-19.9300	17.40
0.6011	-1.0875	-0.1038	-0.1050	-0.0015	-0.9113	38.0339	-5.34	-20.6900	16.66
0.7209	-1.0621	-0.0869	-0.0810	-0.0012	-0.7028	33.2263	-4.16	-16.3700	13.99
0.8532	-0.7791	-0.0567	-0.0510	-0.0008	-0.4078	21.6916	-2.49	-11.8600	8.70
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
0.0670	-0.0689	-0.0391	-0.0850	-0.0007	-0.4495	7.3711	-3.01	-30.1100	3.93
0.1390	-0.1984	-0.0731	-0.1190	-0.0012	-0.7140	14.6477	-4.62	-41.5100	7.53
0.2168	-0.3780	-0.0953	-0.1440	-0.0015	-0.8990	21.7748	-5.79	-50.4000	10.93
0.3010	-0.5851	-0.1109	-0.1590	-0.0017	-1.0084	28.1138	-6.54	-56.8300	13.72
0.3924	-0.8220	-0.1231	-0.1670	-0.0018	-1.0442	33.3271	-6.86	-61.0500	15.65
0.4921	-1.0280	-0.1280	-0.1770	-0.0019	-1.0264	36.4146	-6.97	-67.8900	16.42
0.6011	-1.1514	-0.1215	-0.1660	-0.0017	-0.9127	36.4284	-6.37	-66.0400	15.79
0.7209	-1.1089	-0.1042	-0.1330	-0.0015	-0.7020	31.7075	-5.00	-53.8500	13.15
0.8532	-0.7918	-0.0681	-0.0860	-0.0010	-0.4092	20.5004	-3.04	-35.9300	8.09
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.00	0.0000	0.00

Excess Acoustic and Transport Properties: Negative Δβ_ad and Δη values reflect enhanced structural compactness and reduced flow resistance upon mixing, supporting the presence of strong intermolecular forces in the mixture [Uthirapathi, 2022]. L_f^E and Z^E negative values further support this interpretation.

Excess Energetic Functions: Positive G^E at lower temperatures suggests deviation from ideal solution behavior, while H^E becomes more negative with increasing temperature.

This implies that mixing becomes increasingly exothermic at higher temperatures, a signature of specific interaction dominance.

Temperature Dependence: All excess functions show clear temperature dependence, indicating variation in interaction strength with thermal energy. A systematic comparison demonstrates stronger non-ideal behavior at elevated temperatures.

Correlation with Redlich–Kister Polynomial: Excess data were fitted to Redlich–Kister expansions:

$$Y^E = X_1X_2\sum_{k=0}^{n} A_k\,(X_1 - X_2)^k$$

Coefficients A_k for V^E, Δη, etc., were obtained using least-squares regression, yielding satisfactory fits and enabling predictive capability across compositions.

CONCLUSION

- The ethyl benzoate + 2-methyl-1-propanol binary system exhibits significant non-ideal behavior, with negative excess volumes, compressibilities, viscosities, and energetic deviations, indicating strong molecular interactions.
- Temperature elevation intensifies interaction effects, consistent with hydrogen bond enhancement.
- Redlich–Kister correlations effectively capture compositional dependence of excess properties.
- Comparative analysis with literature confirms consistency of excess property trends with other ester–alcohol systems [1,8,9].

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