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Molar excess Gibbs free energy of 1-Propanol or 2-Propanol + aromatic hydrocarbons at 298.15 K in terms of an association model with a Flory contribution term

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Abstract

Molar excess Gibbs free energy of mixing values for 1-propanol or 2-propanol + benzene, toluene, o- m- or p-xylene at 298.15 K have been calculated by the Barker method from vapour pressure data measured by a static method. The free energies of mixing for these binary systems are also predicted in terms of the Mecke-Kempter type of association model with a Flory contribution term using two interaction parameters. The predicted values agree reasonably well with the experimental values.

Keywords: Aromatic hydrocarbons; Association model; Flory contribution term; Gibbs free energy of mixing

List of symbols

G^E	excess Gibbs free energy of mixing
G_0, G_1, G_2	adjustable parameters of Eq. (1)
H^E	excess enthalpy of mixing
K_T	isothermal compressibility
K^{ϕ}	constant defined by Eq. (6)
P_i	partial pressure of component *i*
P^*	characteristic pressure
P^0	vapour pressure of pure component

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$\tilde{P}$	reduced pressure
Q_{12}	interchange interaction parameters in entropy Eq. (9)
R	gas constant
r	residual pressure
S^E	excess molar entropy
T	thermodynamic temperature
T_i^*	characteristic temperature of component i
$\tilde{T}$	reduced temperature of mixture
$\tilde{T}_i$	reduced temperature of component i
V^E	excess volume of mixing
$\tilde{V}_i$	reduced volume of component i
$\tilde{V}$	reduced volume of mixture
V_i^*	characteristic molar volume of component i
x_i	mole fraction of component i
χ_{12}	interchange interaction parameter in Flory theory
Δh_H^0	standard molar enthalpy of H-bond formation
Δs_H^0	standard molar entropy of H-bond formation
Δv_H^0	standard molar volume of H-bond formation
ϕ	segment fraction
θ_2	contact surface fraction
γ_i	activity coefficient of component i
α	isobaric thermal expansivity
β	virial coefficient

1. Introduction

In our earlier work [1], we analysed the excess molar volume V^E and excess molar enthalpy H^E data of 1-propanol or 2-propanol + benzene, toluene, o-, m- or p-xylene at 298.15 K in terms of an association model proposed by Treszczanowicz and Benson [2]. In this paper, Gibbs free energies of mixing of these systems at 298.15 K calculated using the Barker method, and their interpretation in terms of the Mecke-Kempter (MK) type of association model combined with a Flory contribution term, are presented.

2. Experimental

1-Propanol, 2-propanol, benzene, toluene, *o*,*m*- and *p*-xylenes (E. Merck) were purified by standard procedures [3]. The purities of the final samples were checked by measuring their densities at 298.15 ± 0.01 K; these agreed to within $\pm 5 \times 10^{-5}$ g cm^{-3} with the corresponding literature values [4–7]. The total vapour pressures of 1-propanal or 2-propanal (1) + benzene, toluene, *o*-, *m*- or *p*-xylene (2) mixtures were measured as a function of liquid phase mole fraction x_1 at 298.15 ± 0.01 K by a static method [8] in the manner described by Nigam and Mahl [9] and recorded in Table 3,

Table 1

Molar volume (V), thermal expansivity (α), isothermal compressibility (K_T), virial coefficient (β) and vapour pressure (P^0) for the pure components at 298.15 K

Compound	V/cm^{3}mol^{-1}	$\alpha \times 10^3$/K^{-1}	$K_T \times 10^6$/cm^3 J^{-1}	β/cm^3 mol^{-1}	P^0/Torr	
					Our value	Literature
1-Propanol	75.164	0.9964	644.00	−1120.03	19.71	19.7[10]
2-Propanol	76.953	1.1167	795.00	−1024.78	44.01	44.0[10]
Benzene	89.399	1.217	937.78	−1355.94	94.21	94.2[13]
Toluene	106.861	1.071	1136.19	−1879.04	28.52	28.5[11]
o-Xylene	121.222	0.963	820.13	−2653.37	6.47	6.45[12]
m-Xylene	123.455	1.004	873.62	−2560.67	7.98	7.97[12]
p-Xylene	123.925	1.017	908.17	−2608.08	8.39	8.38[12]

below. The height of mercury column in the manometer was read to 0.001 cm. All the vapour pressure measurements were reproducible to better than ±0.02 Torr. Our experimental values for the vapour pressures of the pure compounds compared well with the literature values [10–13] as shown in Table 1.

The composition of the liquid phase was determined by measuring the refractive index using an Abbé refractometer in the manner described by Strubl et al. [14]. The uncertainties in the liquid phase composition were about 0.01 mol%.

3. Results

The excess Gibbs free energy of mixing G^E for the present alkanol (1) + aromatic hydrocarbon (2) mixtures were calculated from their vapour pressure data using Barker's method [15] and are recorded in Table 3. The form of function used for G^E following Redlich and Kister [16] is

$$G^E = x_1(1 - x_1) \sum_{n=1}^{2} [RTG_n(2x_1 - 1)^n] \tag{1}$$

where $G_n(n = 0\text{–}2)$ are the adjustable parameters. These parameters are recorded in Table 3. The virial coefficients required in these calculations were obtained from Berthelot's equation [17] and the critical constant data were taken from the literature [18].

4. Discussion

Ashcroft et al. [19] have determined the G^E values for the 2-propanol (1) + toluene (2) system at 298.15 K. Our values are in agreement with their values. However in the intermediate range our values are slightly more (at most 8%) than the literature values [19]. G^E values for all these systems are positive over the whole composition range.

Plots of G^E versus x_1 are symmetrical for the 1–propanol or 2–propanol (1) + benzene, toluene or *p*–xylene (2) systems, while these are slightly skewed towards low mole fraction of alkanol for 1-propanol or 2-propanol (1) + *o*- or *m*-xylene (2) systems. For an equimolar fraction, G^E values for 1-propanol or 2-propanol (1) + an aromatic hydrocarbon (2) vary in the order benzene < toluene < *p*-xylene < *o*-xylene ≈ *m*-xylene. The high positive value of G^E for these systems indicates the dissociation of hydrogen bonding in 1-propanol or 2-propanol by the addition of aromatic hydrocarbon.

Next we analysed the excess molar Gibbs free energy for the present binary systems in term of an association model proposed by Treszczanowicz and Benson [2]. According to this model, the excess Gibbs free energy of mixing G^E is composed of three type of contributions: the combinatorial contribution as described by the Flory–Huggin theory, the chemical (MK type of association of alkanol) contribution [2], and a physical contribution described by Flory theory [20, 21].

$$G^E = G^E_{comb} + G^E_{MK} + G^E_F \tag{2}$$

The combinatorial contribution is given by relation

$$G^E_{comb} = -TS^E_{comb} \tag{3}$$

where

$$S^E_{comb} = -R\sum_{i=1}^{2}[x_i \ln(\phi_i/x_i)] \tag{4}$$

The chemical (MK) contribution is given by [2]

$$G^E_{MK} = (x_1RT/K^\phi\phi_1)[\phi_1(1+K^\phi)\ln(1+K^\phi) - (1+K^\phi\phi_1)\ln(1+K^\phi\phi_1)] \tag{5}$$

where

$$K^\phi = \exp[1 - (\Delta h^0_H - T\Delta s^0_H)/RT - \ln(V^*/17.12\,\mathrm{cm^3\,mol^{-1}})] \tag{6}$$

and the physical contribution given by Flory

$$G^E_F = H^E_F - TS^E_F \tag{7}$$

where

$$H^E_F = x_1\theta_2(V^*_1/\tilde{V})\chi_{12} + \sum_{i=1}^{2}[x_iP^*_iV^*_i(\tilde{V}_i^{-1} - \tilde{V}^{-1})] \tag{8}$$

and

$$S^E_F = x_1\theta_2V^*_1Q_{12} - 3\sum_{i=1}^{2}(x_iP^*_iV^*_i/T_i^*)\ln[(\tilde{V}_i^{-1/3} - 1)/(\tilde{V}^{-1/3} - 1)] \tag{9}$$

The values of association constants like Δv^0_H, Δh^0_H and Δs^0_H for these binary systems were calculated in our earlier work [1] as suggested by Treszczanwicz and Benson [2]. These are reported again in Table 2. Using these values of Δh^0_H and Δs^0_H, K^ϕ was calculated from Eq.(6). Using this value of K^ϕ, G^E_{MK} was computed from Eq. (5).

Table 2
Values of various parameters (Δh_H^0, Δs_H^0 and Δv_H^0) of the Mecke-Kempter model along with the Flory interaction parameters χ_{12} and Q_{12} for alkanol (1) + aromatic hydrocarbon (2) at 298.15 K.

System	χ_{12}/J cm^{-3}	Q_{12}/J cm^{-3}	Δh_H^0/J mol^{-1}	Δs_H^0/J K^{-1}mol^{-1}	Δv_H^0/cm^3 mol^{-1}
1-Propanol(1) + benzene(2)	8.9504	0.0057	−23930.95	−35.32	−5
1-Propanol(1) + toluene(2)	−6.4079	−0.0460	−19887.91	−26.17	−5
1-Propanol(1) + o-xylene	−44.0099	−0.2491	−19024.19	−34.99	−5
1-Propanol(1) + m-xylene	−28.3810	−0.1932	−17807.91	−27.50	−5
1-Propanol(1) + p-xylene	−32.0774	−0.1811	−18102.67	−29.88	−5
2-Propanol(1) + benzene(2)	6.2426	−0.0386	−19805.54	−30.07	−5
2-Propanol(1) + toluene(2)	−20.5979	−0.1295	−18675.93	−31.22	−5
2-Propanol(1) + o-xylene	−38.1949	−0.1894	−20187.11	−40.69	−5
2-Propanol(1) + m-xylene(2)	−18.2970	−0.1441	−17945.83	−29.20	−5
2-Propanol(1) + p-xylene(2)	−30.3458	−0.1649	−19431.10	−37.34	−5

Calculation of the physical contribution G_F^E from Eq. (7) requires two unknown interaction parameters χ_{12} and Q_{12}. In order to calculate χ_{12}, V_F^E at equimole fractions is calculated from the relation

$$V_F^E = V_{\text{exptl}}^E - V_{\text{MK}}^E \tag{10}$$

where

$$V_{\text{MK}}^E = \Delta v_H^0 x_1 h(K^\phi, \phi_1) \tag{11}$$

and

$$h(K^\phi, \phi_1) = [\phi_1 \ln(1 + K^\phi) - \ln(1 + K^\phi \phi_1)]/K^\phi \phi_1 \tag{12}$$

This value of V_F^E was then used to calculate the Flory interaction parameter χ_{12} using the following set of equations [20,21]

$$V_F^E = V^* [\tilde{V} - \sum_{i=1}^{2} (\tilde{V}_i/\phi_i)] \tag{13}$$

$$\tilde{T} = (\tilde{V}^{1/3} - 1)/\tilde{V}^{4/3} \tag{14}$$

$$\chi_{12} = [\sum_{i=1}^{2} (\phi_i P_i^*) - \sum_{i=1}^{2} \phi_i P_i^* \tilde{T}_i/\tilde{T})]\phi_1 \theta_2 \tag{15}$$

Table 3

Measured total vapour pressure, P, partial pressure, P_1 and P_2 activity coefficients, γ_1 and γ_2, residual vapour pressure, $r = P_{\mathrm{exptl}} - P_{\mathrm{calcd}}$, Gibbs free energy of mixing, G^E, for different mole fractions x_1 of alkanol at 298.15 K; also included are the RTG_n ($n = 0$–2) J mol^{-}1) parameters of Eq. (1)

x_1	P/Torr	P_1/Torr	P_1/Torr	γ_1	γ_2	r/Torr	G^E/J mol^{-1}
1-Propanol (1) + benzene (2)							
0.0000	94.21	–	–	–	–	–	–
0.0481	97.60	7.61	90.85	8.0075	1.0128	−0.88	278.03
0.1211	100.31	10.34	88.75	4.3080	1.0713	1.22	588.52
0.2010	100.92	10.67	88.26	2.6802	1.1719	1.98	805.48
0.3052	98.40	11.02	87.20	1.8242	1.3317	0.17	948.17
0.3821	95.11	11.68	84.57	1.5426	1.4526	−1.13	982.51
0.4653	90.32	12.69	79.40	1.3783	1.5767	−1.78	973.69
0.5342	85.35	13.70	73.51	1.2960	1.6764	−1.87	939.90
0.6201	79.20	15.00	64.91	1.2224	1.8157	−0.70	870.39
0.6720	74.81	15.73	59.42	1.1836	1.9260	−0.35	813.75
0.7145	70.03	16.29	54.92	1.1526	2.0453	−1.16	758.01
0.8041	60.21	17.29	45.25	1.0884	2.4580	−2.33	605.59
0.8734	60.12	18.01	36.50	1.0434	3.0700	5.59	444.08
0.9342	37.31	18.68	24.99	1.0135	4.0504	−6.37	259.34
1.0000	19.71	–	–	–	–	–	–
$RTG_0 = 3887.15$; $RTG_1 = -987.61$; $RTG_2 = 1643.54$							
1-Propanol (1) + toluene (2)							
0.0000	28.52	–	–	–	–	–	–
0.0711	36.22	10.35	27.13	7.3933	1.0230	−1.27	404.87
0.1502	39.11	12.55	26.57	4.2414	1.0953	−0.04	729.82
0.2374	40.24	12.52	26.64	2.6686	1.2231	1.10	958.42
0.3117	40.45	12.23	26.86	1.9894	1.3661	1.36	1063.75
0.4171	39.77	12.23	26.82	1.4861	1.6119	0.71	1099.48
0.4826	38.92	12.50	26.34	1.3129	1.7831	0.07	1067.47
0.5490	38.18	12.97	25.31	1.1981	1.9649	−0.10	1001.06
0.6131	36.76	13.61	23.67	1.1248	2.1437	−0.52	910.14
0.6602	35.77	14.17	22.07	1.0872	2.2752	−0.46	829.26
0.7253	33.89	15.04	19.25	1.0508	2.4556	−0.40	700.90
0.8061	30.90	16.27	14.82	1.0230	2.6793	−0.19	519.15
0.8895	27.11	17.67	9.20	1.0072	2.9209	−0.24	309.38
0.9461	23.53	18.68	4.78	1.0017	3.1033	0.08	155.36
1.0000	19.71	–	–	–	–	–	–
$RTG_0 = 4212.46$; $RTG_1 = -1780.37$; $RTG_2 = 530.74$							
1-Propanol (1) + *o*-xylene (2)							
0.0000	6.47	–	–	–	–	–	–
0.0510	17.60	10.18	6.22	10.0821	1.0113	1.25	318.64
0.1091	20.14	14.39	6.05	6.6913	1.0477	−0.03	614.93
0.1910	22.31	16.15	5.94	4.2958	1.1319	0.20	938.62
0.2682	23.50	16.71	5.89	3.1585	1.2397	0.92	1154.50
0.3431	24.20	16.94	5.83	2.5212	1.3684	1.31	1297.97
0.4282	24.70	17.47	5.74	2.0699	1.5481	1.48	1391.75
0.4910	24.81	17.77	5.66	1.8359	1.7144	1.38	1419.63

Table 3 (*Continued*)

x_1	P/Torr	P_1/Torr	P_1/Torr	γ_1	γ_2	r/Torr	G^E/J mol^{-1}
0.5672	24.81	18.05	5.56	1.6147	1.9807	1.18	1407.02
0.6214	24.60	18.18	5.51	1.4844	2.2409	0.91	1365.89
0.7031	24.20	18.25	5.48	1.3168	2.8376	0.48	1247.33
0.7844	23.41	18.25	5.47	1.1807	3.9045	-0.31	1050.92
0.8775	22.10	18.42	5.16	1.0649	6.5293	-1.51	706.62
0.9491	20.80	18.94	3.70	1.0124	11.2200	-1.84	333.93
1.0000	19.71	–	–	–	–	–	–
$RTG_0 = 5683.21$; $RTG_1 = 182.70$; $RTG_2 = 1320.03$							
1-Propanol (1) + *m*-xylene (2)							
0.0000	7.98	–	–	–	–	–	–
0.0372	16.01	6.94	7.72	9.5066	1.0036	1.32	216.27
0.0951	20.80	13.41	7.40	7.1703	1.0239	-0.05	517.31
0.1605	22.89	16.83	7.18	5.3272	1.0694	-1.15	805.23
0.2323	24.30	18.10	7.06	3.9516	1.1504	-0.86	1057.90
0.3231	25.32	18.01	7.08	2.8272	1.3083	-0.22	1283.33
0.4102	25.56	17.37	7.24	2.1473	1.5339	0.95	1402.62
0.4555	25.51	17.01	7.36	1.8948	1.6876	1.14	1427.97
0.5092	25.20	16.66	7.50	1.6596	1.9092	1.04	1426.28
0.5991	24.63	16.30	7.70	1.3805	2.3994	0.63	1348.69
0.6746	23.88	16.29	7.69	1.2250	2.9580	-0.11	1214.19
0.7457	23.00	16.54	7.39	1.1252	3.6409	-0.95	1032.76
0.8349	22.10	17.24	6.29	1.0474	4.7647	-1.43	734.88
0.9075	21.10	18.13	4.39	1.0137	5.9390	-1.43	439.12
1.0000	19.71	–	–	–	–	–	–
$RTG_0 = 5715.94$; $RTG_1 = -479.43$; $RTG_2 = -141.55$							
1-Propanol (1) + *p*-xylene (2)							
0.0000	8.39	–	–	–	–	–	–
0.0421	16.25	7.32	8.09	8.8176	1.0053	0.85	239.70
0.0810	19.14	11.39	7.87	7.1164	1.0195	-0.09	438.05
0.1411	21.30	14.56	7.65	5.2364	1.0593	-0.91	701.71
0.2201	22.80	15.88	7.52	3.6588	1.1462	-0.59	971.52
0.2982	23.40	15.85	7.52	2.6963	1.2751	0.02	1156.02
0.3721	23.61	15.49	7.62	2.1100	1.4426	0.51	1259.12
0.4613	23.60	15.06	7.76	1.6565	1.7140	0.77	1296.74
0.5372	23.40	14.92	7.83	1.4085	2.0142	0.64	1259.44
0.6012	23.10	14.98	7.78	1.2644	2.3223	0.33	1182.55
0.6624	22.70	15.23	7.57	1.1665	2.6659	-0.10	1073.47
0.7433	22.10	15.83	6.89	1.0808	3.1902	-0.62	881.40
0.8162	21.45	16.65	5.72	1.0349	3.7159	-0.94	667.59
0.9091	20.61	18.04	3.35	1.0066	4.4088	-0.80	349.20
1.0000	19.71	–	–	–	–	–	–
$RTG_0 = 5141.32$; $RTG_1 = -1004.47$; $RTG_2 = -140.06$							
2-Propanol (1) + benzene (2)							
0.0000	94.21	–	–	–	–	–	–
0.0541	106.40	20.85	90.53	8.7239	1.0149	-4.98	325.22

Table 3 (*Continued*)

x_1	P/Torr	P_1/Torr	P_1/Torr	γ_1	γ_2	r/Torr	G^E/J mol^{-1}
0.1011	112.12	26.22	88.97	5.8651	1.0492	−3.05	550.32
0.1492	115.71	27.46	88.44	4.1668	1.1015	−0.21	731.76
0.2420	118.62	26.93	88.95	2.5171	1.2432	2.74	962.86
0.3551	117.53	26.51	89.45	1.6888	1.4696	1.57	1076.72
0.4433	114.34	27.25	87.72	1.3909	1.6700	−0.63	1070.27
0.4972	112.05	28.13	85.23	1.2803	1.7970	−1.32	1035.10
0.5562	108.71	29.39	81.10	1.1963	1.9374	−1.78	974.74
0.6201	104.32	31.05	74.90	1.1338	2.0910	−1.63	887.80
0.7190	94.07	34.02	62.01	1.0717	2.3427	−1.96	716.39
0.7881	84.08	36.25	50.83	1.0426	2.5480	−3.00	572.89
0.8613	71.62	38.73	36.86	1.0200	2.8264	−3.97	399.57
0.9431	56.04	41.69	17.53	1.0039	3.2825	−3.20	176.71
1.0000	44.01	–	–	–	–	–	–

$RTG_0 = 4130.90$; $RTG_1 = -1717.41$; $RTG_2 = 871.10$

2-Propanol (1) + toluene (2)

0.0000	28.52	–	–	–	–	–	–
0.0451	43.71	14.91	27.46	7.5331	1.0071	1.28	242.61
0.1122	50.34	25.02	26.43	5.0652	1.0415	−1.11	540.78
0.1741	53.25	28.69	25.87	3.7412	1.0953	−1.30	755.88
0.2533	55.76	30.48	25.47	2.7336	1.1923	−0.20	957.00
0.3460	57.04	31.40	25.16	2.0607	1.3446	0.48	1100.21
0.4162	57.25	31.98	24.87	1.7450	1.4892	0.39	1150.75
0.4790	57.75	32.60	24.48	1.5453	1.6430	0.66	1158.10
0.5444	57.65	33.38	23.88	1.3919	1.8330	0.38	1130.65
0.6152	57.23	34.36	22.94	1.2685	2.0834	−0.07	1062.84
0.7071	56.78	35.91	21.03	1.1531	2.5095	−0.16	917.76
0.7850	55.59	37.46	18.52	1.0837	3.0120	−0.40	744.15
0.8721	53.35	38.59	14.05	1.0310	3.8380	−0.28	492.36
0.9372	49.52	41.58	8.53	1.0078	4.7652	0.62	261.23
1.0000	44.01	–	–	–	–	–	–

$RTG_0 = 4612.31$; $RTG_1 = -651.47$; $RTG_2 = 517.60$

2-Propanol (1) + *o*-xylene (2)

0.0000	6.47	–	–	–	–	–	–
0.0821	31.00	25.04	6.11	6.9363	1.0255	−0.15	451.48
0.1252	35.31	29.54	6.00	5.3618	1.0564	−0.22	640.13
0.1560	37.28	31.29	5.94	4.5611	1.0847	0.03	756.89
0.2144	38.56	33.07	5.88	3.5075	1.1511	−0.40	940.99
0.2732	39.66	33.98	5.83	2.8274	1.2336	−0.16	1082.20
0.3612	40.71	34.92	5.75	2.1975	1.3860	0.03	1221.86
0.4201	41.40	35.53	5.69	1.9227	1.5097	−0.16	1272.96
0.4732	42.01	36.12	5.63	1.7347	1.6403	0.27	1292.47
0.5542	42.70	37.01	5.48	1.5173	1.8896	0.22	1276.01
0.6212	43.05	37.69	5.33	1.3785	2.1667	0.02	1220.39
0.7250	43.59	38.66	5.07	1.2114	2.8318	−0.13	1054.26
0.8190	43.84	39.63	4.66	1.0992	3.9472	−0.43	807.45
0.9234	44.00	41.46	3.30	1.0201	6.6086	−0.75	404.04
1.0000	44.01	–	–	–	–	–	–

Table 3 (*Continued*)

x_1	P/Torr	P_1/Torr	P_1/Torr	γ_1	γ_2	r/Torr	G^E/J mol^{-1}
$RTG_0 = 5172.55$; $RTG_1 = -176.25$; $RTG_2 = 960.84$							
2-Propanol (1) + *m*-xylene (2)							
0.0000	7.98	–	–	–	–	–	–
0.0431	29.10	20.48	7.73	10.8347	1.0097	0.83	277.55
0.0892	34.51	28.46	7.58	7.2596	1.0385	−1.55	523.67
0.1362	37.14	31.12	7.50	5.1959	1.0833	−1.49	727.72
0.1842	38.82	31.92	7.47	3.9409	1.1417	−0.58	894.19
0.2502	39.92	32.38	7.44	2.9406	1.2376	0.11	1065.19
0.3333	41.25	33.24	7.36	2.2662	1.3764	0.65	1203.99
0.4112	42.32	34.59	7.18	1.9120	1.5215	0.54	1273.30
0.4922	43.51	36.32	6.90	1.6768	1.6948	−0.29	1294.73
0.5784	44.44	38.08	6.53	1.4958	1.9334	−0.18	1266.38
0.6745	45.20	39.52	6.15	1.3310	2.3549	−0.46	1169.21
0.7814	45.64	40.37	5.80	1.1740	3.3120	−0.55	959.75
0.8821	45.53	41.13	5.28	1.0594	5.5634	−0.86	627.69
0.9802	44.34	43.23	1.95	1.0020	12.1871	−0.82	127.56
1.0000	44.01	–	–	–	–	–	–
$RTG_0 = 5177.26$; $RTG_1 = -162.12$; $RTG_2 = 1681.71$							
2-Propanol (1) + *p*-xylene (2)							
0.0000	8.39	–	–	–	–	–	–
0.0721	29.52	20.52	7.96	6.4747	1.0188	1.04	376.75
0.1371	33.32	26.94	7.73	4.4680	1.0636	−1.35	640.60
0.1852	35.41	28.99	7.62	3.5572	1.1110	−1.19	795.28
0.2490	37.62	30.30	7.54	2.7672	1.1908	−0.23	953.43
0.3201	39.10	31.16	7.45	2.2133	1.3010	0.47	1073.92
0.4102	40.24	32.15	7.32	1.7813	1.4731	0.76	1153.52
0.4972	41.02	33.26	7.12	1.5200	1.6801	0.65	1162.67
0.5613	41.33	34.17	6.91	1.3834	1.8674	0.25	1130.77
0.6723	42.04	35.91	6.36	1.2140	2.3050	−0.24	1001.47
0.7254	42.35	36.82	6.00	1.1534	2.5957	−0.48	905.97
0.7903	42.91	38.02	5.44	1.0932	3.0716	−0.54	757.89
0.8782	43.32	39.96	4.20	1.0340	4.0742	−0.83	496.86
0.9372	43.85	41.64	2.73	1.0096	5.1575	−0.52	277.68
1.0000	44.01	–	–	–	–	–	–
$RTG_0 = 4647.76$; $RTG_1 = -541.15$; $RTG_2 = 710.71$							

The other interaction parameter Q_{12} was calculated by assuming that at equimolar fractions $G_F^E = G_{\text{exptl}}^E - G_{\text{comb}}^E - G_{\text{MK}}^E$, and by using Eq. (7)–(9). The values of χ_{12} and Q_{12}, along with association parameters Δh_H^0 and Δs_H^0, for all the present systems are recorded in Table 2. G^F at other mole fractions for all these (1 + 2) binary systems were calculated from Eq. (2) and are recorded in Table 3. It has been observed from plots of G_{calcd}^E and G_{exptl}^E against x_1 (Fig. 1 and Fig. 2) that the G^E values are in reasonable agreement with G_{exptl}^E.

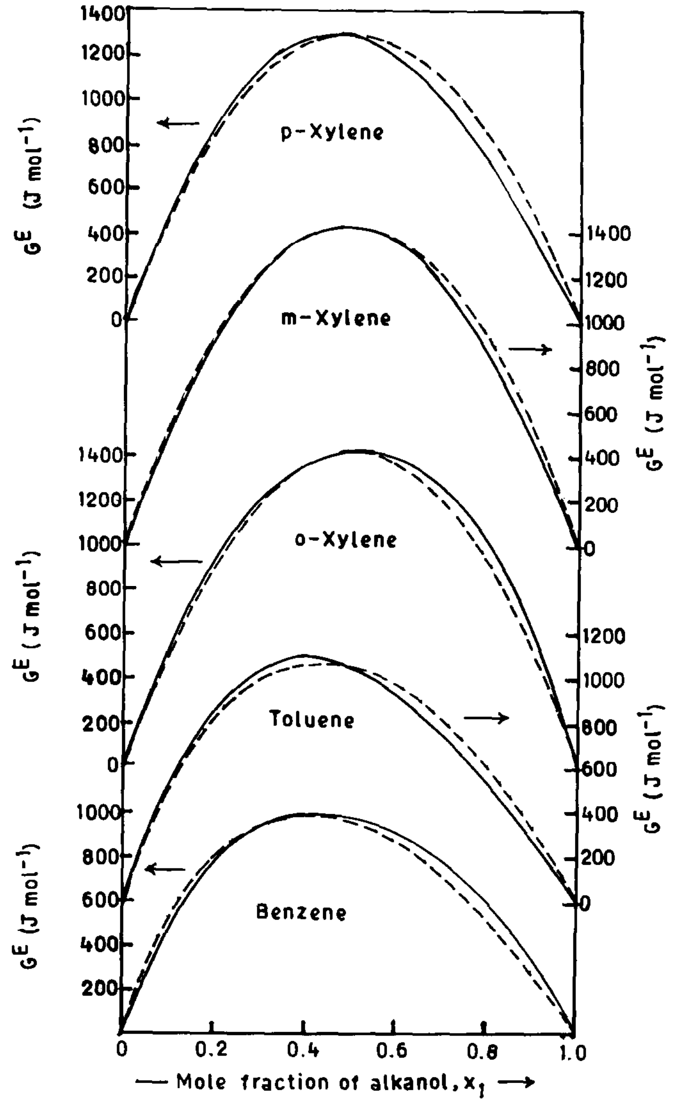

Fig. 1. Molar excess Gibbs free energy, G^E, of 1-propanol (1) + aromatic hydrocarbons (2) at 298.15 K: —, G^E(exptl); – – G^E(calcd).

Thus it may be concluded that the G^E values for 1-propanol or 2-propanol(1) + benzene, toluene, *o*-, *m*- or *p*-xylene (2) at 298.15 K may be represented by an MK-type association model with a Flory contribution term [2] using two interaction parameters χ_{12} and Q_{12}.

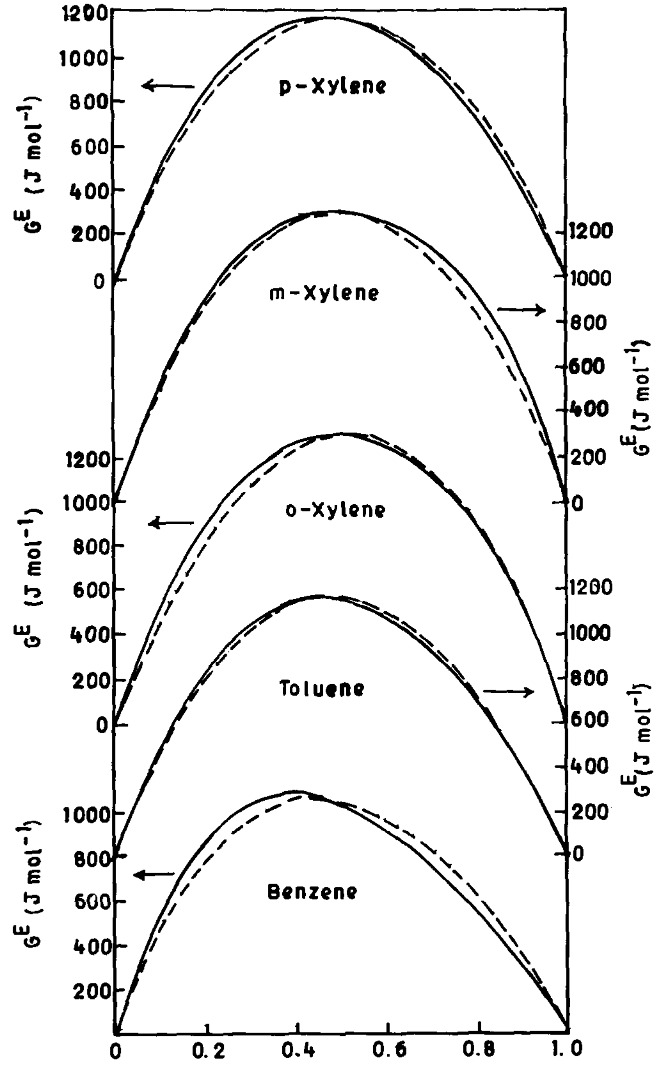

Fig. 2. Molar excess Gibbs free energy, G^E, of 2-propanol (1) + aromatic hydrocarbons (2) at 298.15 K: —, G^E(exptl); – – G^E(calcd).

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