J. Chem. Eng. Data 1989, 34, 409-412

Vapor–Liquid Equilibria for the Systems 1,3,5-Trimethylbenzene–1-Propyl Alcohol and 1,3,5-Trimethylbenzene–2-Propyl Alcohol

Fernando Aguirre-Ode* and Jenny Aldoney

Departamento de Química, Facultad de Ciencia, Universidad Técnica Federico Santa María, Valparaíso, Chile

Isothermal vapor–liquid equilibrium data at four different temperatures over the entire range of composition were obtained by using a vapor-recirculating equilibrium still for the binary systems formed by 1,3,5-trimethylbenzene and either 1-propyl alcohol or 2-propyl alcohol. Fits to NRTL, Wilson, UMAS, UNIQUAC, and other models by a nonlinear regression method based on the maximum-likelihood principle were tried. The best fits for both systems are obtained successively in the same order in which the models are mentioned above, the deviations being not significantly different from one model to the other. Calculated values with UNIFAC show considerable deviation.

Introduction

Vapor–liquid equilibrium data for the binary systems formed by 1,3,5-trimethylbenzene (1,3,5-TMB), also known as mesitylene, and either 1-propyl alcohol (1-PrOH) or 2-propyl alcohol (2-PrOH) were not found in the available literature. For this reason their measurement and correlation to current models was considered to be an interesting contribution, especially due to the fact that they are examples of associated solutions formed by pure fluids showing important boiling point differences.

Experimental Section

1,3,5-Trimethylbenzene was a Fluka analytical grade reagent with a certified minimum purity of 99.5%. It was redistilled in a high-efficiency packed column. The heart cut was collected by discarding the first 20% distillate and the last 20% residue. Both 1-propyl alcohol and 2-propyl alcohol were Merck analytical grade reagents with a certified minimum purity of 99.0%. The treatment was similar to that described for 1,3,5-trimethylbenzene, except for the addition of magnesium to the latter during the distillations. A chromatographic analysis made to each heart cut showed no significant peak other than the main one. Refractive indices showed good agreement with literature values and they are given in Table I. Vapor pressures of the pure fluids were measured with the still described below and showed to be accurate within ±0.3 Torr when compared with Antoine-type equations:

$$\ln P = 16.2893 - 3614.19/(T - 63.57) \qquad (1)$$

for 1,3,5-trimethylbenzene (*1*),

$$\ln P = 18.0699 - 3452.06/(T - 68.51) \qquad (2)$$

for 1-propyl alcohol (*2*), and

$$\ln P = 18.6919 - 3640.20/(T - 53.54) \qquad (3)$$

for 2-propyl alcohol (*2*). P is given in Torr and T in kelvin in eq 1–3.

Vapor pressures of the solutions were measured at constant temperature as a function of composition by using a vapor-recirculating equilibrium still, which was a simplified version of that described by Hipkin and Myers (*3*). Instead of the vapor jacket used in the original design, the contactor is self-lagged with its own vapor so as to assure adiabatic conditions. A schematic view of the apparatus has been shown elsewhere (*4*). The equilibrium still was connected through a cold trap to the regulating and measuring pressure devices. Pressures were measured by a mercury manometer and were corrected to give the equivalent heights of a mercury column at 273.15 K and standard gravity. Experimental vapor pressures are considered to be accurate to approximately ±0.5 Torr. Temperatures were measured by a certified thermometer (Will Scientific 710-5) with a stated accuracy of ±0.1 K. Compositions of the liquid and condensed vapor were determined from measurements of their refractive indices at 298.15 K by using an Abbe-type refractometer with an accuracy of ±0.0002. The best fits of the refractive index to polynomials are given in Table I. Compositions were estimated to be within ±0.002 mole fraction accuracy for the liquid phase and within ±0.010 for the vapor phase.

Table I. Refractive Indices of Pure Fluids and Their Solutions at 298.15 K as Given by the Polynomial

$$n_D = x_1n_1 + x_2n_2 + x_1x_2(a_0 + a_1x_2 + a_2x_2^2 + a_3x_2^3 + a_4x_2^4)$$

	1,3,5-Trimethylbenzene (1) +	
	1-propyl alcohol (2)	2-propyl alcohol (2)
n_1	1.4973 (1.4967)[a]	1.4973
n_2	1.3835 (1.3837)[b]	1.3755 (1.3752)[b]
a_0	0.08400	0.06184
a_1	−0.23194	−0.06866
a_2	0.70268	0.34268
a_3	−0.78112	0.49725
a_4	0.32778	0.27015
std dev	±0.00025	±0.00018

[a] Reference *1*. [b] Reference *2*.

Results and Discussion

The vapor–liquid equilibrium data for the binary systems 1,3,5-trimethylbenzene with 1- and 2-propyl alcohol are given respectively in Tables II and III. In order to appraise the interpretative ability of different models, the experimental data were tested with several of them given in the current literature. In this report, only those that gave relatively good correlations are informed: the Renon–Prausnitz NRTL equation (*5*), Wilson equation (*6*), unified model of athermal associated solutions (UMAS) (*7*), modified UNIQUAC equation (*8*, *9*), and generalized model of ideal associated solutions (GMAS) (*10*). The computer program developed by Prausnitz et al. (*11*) with convenient modifications was used to estimate the best parameters of the respective activity coefficients by a nonlinear regression method based on the maximum-likelihood principle (*12*). The equations for the corresponding activity coefficients for the above-mentioned models are shown in Table IV.

The objective function

$$\psi = \sum_{i=1}^{N}\sum_{j=1}^{n}[(y_j - \hat{y}_j)/\sigma_j]_i^2 \qquad (4)$$

in which N is the total number of experimental points, n is the

Table II. Vapor–Liquid Equilibrium Data for the Binary System 1,3,5-Trimethylbenzene (1)–1-Propyl Alcohol (2)

no.	P, Torr	t, °C	x_1	y_1
1	116.1	55.0	0.093	0.048
2	112.6	55.0	0.163	0.066
3	110.4	55.0	0.247	0.080
4	109.1	55.0	0.291	0.088
5	107.8	55.0	0.357	0.092
6	106.1	55.0	0.362	0.092
7	104.7	55.0	0.417	0.091
8	100.1	55.0	0.512	0.093
9	99.2	55.0	0.545	0.101
10	98.7	55.0	0.559	0.098
11	87.5	55.0	0.752	0.121
12	85.3	55.0	0.793	0.131
13	84.9	55.0	0.796	0.120
14	149.2	60.0	0.087	0.045
15	147.3	60.0	0.151	0.061
16	141.7	60.0	0.243	0.075
17	140.0	60.0	0.271	0.081
18	137.9	60.0	0.314	0.085
19	137.3	60.0	0.361	0.088
20	135.8	60.0	0.364	0.088
21	135.3	60.0	0.396	0.092
22	133.8	60.0	0.402	0.097
23	131.4	60.0	0.473	0.085
24	129.3	60.0	0.488	0.092
25	121.2	60.0	0.658	0.115
26	112.6	60.0	0.762	0.120
27	107.7	60.0	0.789	0.132
28	106.6	60.0	0.810	0.130
29	103.4	60.0	0.829	0.136
30	102.7	60.0	0.834	0.131
31	190.3	65.0	0.086	0.042
32	183.6	65.0	0.158	0.063
33	183.3	65.0	0.229	0.073
34	175.1	65.0	0.311	0.082
35	175.8	65.0	0.319	0.079
36	174.8	65.0	0.356	0.085
37	169.7	65.0	0.396	0.085
38	167.3	65.0	0.459	0.086
39	160.5	65.0	0.614	0.084
40	149.1	65.0	0.703	0.104
41	142.6	65.0	0.734	0.108
42	140.9	65.0	0.758	0.107
43	131.1	65.0	0.818	0.129
44	132.9	65.0	0.829	0.127
45	239.3	70.0	0.086	0.042
46	233.6	70.0	0.148	0.058
47	225.6	70.0	0.248	0.073
48	222.7	70.0	0.269	0.077
49	217.4	70.0	0.338	0.078
50	219.8	70.0	0.352	0.087
51	220.0	70.0	0.354	0.081
52	211.3	70.0	0.424	0.094
53	208.3	70.0	0.465	0.089
54	203.0	70.0	0.537	0.095
55	200.3	70.0	0.584	0.093
56	198.0	70.0	0.639	0.094
57	195.3	70.0	0.628	0.103
58	198.0	70.0	0.639	0.094
59	184.9	70.0	0.705	0.104

Table III. Vapor–Liquid Equilibrium Data for the Binary System 1,3,5-Trimethylbenzene (1)–2-Propyl Alcohol (2)

no.	P, Torr	t, °C	x_1	y_1
1	176.8	50.0	0.005	0.004
2	168.0	50.0	0.079	0.024
3	170.0	50.0	0.082	0.024
4	166.1	50.0	0.137	0.030
5	164.6	50.0	0.139	0.033
6	163.5	50.0	0.187	0.036
7	161.1	50.0	0.215	0.036
8	158.9	50.0	0.227	0.041
9	161.1	50.0	0.239	0.037
10	156.1	50.0	0.300	0.043
11	149.9	50.0	0.412	0.048
12	150.0	50.0	0.426	0.045
13	149.8	50.0	0.470	0.050
14	138.4	50.0	0.574	0.057
15	139.9	50.0	0.637	0.064
16	126.9	50.0	0.740	0.066
17	126.1	50.0	0.769	0.053
18	284.2	60.0	0.034	0.014
19	279.0	60.0	0.059	0.019
20	278.3	60.0	0.082	0.023
21	276.2	60.0	0.092	0.023
22	273.0	60.0	0.109	0.026
23	269.7	60.0	0.127	0.031
24	270.0	60.0	0.139	0.031
25	267.5	60.0	0.163	0.029
26	266.4	60.0	0.172	0.032
27	257.6	60.0	0.236	0.037
28	260.6	60.0	0.239	0.037
29	252.2	60.0	0.320	0.042
30	252.2	60.0	0.341	0.039
31	246.7	60.0	0.386	0.042
32	244.7	60.0	0.416	0.047
33	229.7	60.0	0.519	0.055
34	226.8	60.0	0.533	0.061
35	233.5	60.0	0.568	0.056
36	223.1	60.0	0.589	0.054
37	220.5	60.0	0.650	0.052
38	188.3	60.0	0.818	0.075
39	442.8	70.0	0.051	0.014
40	436.6	70.0	0.072	0.020
41	437.0	70.0	0.075	0.014
42	429.3	70.0	0.097	0.023
43	426.7	70.0	0.121	0.023
44	424.9	70.0	0.139	0.025
45	418.0	70.0	0.155	0.029
46	419.4	70.0	0.169	0.026
47	402.9	70.0	0.261	0.028
48	398.4	70.0	0.273	0.047
49	403.2	70.0	0.285	0.032
50	400.1	70.0	0.317	0.031
51	384.5	70.0	0.342	0.044
52	377.6	70.0	0.420	0.045
53	383.7	70.0	0.428	0.038
54	347.8	70.0	0.591	0.057
55	343.9	70.0	0.641	0.061
56	687.0	80.0	0.029	0.010
57	677.8	80.0	0.052	0.011
58	671.6	80.0	0.069	0.014
59	665.3	80.0	0.081	0.019
60	664.4	80.0	0.088	0.021
61	656.5	80.0	0.115	0.026
62	651.1	80.0	0.125	0.030
63	645.8	80.0	0.155	0.020
64	643.0	80.0	0.175	0.024
65	604.5	80.0	0.299	0.035
66	604.4	80.0	0.313	0.045
67	593.5	80.0	0.327	0.047
68	577.3	80.0	0.385	0.047
69	569.9	80.0	0.480	0.053
70	555.7	80.0	0.482	0.050
71	531.4	80.0	0.633	0.059

total number of variables, σ_j are the estimated standard deviations for the respective measured variables, y_j, and $\hat{y}_j$ are the respective calculated values of the variables. The magnitude of each σ_j was taken as that already indicated under Experimental Section.

The fugacity coefficients were calculated by the virial equation of state in terms of pressure, neglecting third and higher order coefficients. Second virial coefficients were obtained through the Hayden and O'Connell correlation (*13*). Molar volumes were calculated with the Rackett equation as modified by Spencer and Danner (*14*).

For the liquid phase, the standard-state fugacities at the saturation pressure of the pure fluids were calculated with eq 1–3. The constants used for the calculation of both fugacity and activity coefficients are given in Tables V and VI.

The resulting parameters from the fit to each model of the liquid phase for both binary systems are shown in Table VII, with the assumption that all of them are independent of tem-

Table IV. Equations for the Activity Coefficients of the Models

NRTL Equation (*5*)

$\gamma_i = \exp[x_j^2\{(\tau_{ji}G_{ji}^2/\Omega_j) - (\tau_{ij}G_{ij}/\Omega_i)\}]; \quad i = 1, 2; j = 3 - i$

in which

$G_{ij} = \exp(-\alpha_{ij}\tau_{ij})$

$\tau_{ij} = \Delta_{ij}/RT$

$\Omega_i = (x_j + x_iG_{ij})^2$

Δ_{ij}: adjustable energy parameter

α_{ij}: adjustable parameter (when given, $\alpha_{ij} = 0.47$)

Wilson Equation (*6*)

$\gamma_i = \Omega_i^{-1} \exp[x_j\{(\Lambda_{ij}/\Omega_i) - (\Lambda_{ji}/\Omega_j)\}]; \quad i = 1, 2, j = 3 - i$

in which

$\Omega_i = x_i + x_j\Lambda_{ij}$

$\Lambda_{ij} = (v_j/v_i) \exp(-\Delta_{ij}/RT)$

v_i: molar liquid volume

Δ_{ij}: adjustable energy parameter

UMAS Equations (*7*)

$\gamma_1 = (\epsilon r/x) \exp[1 - (\epsilon v_1/v) + x_2\Omega + \Phi v_1 x_2^2(1 + \eta)]$

$\gamma_2 = (\phi/x_2\phi^\circ) \exp[v_2(v - v^\circ)/vv^\circ - x_1\Omega + \Phi v_2 r x_1^2(\epsilon^2 r + \eta)]$

in which

$\Phi = \chi/RTx^2$

$x = x_2 + r\epsilon x_1$

$\epsilon = \epsilon^\circ x_2 + x_1$

$\Omega = x_1(\epsilon^\circ - 1)(v_1/v - 1/\epsilon)$

$\eta = (\epsilon^\circ - 1)x_2^2 = (\epsilon - 1)x_2$

$v = v_2/[x_1/x + (\phi/\alpha)\{\beta + (\beta - 1)\alpha \ln \alpha/K\phi\}]; \quad v^\circ$ when $x_2 = 1$

$\alpha = 1 - K\phi$

$\phi = 2x_2/[2Kx_2 + x + \{x(x + 4\beta Kx_2)\}^{1/2}]; \quad \phi^\circ$ when $x_2 = 1$

v_1, v_2: molar liquid volumes

K: equilibrium constant for association according to Nath and Bender (*17*)

Modified UNIQUAC Equation (*8, 9*)

$\gamma_i = (\phi_i/x_i)(\theta_i/\phi_i)^{zq_i/2}\Omega_i^{-q_i'} \exp(\eta_j); \quad i = 1, 2; j = 3 - i$

in which

$\phi_i = x_ir_i/(x_ir_i + x_jr_j)$

$\theta_i = x_iq_i/(x_iq_i + x_jq_j); \quad \theta_i'$ when q_i'

$\Omega_i = \theta_i' + \theta_j'\tau_{ji}$

$\tau_{ij} = \exp(-\Delta_{ij}/RT)$

$\eta_i = \phi_i(l_j - r_jl_i/r_i) + q_i'\theta_j'\{(\tau_{ji}/\Omega_i) - (\tau_{ij}/\Omega_j)\}$

$l_i = (z/2)(r_i - q_i) - (r_i - 1)$

z: coordination number, equal to 10

r_i: structural size parameter

q_i, q_i': structural area parameters

Δ_{ij}: adjustable energy parameter

GMAS Equations (*10*)

$\gamma_1 = \{(1 - x)/x)/x_1\} \exp[(\chi v_1/RT)/\{1 + (x_2/rx_1)\}^2]$

$\gamma_2 = (x_m/x_m^\circ x_2) \exp[(\chi v_2/RT)/\{1 + (rx_1/x_2)\}^2]$

in which

$x = \{(1 - x_m)^{-\beta} - 1\}/\beta\Omega$

$\Omega = 2[\exp(\Delta_{ij}/RT)]/(\beta + 1)$

x_m calculated iteratively from

$x_2 = \beta\Omega x_m/[(1 - \Omega x_m)^{\beta+1}(1 + \beta\Omega) + (\beta + 1)\Omega x_m - 1]; x_m^\circ$ for $x_2 = 1$

Δ_{ij}: adjustable energy parameter

β: adjustable binary parameter

χ: adjustable Scatchard–Hildebrand-type parameter

UNIFAC Equations (*15, 16*)

$\gamma_i = (\phi_i/x_i)(\theta_i/\phi_i)^{zq_i/2}[\prod_k(\Gamma_k/\Gamma_k^{(i)})^{\nu_{ki}}] \exp(\eta_j); \quad i = 1, 2; j = 3 - i$

in which

$\ln r_i = q_k[1 - \ln (\sum_l\theta_l\tau_{lk}) - (\sum_l\theta_l\tau_{lk})/(\sum_m\theta_m\tau_{ml})];$ $\Gamma_k^{(i)}$ for $x_i = 1$

$\tau_{lm} = \exp(-\Delta_{lm}/T)$

$\eta_i = \phi_i(l_j - r_jl_i/r_i)$

$r_i = \sum_k\nu_{ki}r_k$

$q_i = \sum_k\nu_{ki}q_k$

ν_{ki}: number of groups of type k in molecule i

ϕ_i, θ_i, l_i, z: defined as in UNIQUAC equation

$\theta_l, q_k, r_k, \Delta_{lm}$: as in UNIQUAC but applied to groups

Table V. Fixed Parameters for the Calculation of both Fugacity and Activity Coefficients (*1, 2, 17*)

parameter	1,3,5-TMB	1-PrOH	2-PrOH
critical temperature, K	637.3	536.71	508.32
critical pressure, bar	30.9	51.70	47.64
Rackett parameter	0.255	0.2485	0.254
mean radius of gyration, Å	4.34	2.736	2.726
dipole moment, D	0.10	1.68	1.66
association parameter[a]	0.0	1.40	1.32
UNIQUAC r	4.07	2.78	2.78
UNIQUAC q	3.32	2.51	2.51
UNIQUAC q'	3.32	0.89	0.89
vaporization entropy, J/(mol K)		−115.2	−117.5
vaporization enthalpy, kJ/mol		−42.68	−41.76
ideal temperature of vaporization, K		274.9	274.9

[a] Solvation parameter was taken as zero for both systems.

Table VI. UNIFAC Parameters (*15, 16*)

	no. of subgroups			parameters	
subgroup	1,3,5-TMB	1-PrOH	2-PrOH	r	q
CH_3		1	2	0.9011	0.848
CH_2		2		0.6744	0.540
CH			1	0.4469	0.228
OH		1	1	1.000	1.200
ACH	3			0.5313	0.400
$ACCH_3$	3			1.2663	0.968

	interaction energies					
subgroup	CH_3	CH_2	CH	OH	ACH	$ACCH_3$
CH_3				986.5	61.13	76.5
CH_2				986.5	61.13	76.5
CH				986.5	61.13	76.5
OH	156.4	156.4	156.4		89.6	25.82
ACH	−11.12	−11.12	−11.12	636.1		167.0
$ACCH_3$	69.7	69.7	69.7	803.2	−146.8	

perature. This assumption may not apply strictly, but it allows testing of the data more severely against the models. Table VII gives also a measure of the overall fit of the respective equation to the experimental data, defined as

$$\sigma = [\psi/(N - n_p)]^{1/2} \tag{5}$$

in which n_p is the number of adjustable parameters. This quantity approximates to the overall variance of errors. The magnitudes of the correlation coefficients give an indication of the degree of independence between the parameters of a model. When the parameters are completely independent, the value of the correlation coefficients is zero; as the parameters become more and more correlated, they approach a value of +1 or −1.

The three-parameter NRTL equation gives the best fit in both binary systems, followed quite closely by the two-parameter Wilson equation and the two-parameter version of the NRTL model. Slight increases of the overall fit follow the same order given in Table VII for the different models. Values of the variables calculated with the UNIFAC equation (*15*, *16*) given an overall variance of errors almost 2 orders of magnitude higher, a fact that suggests a revision of some of its fixed parameters.

From the analysis of both the quality of the overall fit and the degree of independence of the parameters, the three-parameter NRTL model is the one that represents the data more closely.

Bubble point pressure deviations shown in the last column of Table VII are within experimental error in all models, and they are reasonably scattered. Vapor mole fraction deviations are mostly of the same sign, which may be an indication of either some lack of thermodynamic consistency of this kind of data or inadequacy of the models. However, experimental vapor compositions are almost within experimental error in the system with 2-propyl alcohol and not too far from experimental error in the system with 1-propyl alcohol.

Glossary

A, *B*, *C*	generalized parameters for models (Table VII)
a_i	coefficient of the *i*th power of polynomial
G_{ij}	abbreviated quantity in NRTL equation
K	Nath and Bender association equilibrium constant

Table VII. Parameters and Standard Deviations for the Models Applied to the Systems Formed by 1,3,5-Trimethylbenzene with either 1-Propyl or 2-Propyl Alcohol

model	system[a]	A^b	B^c	C^d	σ	σ_p
NRTL-3	TMB/1-P	944.4 ± 53.9	817.8 ± 28.2	0.540 ± 0.020	5.76	0.40
	TMB/2-P	994.5 ± 63.8	813.1 ± 20.4	0.536 ± 0.014	5.45	0.38
Wilson	TMB/1-P	306.4 ± 17.3	1311.1 ± 26.7		6.03	0.46
	TMB/2-P	366.9 ± 16.0	1268.5 ± 38.2		5.65	0.40
NRTL-2	TMB/1-P	822.9 ± 20.5	751.7 ± 13.9	0.47	6.31	0.50
	TMB/2-P	824.7 ± 30.0	756.5 ± 12.6	0.47	6.20	0.42
UMAS	TMB/1-P	1.701 ± 0.112	25.7 ± 8.12	1.00	6.70	0.41
	TMB/2-P	1.988 ± 0.124	27.0 ± 12.86	1.00	6.36	0.42
UNIQUAC	TMB/1-P	907.7 ± 19.9	−132.0 ± 2.8		7.55	0.56
	TMB/2-P	924.5 ± 29.5	−132.9 ± 2.7		6.83	0.45
GMAS	TMB/1-P	1248 ± 108	2.92 ± 0.72	−0.165 ± 0.042	6.86	0.47
	TMB/2-P	2019 ± 382	18.1 ± 22.1	−0.048 ± 0.016	6.53	0.39
UNIFAC	TMB/1-P				618.1	
	TMB/2-P				375.1	

[a] TMB, 1,3,5-trimethylbenzene; 1-P, 1-propyl alcohol; 2-P, 2-propyl alcohol. [b] A: Δ_{12} for NRTL, Wilson, UNIQUAC, and GMAS; χ/R for UMAS. [c] B: Δ_{21} for NRTL, Wilson, and UNIQUAC; β for UMAS and GMAS. [d] C: α_{12} for NRTL; χ/R for GMAS; ϵ° for UMAS.

l_i	abbreviated quantity in UNIQUAC and UNIFAC equations
n	number of variables
n_D	refractive index of solutions
n_i	refractive index of pure component i
n_p	number of parameters
N	number of experimental points
P	saturation pressure
q_i, q_i'	structural area parameters
r	liquid volume ratio
r_i	structural size parameter
R	universal gas constant
v	molar volume of liquid mixture
v_i	molar volume of pure liquid i
x	abbreviated quantity in UMAS and GMAS equations
x_i	liquid mole fraction of component i
x_m	mole fraction of monomeric species
y_i	vapor mole fraction of component i
y_j	generalized calculated variable
$\hat{y}_j$	generalized experimental variable
z	coordination number in UNIQUAC and UNIFAC equations

Greek Letters

α	abbreviated quantity in UMAS equations
α_{ij}	adjustable or fixed parameter in NRTL equation
β	adjustable parameter in UMAS and GMAS equations
γ_i	activity coefficient of component i
Γ_k	activity coefficient of group k in UNIFAC equations
Δ_{ij}	adjustable energy parameter
ϵ	abbreviated quantity in UMAS equations
ϵ°	adjustable volumetric parameter in UMAS equations
η	abbreviated quantity in UMAS equations
η_i	abbreviated quantity for component i in UNIQUAC equation
θ_i	surface fraction of either group or component i
Λ_{ij}	abbreviated quantity in Wilson equation
ν_{ki}	number of groups of type k in molecule i
σ	total variance of the fit
σ_j	estimated standard deviation for variable j
τ_{ij}	abbreviated quantity in NRTL, UNIQUAC, and UNIFAC equations
ϕ	volume fraction of monomeric species
ϕ_i	size fraction or volume fraction of component i
Φ	abbreviated quantity in UMAS equations
χ	adjustable Scatchard–Hildebrand type parameter
ψ	objective function or total sum of squares
Ω	abbreviated quantity in UMAS and GMAS equations
Ω_i	abbreviated quantity in Wilson, NRTL, and UNIQUAC equations

Registry No. 1,3,5-TMB, 108-67-8; 1-PrOH, 71-23-8; 2-PrOH, 67-63-0.

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Received for review October 11, 1988. Accepted June 6, 1989. Financial support by FONDECYT (Chile) is duly acknowledged.