Densities and viscosities of the binary mixtures of phenylmethanol with 2-butanone

Densities and Viscosities of the Binary Mixtures of Phenylmethanol with 2–Butanone

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1 **Abstract**

2   Densities and viscosities of the binary systems of phenylmethanol with 2–butanone were measured for

3 the entire composition range at T = (303.15, 308.15, 313.15, 318.15 and 323.15) K and at the

4 atmospheric pressure. The excess molar volumes were derived from the experimental data, and were

5 fitted with the Redlich–Kister equation to obtain their coefficients and standard deviations. The

6 Grunberg–Nissan equation was used to correlate the viscosity data. Furthermore, kinematic viscosities

7 were compared with those predicted by UNIFAC–VISCO model. The cause of relatively large

8 deviations between the experimental and predicted kinematic viscosities was explored by comparing

9 combinatorial and residual term of UNIFAC–VISCO model.

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1   **Introduction**

2   The fluid property data are essential to explore their usability in the analytical applications that work

3   with mixed solvents, process engineering design applications and other related areas, and have drawn

4   considerable interest in recent years. We are interested in the accumulation of the physical property data

5   of organic liquid mixtures, [1-5] and as a continuation of our effort, we are reporting here the density and

6   viscosity data of the binary mixtures of phenylmethanol with 2–butanone at T = (303.15, 308.15, 313.15,

7   318.15 and K. 3.15) K.

8   Phenylmethanol is a polar solvent with strong self–associating nature via hydrogen bonding, while 2–

9   butanone is an aprotic and protophilic solvent, and both the liquids are widely used as a solvent in the

10 laboratory and industrial processes. In this study, density and viscosity of the binary liquid mixtures of

11 different compositions covering the entire range were measured. The experimental density data were

12 used to derive the excess molar volume, V_m^E, and Redlich–Kister type polynomial equation[6] was used to

13 estimate the binary coefficients and the standard deviations. The Grunberg–Nissan interaction parameter

14 which indicates the strength of interactions of the components was calculated using the correlation

15 equation.[7] Kinematic viscosities for the binary system predicted by UNIFAC–VISCO model[8, 9] were

16 compared with the experimental values. The experimental data and the derived quantities were used to

17 understand the likely interactions of the >C=O group of 2–butanone either with the –OH group of

18 phenylmethanol or with the delocalized π–electrons the benzene ring in phenylmethanol.

19   Our survey of the literature shows that there have not been any density or viscosity data reported for

20 the binary system of phenylmethanol with 2–butanone.

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22 **Experimental**

23   Phenylmethanol (Aldrich, 0.99 mass fraction purity) and 2–butanone (Aldrich, >0.99 mass fraction

24 purity) were used without additional treatment. Density and viscosity data from literatures have been

25 used to ascertain the solvent purity (Table 1).

1   An analytical balance (Model: B 204–S, Mettler Toledo, Switzerland) with uncertainty of ± 0.0001 g

2   was used to prepare the binary mixtures. Mixtures were prepared by mass just before use, and were

3   completely miscible over the entire composition range. The uncertainty in the mole fraction was less

4   than $\pm\ 1\cdot10^{-4}$. A 25 mL specific gravity bottle and A–type Ostwald viscometer, previously calibrated

5   with redistilled water, were used for the measurement of density and viscosity correspondingly. The

6   mean uncertainties in densities and viscosities, respectively, were estimated to be 0.0004 g·cm^{-3} and ±

7   0.5%. A thermostatic water bath equipped with the Thermo Haake DC10 controller (Thermo Fisher

8   Scientific, MA, USA) was used to maintain the temperatures with an average uncertainty of ± 0.05 K.

9   All the measurements were conducted in triplicate and averaged for calculations. LAB Fit[10] and LSM

10   [11] curve–fitting programs were used for least–square regression analyses.

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12   **Results and Discussion**

13   Experimental densities, ρ_{exp} and excess molar volume, V_m^E for different binary compositions of

14   phenylmethanol with 2–butanone at T = (303.15, 308.15, 313.15, 318.15 and 323.15) K is listed in

15   Table 2. Excess molar volumes were calculated using the following relation:

16   $$V_m^E = \left[(x_1 M_1 + x_2 M_2)/\rho_{exp} - \{(x_1 M_1)/\rho_1 + (x_2 M_2)/\rho_2\}\right] \tag{1}$$

17   where ρ_{exp} is for density of the binary mixtures. The mole fraction, molar mass and density of

18   phenylmethanol are represented with x_1, M_1 and ρ_1, and the corresponding quantities of 2–butanone are

19   denoted with x_2, M_2 and ρ_2, respectively. Excess molar volume, V_m^E of the (phenylmethanol + 2–

20   butanone) system as a function of the binary compositions at T = (303.15, 308.15, 313.15, 318.15 and

21   323.15) K is shown in Figure 1. The V_m^E values are negative throughout the composition range,

22   decreases with an increase in phenylmethanol concentration up to the mole fraction, $x_1 \approx 0.5$, and then

23   increases further with the change in x_1. Such behavior may be accounted to the change in orientation of

24   the molecules within the mixtures due to the interaction between the components with the addition of

25   H–bonding containing liquid into the system, and partial interstitial accommodation of ketone molecules

1. into the network of alcohol at the phenylmethanol–rich conditions. It is assumed that the latter effect not

2. only compensates the former effect but also predominates largely, resulting in a net negative V_m^E. There

3. are two probable pathways, which may result from the change in orientation of the molecules within the

4. mixtures – (a) interaction between the –OH group of phenylmethanol and the >C=O group of 2–

5. butanone through H–bonding (*i.e* –O–H……O=C<) and (b) interaction between the delocalized π–

6. electrons of the benzene ring in phenylmethanol with the >C=O group of 2–butanone.[12] Decreasing

7. trend in the variations of V_m^E values is observed with the rise of temperatures, *i.e.* $\partial V_m^E/\partial T < 0$. Greater

8. population of intermolecular complex within the system, which is attributable to the increasing

9. proportion of smaller multimers as well as the monomers of phenylmethanol and 2–butanone with the

10. increase in temperature, is thus supposed to explain such behavior.

11. The composition dependence of V_m^E can be represented by a Redlich–Kister type equation: [6]

12. $$Y = x_1 x_2 \sum_{i=0}^{n} A_i (1 - 2x_1)^i \tag{2}$$

13. where Y refers to V_m^E, and the mole fractions of phenylmethanol and 2–butanone are represented with x_1

14. and x_2, respectively. The coefficients A_i in eq 2 were obtained by fitting the equation with the

15. experimental values (Table 4). The standard deviation values, as listed in Table 3, were calculated from

16. the following equation:

17. $$\sigma(Y) = \left[\sum (Y_{expt} - Y_{calc})^2 / (n - p) \right]^{(1/2)} \tag{3}$$

18. where n is the number of experimental points, p is the number of coefficients of eq 2, and Y_{expt} and Y_{calc}

19. are the experimental and calculated values of the properties.

20. Table 4 lists the experimental viscosities, η_{exp} for different binary compositions at $T = (303.15, 308.15,$

21. 313.15, 318.15 and 323.15) K. Figure 2 represents the variation of η_{exp} against the mole fraction of

22. phenylmethanol (x_1) at different temperatures. The viscosity of a mixture strongly depends on the

23. structure of liquids and bond enthalpy, and consequently, on the molecular interactions between the

24. components of the mixture. [13] A gradual increase in the viscosity of the mixtures can be observed with

1   the increasing concentration of phenylmethanol in the binary mixtures with 2–butanone which indicate

2   the formation of more and more flow-resistant species within the system as the proportion of x_1

3   increases. The magnitude of η_{exp} decreases as the temperature is higher and such temperature effect on

4   viscosities is a common phenomenon. [14]

5   Viscosity data was analyzed based on the Grunberg–Nissan treatment [7] whose parameter gives

6   qualitative information about molecular interactions:

7    $$\eta_{mix} = \exp\left(x_1 \ln \eta_1 + x_2 \ln \eta_2 + x_1 x_2 d\right) \tag{4}$$

8   where d is an interaction parameter that is a function of the nature of the components and temperature,

9   and has been regarded as a measure of the strength of molecular interactions between the mixture

10   components. The Grunberg–Nissan interaction parameter (d) values are found to be negative and quite

11   large in magnitude for the whole range of composition, and decrease with the increase of temperature

12   (Table 5). According to Fort and Moore, [15] such pattern in d values indicate the tendency of the systems

13   to move towards more ideal conditions, which are due to the absence of specific interaction and

14   presence of dominant dispersive force between the components.

15   In this study, kinematic viscosities were calculated with the experimental density and viscosity data,

16   and compared with those predicted by UNIFAC–VISCO model.[8, 9] In UNIFAC–VISCO model, the

17   relationship between the kinematic viscosity and the excess Gibbs energy of activation, $\Delta^* G^E$ is

18   expressed in the following form:

19   $$\ln(\nu M) = \sum_{i}^{NC} x_i \ln\left(\nu_i M_i\right) + \frac{\Delta^* G^E}{RT} \tag{5}$$

20   $$\Delta^* G^E = \Delta^* G^{EC} + \Delta^* G^{ER} \tag{6}$$

21   where M is molecular weight, $\Delta^* G^E$, $\Delta^* G^{EC}$ and $\Delta^* G^{ER}$ are excess Gibbs energy of activation and its

22   combinatorial and the residual parts, respectively. In UNIFAC-VISCO model, the combinatorial part

23   expresses the contribution of shape differences among molecules to the $\Delta^* G^E$, while the residual part

24   accounts for the enthalpy effect caused by mixing. In Figure 3, kinematic viscosities predicted by

1   UNIFAC-VISCO model are compared with the experimental ones. For the prediction, the interaction

2   parameters reported by Gaston-Bonhomme et al.[9] are used. Experimental kinematic viscosities, v_{exp},

3   experimental viscosities, η_{exp}, and experimental densities, ρ_{exp}, in Table 2 and 4 have the following

4   relationship:

5    $$v_{exp} = \frac{\eta_{exp}}{\rho_{exp}}$$ (7)

6   As can be seen from the figure, the kinematic viscosities obtained by UNIFAC–VISCO model are

7   smaller than the experimental ones at all temperatures. The relative errors, $E_{v,i}$, and the absolute average

8   differences, AAD, was expressed by the following equations, and shown in Table 6:

9    $$E_{v,i} = \frac{v_{exp,i} - v_{cal,i}}{v_{exp,i}} \times 100$$ (8)

10    $$AAD = \frac{1}{n} \sum_{i}^{N_p} |E_{v,i}|$$ (9)

11   where i denotes the i–th experimental data and n is the number of the experimental data at each

12   temperature. In order to explore the cause of the deviations, $\Delta^* G^E$, $\Delta^* G^{EC}$, $\Delta^* G^{ER}$, and $\Delta^* G^E$ from the

13   experimental data were also compared with each other. The experimental $\Delta^* G^E$ was obtained by the

14   following equation:

15    $$\left. \frac{\Delta^* G^E}{RT} \right|_{exp} = \ln(v_{exp}M) - \sum_{i}^{NC} x_i \ln(v_i M_i)$$ (10)

16   where NC is the number of components. Since the results of comparisons were similar at all

17   temperatures, that at 303.15 K is shown in Figure 4 as an example. As can be seen from the figure, the

18   absolute values for $\Delta^* G^E_{exp}$ are much smaller than the predicted ones. Since absolute values for the

19   combinatorial part are smaller than those for the residual part, the residual part seems to be responsible

20   for the large deviation. The greater absolute values of the residual term mean the individual

21   contributions of constituent groups in the system are overestimated by UNIFAC–VISCO model.

22

1 **Conclusions**

2 Densities and viscosities for the binary mixtures of phenylmethanol with 2–butanone have been

3 determined experimentally as a function of temperature and at the atmospheric pressure. Excess molar

4 volumes have been derived from the experimental density data, and the patterns are negative throughout

5 the composition range. Analysis of viscosity data based on the Grunberg–Nissan treatment show that no

6 specific interaction exists among the component molecules. Furthermore, experimental kinematic

7 viscosities were obtained by densities and viscosities, and compared with those predicted by UNIFAC–

8 VISCO model. The deviations between experimental and predicted kinematic viscosities are large, and

9 larger the temperature higher. By the comparisons among excess Gibbs energies of activation, the

10 residual term in UNIFAC–VISCO model seems to be responsible for those large deviations.

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Table 1. Comparison of Experimental Densities, ρ_{exp} and Viscosities, η_{exp} of Pure Solvents with Literature Values at T = (303.15, 308.15, 313.15, 318.15 and 323.15) K

Component	T/K	ρ /g·cm^{-3}			η /mPa·s		
		Exp.	Lit.	Ref.	Exp.	Lit.	Ref.
Phenylmethanol	303.15	1.0376	1.0376	[16]	4.689	4.670	[17]
	308.15	1.0338	1.0337	[17]	4.058	4.004	[17]
						4.093	[18]
	313.15	1.0301	1.0294	[17]	3.531	3.530	[19]
	318.15	1.0263	1.02572	[20]	3.103	3.120	[20]
	323.15	1.0225	1.0221	[16]	2.747		
2–Butanone	303.15	0.7940	0.7944	[21]	0.362	0.3653	[22]
						0.366	[23]
	308.15	0.7888	0.7888	[24]	0.345	0.3441	[24]
			0.7885	[22]		0.3440	[22]
	313.15	0.7835	0.7831	[25]	0.330		
	318.15	0.7783	0.7785	[26]	0.316	0.311	[26]
	323.15	0.7730	0.7733	[1]	0.303		

Table 2. Composition, Experimental Densities, ρ_{exp} and Excess Molar Volumes, V_m^E for the Binary Mixtures of Phenylmethanol (1) with 2–Butanone (2) at T = (303.15, 308.15, 313.15, 318.15 and 323.15) K

	T/K = 303.15		T/K = 308.15		T/K = 313.15		T/K = 318.15		T/K = 323.15	
x_1	ρ_{exp} /g·cm^{-3}	V_m^E /cm^3·mol^{-1}	ρ_{exp} /g·cm^{-3}	V_m^E /cm^3·mol^{-1}	ρ_{exp} /g·cm^{-3}	V_m^E /cm^3·mol^{-1}	ρ_{exp} /g·cm^{-3}	V_m^E /cm^3·mol^{-1}	ρ_{exp} /g·cm^{-3}	V_m^E /cm^3·mol^{-1}
0.0000	0.7940	0.0000	0.7888	0.0000	0.7835	0.0000	0.7783	0.0000	0.7730	0.0000
0.1003	0.8254	–0.4210	0.8204	–0.4389	0.8154	–0.4670	0.8104	–0.4862	0.8053	–0.5053
0.2000	0.8547	–0.6994	0.8499	–0.7308	0.8451	–0.7706	0.8403	–0.8042	0.8355	–0.8484
0.3010	0.8825	–0.8528	0.8778	–0.8833	0.8730	–0.9090	0.8683	–0.9415	0.8636	–0.9835
0.3991	0.9075	–0.8623	0.9030	–0.9000	0.8984	–0.9312	0.8939	–0.9712	0.8893	–1.0087
0.5001	0.9326	–0.8790	0.9282	–0.9118	0.9238	–0.9463	0.9194	–0.9812	0.9150	–1.0232
0.6000	0.9563	–0.8491	0.9520	–0.8758	0.9478	–0.9123	0.9436	–0.9513	0.9393	–0.9856
0.7008	0.9782	–0.6816	0.9741	–0.7103	0.9699	–0.7258	0.9658	–0.7561	0.9617	–0.7908
0.8001	0.9985	–0.4529	0.9946	–0.4827	0.9905	–0.4868	0.9856	–0.4141	0.9827	–0.5522
0.8997	1.0181	–0.2091	1.0143	–0.2292	1.0104	–0.2315	1.0065	–0.2420	1.0027	–0.2645
1.0000	1.0376	0.0000	1.0338	0.0000	1.0301	0.0000	1.0263	0.0000	1.0225	0.0000

Table 3. Coefficients, A_i, of Redlich–Kister Equation (Equation 2), Expressing Excess Molar Volumes, V_m^E and Standard Deviation, σ for the Binary Mixtures of Phenylmethanol (1) with 2–Butanone (2) at T = (303.15, 308.15, 313.15, 318.15 and 323.15) K

T/K	A_0	A_1	A_2	A_3	σ
303.15	–3.5764	–0.6174	–0.0394	–1.5488	0.0204
308.15	–3.7035	–0.6727	–0.1846	–1.4255	0.0186
313.15	–3.8312	–0.6856	–0.2004	–1.7601	0.0199
318.15	–3.9907	–0.8351	0.1331	–2.0097	0.0385
323.15	–4.1379	–0.7466	–0.4488	–1.7385	0.0222

Table 4. Composition and Experimental Viscosities, η_{exp} for the Binary Mixtures of Phenylmethanol (1) with 2–Butanone (2) at T = (303.15, 308.15, 313.15, 318.15 and 323.15) K

x_1	η_{exp} /mPa·s				
	T/K = 303.15	T/K = 308.15	T/K = 313.15	T/K = 318.15	T/K = 323.15
0.0000	0.362	0.345	0.330	0.316	0.303
0.1003	0.446	0.424	0.403	0.385	0.368
0.2000	0.554	0.524	0.497	0.472	0.451
0.3010	0.697	0.655	0.616	0.582	0.551
0.3991	0.876	0.818	0.765	0.718	0.676
0.5001	1.131	1.046	0.970	0.904	0.845
0.6000	1.476	1.351	1.242	1.146	1.063
0.7008	1.947	1.761	1.599	1.461	1.341
0.8001	2.586	2.307	2.063	1.866	1.694
0.8997	3.452	3.033	2.682	2.391	2.144
1.0000	4.689	4.058	3.531	3.103	2.747

1 **Table 5. Grunberg–Nissan Interaction Parameters (*d*) for the Binary Mixtures of Phenylmethanol**

2 **(1) with 2–Butanone (2) at *T* = (303.15, 308.15, 313.15, 318.15 and 323.15) K**

x_1	$T/\mathrm{K} = 303.15$	$T/\mathrm{K} = 308.15$	$T/\mathrm{K} = 313.15$	$T/\mathrm{K} = 318.15$	$T/\mathrm{K} = 323.15$
0.1003	−0.540	−0.474	−0.413	−0.358	−0.317
0.2000	−0.535	−0.470	−0.406	−0.352	−0.279
0.3010	−0.550	−0.483	−0.422	−0.368	−0.314
0.3991	−0.575	−0.507	−0.439	−0.380	−0.324
0.5001	−0.564	−0.497	−0.429	−0.370	−0.312
0.6000	−0.545	−0.476	−0.405	−0.344	−0.285
0.7008	−0.535	−0.466	−0.396	−0.334	−0.277
0.8001	−0.518	−0.453	−0.399	−0.325	−0.269
0.8997	−0.547	−0.487	−0.413	−0.350	−0.298

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1 **Table 6. Comparison of the Experimental and Calculated Values of the Kinematic Viscosity**

T/K	AAD/%	$|E_v|_{max}$/%	$|\Delta v/v|_{max} \times 100$
303.15	12.27	19.3	15.9
308.15	13.01	20.5	14.0
313.15	13.73	21.7	12.2
318.15	14.37	22.7	10.6
323.15	14.95	23.7	9.0

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T/K	AAD/%	$|E_v|_{max}$/%	$|\Delta v/v|_{max} \times 100$

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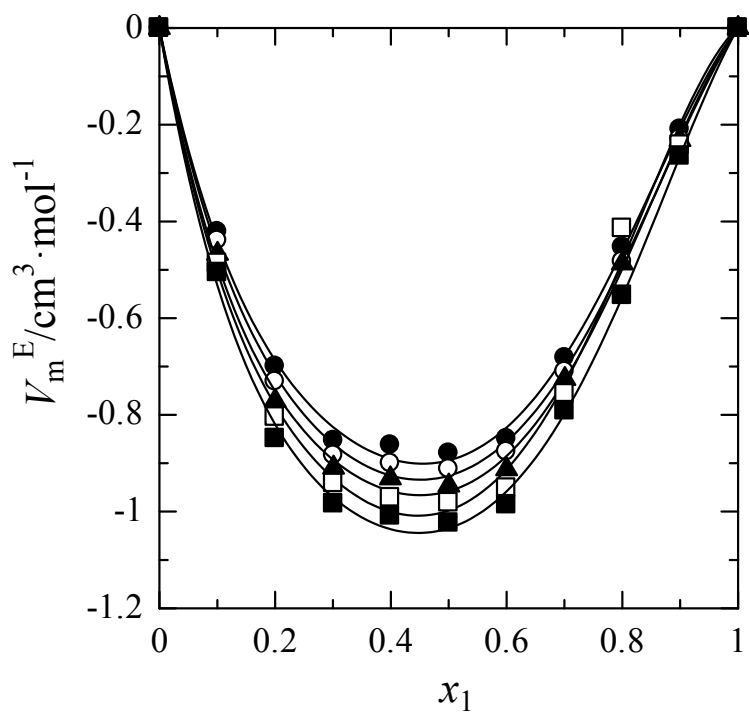
Figure 1. Excess molar volumes for the system phenylmethanol (1) + 2‑butanone (2): ●, 303.15 K; ○,
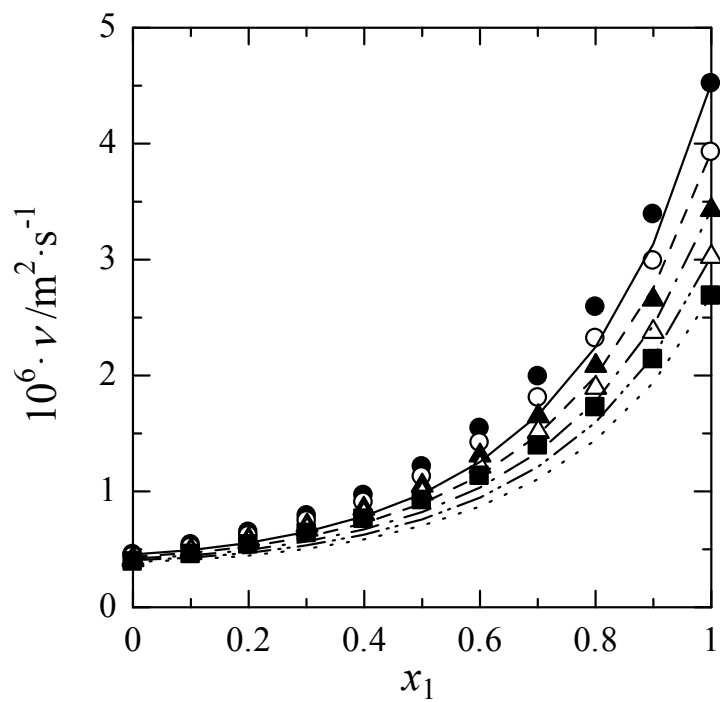
308.15 K; ▲, 313.15 K; □, 318.15 K; ■, 323.15 K.

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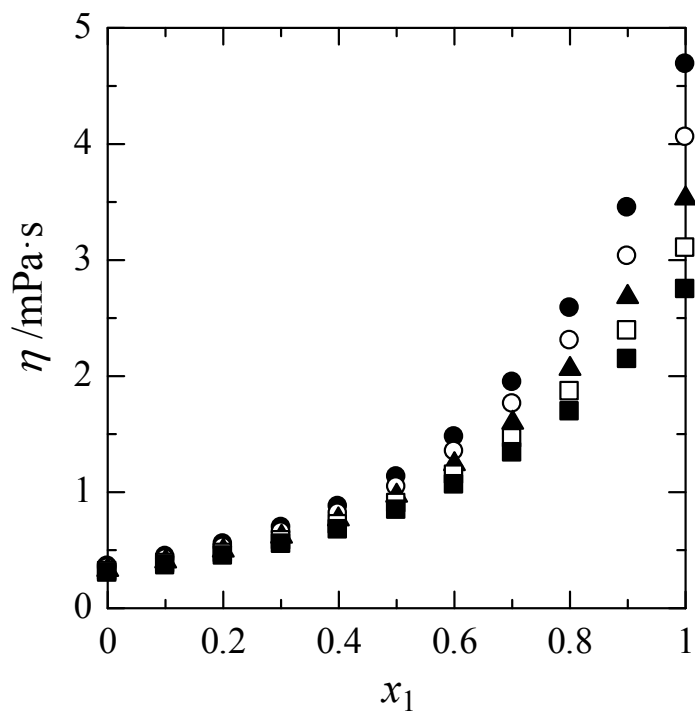
Figure 2. Experimental viscosities for the system phenylmethanol (1) + 2‑butanone (2): ●, 303.15 K;
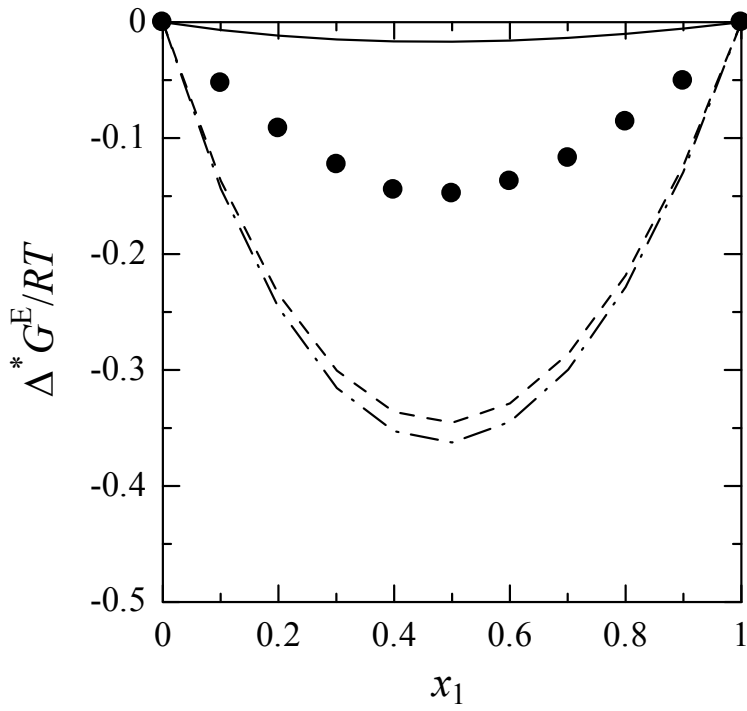
○, 308.15 K; ▲, 313.15 K; □, 318.15 K; ■, 323.15 K.

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Figure 3. Kinematic viscosities for the system phenylmethanol (1) + 2-butanone (2): ●, v_{exp} at 303.15

K; ○, v_{exp} at 308.15 K; ▲, v_{exp} at 313.15 K; □, v_{exp} at 318.15 K; ■, v_{exp} at 323.15 K ; —, v_{cal} at 303.15

K; − −, v_{cal} at 308.15 K; − · −, v_{cal} at 313.15 K; − · · −, v_{cal} at 318.15 K; ······, v_{cal} at 323.15 K.

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Figure 4. Excess Gibbs energy of activation for the system phenylmethanol (1) + 2‑butanone (2) at $T =$

303.15 K: ●, $\Delta^* G^E_{exp}/RT$; —, $\Delta^* G^{EC}_{cal}/RT$; – –, $\Delta^* G^{ER}_{cal}/RT$; – · –, $\Delta^* G^E_{cal}/RT$.

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