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y y

T = (278.15 333.15)

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ABSTRACT

(+)
y y . , (+)
, , , 1- , , , y , y
(y + y)
278.15 333.15 . , y
. (278.15 333.15) ,
y y .
A , B λ ,
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© 2015 . A .

1. Introduction

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. (1, 17 19 3 3 , W345.42, y y .
A : 73590-58-6), , y, y
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278.15 333.15 y -
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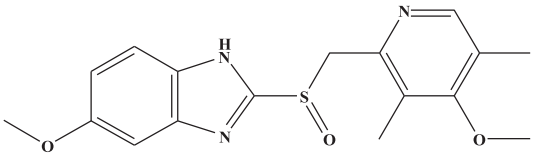

FIGURE 1. .

2. Experimental

2.1. Materials and apparatus

y ⩾0.980
M, M . ., . y -
y y (y
680). W
y (-2),
., .
y y ,
., . y.
.
y y y (
y A 7820A A). -
1.
y (: B A224) -
(B) ., . y
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-2006) y B y ., .
y T = ▪0.05 .

2.2. Methods

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T = 431.15 , T = 430.65 , T = 428.15 T = 428.65 -
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429.15 (u(T) = 0.85).
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y . ,
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24 (+) -
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5,6 .
, , -
y y . A , 1
5
y y -
. . A
y
. A
y, .
y (x)
y . (1). y -
(x_A) y y . (2).

$$x = \frac{m_1/M_1}{m_1/M_1 + m_i/M_i} \quad (1)$$

$$x_A = \frac{m_2/M_2}{m_2/M_2 + m_3/M_3} \quad (2)$$

m1, m2, m3 , y -
, y; M1, M2, M3
, y -
, y.

3. Results and discussion

3.1. In pure solvents

3.1.1. Solubility and correlation models

y (x)
, , , 1- , , , y
y
(278.15 333.15) 2 2.
( )
2.
:

$$RD = \frac{x_i - x_{ci}}{x_i} \quad (3)$$

x_i y , x_ci -
y .
(A) 3 5.
(A) :

$$A = \frac{1}{N}\sum_{i=1}^{N}\frac{x_i - x_{ci}}{x_i} \quad (4)$$

TABLE 1
y .

M			
	M (. −1)	M y A y	
	345.42	0.980	M, M . ., .
W	18.02		y
M	32.04	0.995	y
	46.07	0.997	y
1-B	74.12	0.990	y
A	41.05	0.999	y
A	58.08	0.995	y
y	88.11	0.997	y
y	72.11	0.990	y

TABLE 2
M y (x) (278.15 333.15) 0.1M .[a,b]

T/	1000x	100		
		. (5)	. (6)	. (9)
		Water		
278.15	0.0407	6.14	−9.15	−5.35
283.15	0.0500	2.03	−8.45	−5.81
288.15	0.0615	−0.69	−7.00	−5.39
293.15	0.0764	−1.02	−3.89	−3.14
298.15	0.0936	−1.46	−1.75	−1.69
303.15	0.1145	−0.97	0.52	0.09
308.15	0.1377	−0.95	1.58	0.84
313.15	0.1652	−0.13	2.75	1.87
318.15	0.1959	0.58	3.13	2.33
323.15	0.2297	1.09	2.68	2.15
328.15	0.2631	0.16	0.14	0.11
333.15	0.2994	−0.53	−2.89	−2.11
		Methanol		
278.15	2.058	3.33	−9.66	−7.27
283.15	2.639	0.41	−8.70	−6.98
288.15	3.480	1.65	−3.95	−2.87
293.15	4.350	−1.10	−4.10	−3.50
298.15	5.691	1.97	1.08	1.26
303.15	6.863	−1.90	−1.33	−1.46
308.15	8.573	−1.10	0.39	0.05
313.15	10.55	−0.69	1.21	0.75
318.15	12.89	−0.06	1.73	1.29
323.15	15.62	0.81	2.01	1.69
328.15	18.61	0.81	0.95	0.90
333.15	21.65	−0.62	−2.06	−1.67
		Ethanol		
278.15	1.574	7.74	0.37	3.55
283.15	1.875	2.51	−2.76	−0.43
288.15	2.243	−1.56	−4.89	−3.37
293.15	2.612	−7.61	−9.30	−8.50
298.15	3.465	0.81	0.56	0.70
303.15	4.130	−0.90	−0.20	−0.50
308.15	5.085	1.45	2.70	2.12
313.15	6.047	1.12	2.60	1.87
318.15	7.019	−0.91	0.47	−0.23
323.15	8.316	−0.19	0.70	0.22
328.15	9.818	0.84	0.87	0.83
333.15	11.26	−0.44	−1.66	−1.02
		1-Butanol		
278.15	1.282	6.99	−5.84	−2.64
283.15	1.532	−0.36	−9.60	−7.25
288.15	1.962	0.30	−5.21	−3.78
293.15	2.404	−2.17	−4.88	−4.15
298.15	3.026	−0.71	−1.20	−1.06
303.15	3.702	−0.96	0.08	−0.21
308.15	4.550	0.31	2.25	1.68
313.15	5.401	−0.89	1.43	0.72
318.15	6.504	0.33	2.42	1.75
323.15	7.788	1.86	3.19	2.74
328.15	8.842	−1.03	−0.98	−1.02
333.15	10.35	−0.02	−1.85	−1.23
		Acetonitrile		
278.15	1.177	5.78	−6.29	−3.07
283.15	1.425	−0.26	−8.87	−6.52
288.15	1.821	0.20	−4.97	−3.52
293.15	2.221	−2.80	−5.39	−4.64
298.15	2.732	−3.77	−4.28	−4.12
303.15	3.538	1.57	2.49	2.22
308.15	4.286	1.27	3.04	2.49
313.15	5.126	0.65	2.77	2.09
318.15	6.075	0.05	2.01	1.35
323.15	7.113	−0.88	0.40	−0.06
328.15	8.431	0.27	0.32	0.28
333.15	9.775	0.00	−1.69	−1.09
		Acetone		
278.15	1.463	4.30	−4.47	−0.95
283.15	1.731	−0.89	−7.03	−4.52
288.15	2.155	−0.09	−3.67	−2.17
293.15	2.648	0.35	−1.23	−0.54

(*continued on next page*)

TABLE 2 (*continued*)

T/	1000*x*	100		
		. (5)	. (6)	. (9)
298.15	3.126	−2.25	−2.33	−2.27
303.15	3.773	−1.76	−0.75	−1.18
308.15	4.638	1.41	3.01	2.30
313.15	5.415	0.22	2.05	1.21
318.15	6.372	0.56	2.19	1.41
323.15	7.388	0.13	1.15	0.64
328.15	8.496	−0.45	−0.48	−0.49
333.15	9.815	0.07	−1.47	−0.71
		Ethyl acetate		
278.15	0.9807	3.66	2.86	6.65
283.15	1.124	−0.27	−0.98	1.76
288.15	1.338	0.02	−0.52	1.15
293.15	1.565	−1.03	−1.38	−0.60
298.15	1.854	−0.45	−0.59	−0.54
303.15	2.199	0.66	0.72	0.22
308.15	2.535	−0.74	−0.52	−1.37
313.15	2.927	−1.62	−1.29	−2.29
318.15	3.426	−0.75	−0.41	−1.31
323.15	4.049	1.36	1.62	1.05
328.15	4.696	1.92	1.96	1.97
333.15	5.226	−1.37	−1.71	−0.83
		Tetrahydrofuran		
278.15	4.577	12.68	−6.92	−10.04
283.15	6.437	10.74	−2.96	−5.29
288.15	8.434	4.13	−5.27	−7.03
293.15	11.31	1.43	−4.07	−5.26
298.15	14.62	−3.18	−5.70	−6.42
303.15	19.63	−2.13	−2.37	−2.68
308.15	25.88	−1.20	−0.04	−0.03
313.15	32.73	−2.88	−0.99	−0.77
318.15	42.45	−0.46	1.42	1.74
323.15	54.51	2.34	3.65	3.93
328.15	66.34	1.19	1.46	1.60
333.15	78.86	−1.06	−2.35	−2.53

[a] y $u_r(x) = 2.00\%$. y *u* $u(T) = 0.05$, $u(p) = 2$.

[b] *x* y .

3.1.2. The modi"ed Apelblat model

y A 7 9 :

$$x = A + \frac{B}{(T/K)} + C \quad (T/\ ) \tag{5}$$

T , *A*, *B*, *C* , *x* y . *A* *B* y - y, *C* y, y(△*Cp*) 10,11 . A 3.

3.1.3. Buchowski Ksiazaczak λh model

B λ y B y. λ λ . λ :

$$1 + \frac{\lambda(1-x)}{x} = \lambda h \left(\frac{1}{(T/K)} - \frac{1}{(T_m/K)}\right) \tag{6}$$

x y , *T* - T_m 12 14 . λ 4.

3.1.4. Ideal model

(+) y 15 . :

$$x\gamma = \frac{\Delta_{disso}H}{R}\left(\frac{1}{T_m} - \frac{1}{T}\right) \tag{7}$$

W ($\gamma = 1$), :

$$A \overset{def}{=} \frac{\Delta_{disso}H}{R} \times \frac{1}{T_m}, \quad B \overset{def}{=} -\frac{\Delta_{disso}H}{R} \tag{8}$$

W . (9):

$$x = A + \frac{B}{T} \tag{9}$$

x y , *T* . *A* *B* 5.

3.1.5. Thermodynamic parameters

' y y- . y (Δ H_m^0) :

$$\Delta H_m^0 = -R \times \frac{x}{(1/T)} \tag{10}$$

R (8.314 ∫ · $^{-1}$ · $^{-1}$ *T* . . (5), . (11) 16 :

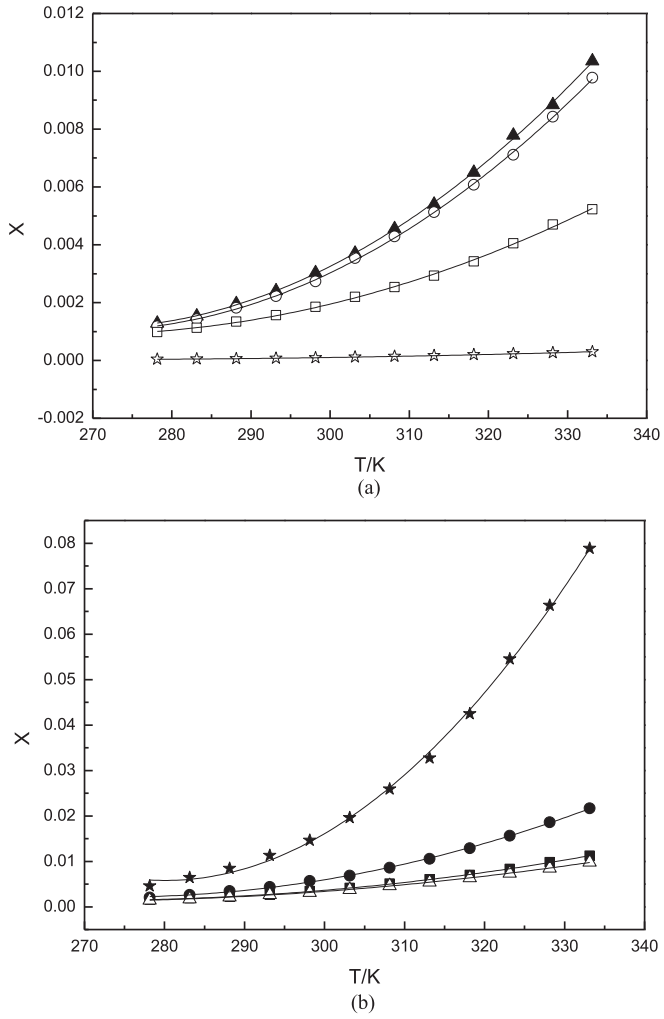


FIGURE 2. M y (x) (T)
: ( ) ☆, W ; □, y ; ○, A ;
▲, 1-B ; ( ) △, A ; ■, ; ●, M ; ★, y .

$$\Delta H_m^0 = -(b - cT)R \tag{11}$$

B y y -
, y
y y
y .
y (Δ G_m^0) :

$$\Delta G_m^0 = -RT \quad x \tag{12}$$

TABLE 3
A
(278.15 333.15) .

	A	B	C	10^2 A
W	128.17	−9170.28	−18.72	1.31
M	110.16	−8641.07	−15.16	1.20
	53.88	−5627.47	−7.14	2.17
1-B	110.12	−8334.80	−15.44	1.33
A	100.63	−7929.87	−14.02	1.46
A	65.40	−6002.12	−8.95	1.04
y	−34.21	−1199.77	5.61	1.15
y	207.2	−13842.9	−28.9	3.62
			(10^2 A) = 13.29	

TABLE 4
λh .

	100λ		10^2 A
W	0.21	1453065	3.66
M	25.80	14540.97	3.10
	8.66	36768.28	2.26
1-B	8.72	37881.21	3.24
A	8.47	39469.21	3.54
A	6.36	46625.85	2.49
y	2.64	100547.6	1.21
y	210.30	2278.137	3.10
		(10^2 A) = 22.60	

TABLE 5
(278.15 333.15) .

	A	B	10^2 A
W	1.84	−3310.50	2.57
M	7.82	−3875.08	2.47
	5.71	−3392.12	1.95
1-B	5.93	−3495.80	2.35
A	5.99	−3533.63	2.62
A	5.00	−3203.27	1.53
y	3.61	−2948.77	1.15
y	11.52	−4676.96	3.94
		(10^2 A) = 18.60	

A ,
y (Δ S_m^0)
y y y 17 .
$\%\xi_H$ $\%\xi_S$
Δ G_m^0 y y y
.

$$\Delta S_m^0 = \frac{\Delta H_m^0 - \Delta G_m^0}{T} \tag{13}$$

$$\%\xi_H = \frac{|\Delta H_m^0|}{|\Delta H_m^0| + |T \cdot \Delta S_m^0|} \times 100\% \tag{14}$$

$$\%\xi_S = \frac{|T \cdot \Delta H_S^0|}{|\Delta H_m^0| + |T \cdot \Delta S_m^0|} \times 100\% \tag{15}$$

Δ H_m^0, Δ S_m^0, Δ G_m^0, $\%\xi_H$ $\%\xi_S$
278.15 333.15 6.

3.2. Binary solvent mixtures

3.2.1. Solubility and correlation models

y (x)
(y + y) y

TABLE 6
y
278.15 333.15 .

	Δ H_m/ J · mol^{-1}	Δ S_m/ J · K^{-1} · mol^{-1}	Δ G_m/ J · mol^{-1}	% ξ_H(%)	% ξ_S(%)
W	28.67	19.49	22.87	83.84	16.16
M	33.32	68.88	12.39	61.40	38.60
	28.64	49.04	13.71	65.72	34.28
1-B	30.06	52.93	14.01	65.21	34.79
A	30.30	53.10	14.18	65.28	34.72
A	27.16	43.47	13.94	67.26	32.74
y	24.23	28.93	15.34	73.30	26.70
y	41.65	105.44	9.66	56.51	43.49

TABLE 7
M. y (x) (y + y) y 278.15 333.15 0.1M. .[a,b]

x_A	100x	100 $x - x$ /x(. (5))	100 $x - x$ /x(. (17))	100 $x - x$ /x(. (20))
		T = 278.15 K		
0.0000	0.0981	3.6649	0.0000	5.5665
0.1748	0.1348	5.9638	5.5327	1.8428
0.3397	0.1652	1.2125	4.1823	1.5203
0.4955	0.2227	5.2449	0.1319	1.9871
0.6429	0.2767	6.7786	1.2538	2.1144
0.7826	0.3242	5.5088	0.0160	2.2598
0.9153	0.3882	8.9930	0.5848	1.7342
1.0000	0.4577	12.6848	0.0000	0.7236
		T = 283.15 K		
0.0000	0.1124	0.2684	0.0000	4.8445
0.1748	0.1714	2.3923	3.5859	1.5088
0.3397	0.2358	4.2893	0.5303	0.6774
0.4955	0.3108	4.0902	1.5784	1.3937
0.6429	0.3905	5.7810	0.1742	1.4349
0.7826	0.4756	7.3272	2.1831	1.1860
0.9153	0.5453	6.3833	1.9287	1.2373
1.0000	0.6437	10.7355	0.0000	0.2921
		T = 288.15 K		
0.0000	0.1338	0.0192	0.0000	8.5736
0.1748	0.2260	3.4979	0.9541	3.1181
0.3397	0.3254	5.7285	0.7396	0.2739
0.4955	0.4389	5.9433	0.3892	1.1966
0.6429	0.5454	5.7368	0.3353	1.5966
0.7826	0.6589	5.8666	0.3530	1.3970
0.9153	0.7654	5.7591	0.2405	1.3186
1.0000	0.8434	4.1327	0.0000	0.9861
		T = 293.15 K		
0.0000	0.1565	1.0316	0.0000	9.0428
0.1748	0.2832	0.7754	1.2106	3.1296
0.3397	0.4197	2.3069	0.8292	0.5059
0.4955	0.5756	2.5284	0.3702	1.2927
0.6429	0.7218	2.4412	0.3262	1.6508
0.7826	0.8778	2.5783	0.3813	1.3477
0.9153	1.024	2.5414	0.2698	1.2624
1.0000	1.131	1.4290	0.0000	0.8699
		T = 298.15 K		
0.0000	0.1854	0.4524	0.0000	7.5555
0.1748	0.3514	1.9198	1.4146	2.3090
0.3397	0.5301	1.7739	0.8929	0.9857
0.4955	0.7344	2.0184	0.3503	1.5828
0.6429	0.9259	2.2710	0.3160	1.9021
0.7826	1.130	2.3162	0.4016	1.6145
0.9153	1.322	2.4211	0.2918	1.5817
1.0000	1.462	3.1847	0.0000	1.2283
		T = 303.15 K		
0.0000	0.2199	0.6572	0.0000	12.2283
0.1748	0.4465	1.1276	1.7652	4.4016
0.3397	0.6905	1.2900	0.9918	0.9167
0.4955	0.9694	1.4826	0.3114	1.5215
0.6429	1.231	1.6392	0.2955	1.9652
0.7826	1.510	1.6802	0.4334	1.3696
0.9153	1.771	1.7388	0.3275	1.3651
1.0000	1.963	2.1316	0.0000	0.7413
		T = 308.15 K		
0.0000	0.2535	0.7413	0.0000	8.2666
0.1748	0.5570	1.2135	2.2370	3.7023
0.3397	0.8838	1.1731	1.1098	0.3657
0.4955	1.257	1.1371	0.2545	0.4095
0.6429	1.607	1.1322	0.2656	0.6697
0.7826	1.981	1.1100	0.4722	0.0570
0.9153	2.331	1.0983	0.3720	0.1113
1.0000	2.588	1.2049	0.0000	0.4408
		T = 313.15 K		
0.0000	0.2927	1.6211	0.0000	8.6342
0.1748	0.6801	2.5013	2.6160	4.6684
0.3397	1.097	2.7898	1.1954	1.9404
0.4955	1.574	2.8591	0.2072	1.4026
0.6429	2.021	2.8849	0.2411	1.8411
0.7826	2.498	2.9148	0.5011	0.7072
0.9153	2.945	2.9194	0.4055	1.0413
1.0000	3.273	2.8761	0.0000	0.1045

TABLE 7 (*continued*)

x_A	100x	100 $x - x$ /x(. (5))	100 $x - x$ /x(. (17))	100 $x - x$ /x(. (20))
		T = 318.15 K		
0.0000	0.3426	0.7523	0.0000	2.0653
0.1748	0.8499	0.5386	3.1017	4.7896
0.3397	1.396	0.6556	1.2962	0.0444
0.4955	2.021	0.6305	0.1458	1.2213
0.6429	2.606	0.5997	0.2098	0.9049
0.7826	3.230	0.6067	0.5358	1.9213
0.9153	3.816	0.5905	0.4461	1.3964
1.0000	4.245	0.4593	0.0000	2.1521
		T = 323.15 K		
0.0000	0.4049	1.3603	0.0000	3.2393
0.1748	1.061	2.1093	3.5451	5.4543
0.3397	1.767	2.0965	1.3810	2.1463
0.4955	2.575	2.1482	0.0896	3.7452
0.6429	3.332	2.1898	0.1816	3.4442
0.7826	4.139	2.1907	0.5659	4.2983
0.9153	4.896	2.2087	0.4813	3.5521
1.0000	5.451	2.3398	0.0000	4.1167
		T = 328.15 K		
0.0000	0.4696	1.9167	0.0000	10.1601
0.1748	1.271	1.5017	3.8228	2.8242
0.3397	2.134	1.2996	1.4312	0.2445
0.4955	3.120	1.2209	0.0545	2.0362
0.6429	4.045	1.1883	0.1641	1.6015
0.7826	5.032	1.1547	0.5841	2.2424
0.9153	5.956	1.1398	0.5026	1.1901
1.0000	6.634	1.1873	0.0000	1.5623
		T = 333.15 K		
0.0000	0.5226	1.3652	0.0000	10.8603
0.1748	1.480	1.2143	4.2287	1.0755
0.3397	2.511	1.0496	1.5010	1.8659
0.4955	3.689	1.0167	0.0034	0.7902
0.6429	4.793	1.0105	0.1390	1.0476
0.7826	5.972	0.9886	0.6099	0.8115
0.9153	7.076	0.9870	0.5328	1.4920
1.0000	7.886	1.0636	0.0000	1.3953

[a] y $u_r(x) = 2.0000\%$, $u_r(x_A) = 2.00\%$. u $u(T) = \pm 0.05$, $u(p) = \pm 2$.

[b] x_A y y .x y ; x y.

278.15 333.15 7. y 3.

3.2.2. Modi ed Apelblat model

A y 3.1 8.

3.2.3. CNIBS/R K Model

y y y B y / (B /) 18 22 , y y . (4):

$$x = x_A \quad X_A + x_B \quad X_B + x_A x_B \sum_{i=0}^{N} S_i (x_A - x_B)^i \tag{16}$$

x y , x_A x_B y , X_A X_B y - y y- y . S_i N 0, 1, 2 3. W $N = 2$ $(1 - x_A)$ x_B, . (16) :

$$x - (1 - x_A) \quad X_B - x_A \quad X_A = (1 - x_A) x_A [S_0 + S_1 (2x_A - 1) + S_2 (2x_A - 1)^2] \tag{17}$$

B / . S_i y { $x - (1 - x_A)$ $X_B - x_A$ X_A} {$(1 - x_A) x_A [S_0 + S_1 (2x_A - 1) + S_2 (2x_A - 1)^2]$} 9. , B / y y y . - y , .

3.2.4. Jouyban Acree model

y - y y 23 :

$$x = x_A \quad X_A + x_B \quad X_B + x_A x_B \sum_{i=0}^{N} \frac{J_i (x_A - x_B)^i}{T} \tag{18}$$

J_i T . y . (16). W $N = 2$ $(1 - x_A)$ x_B, . (18) :

TABLE 8

A y
.

x_A	A	$B/100$	C	M
0.0000	−34.21	−12.00	5.61	1.1542
0.1748	69.05	−69.08	−9.04	2.0630
0.3397	150.4	−109.65	−20.9	2.1388
0.4955	185.1	−127.02	−25.9	2.5267
0.6429	200.8	−134.88	−28.1	2.8044
0.7826	215.8	−142.27	−30.3	2.8536
0.9153	223.1	−145.89	−31.3	3.0650
1.0000	207.2	−138.43	−28.9	3.6191
				M) = 20.2248

TABLE 9

B / y .

$T/$	S_0	S_1	S_2	M
278.15	0.23	−0.07	−0.79	1.4627
283.15	0.67	−0.25	−0.65	1.2476
288.15	1.08	−0.37	0.02	0.3765
293.15	1.27	−0.50	0.08	0.4234
298.15	1.39	−0.59	0.13	0.4584
303.15	1.58	−0.73	0.20	0.5156
308.15	1.78	−0.89	0.29	0.5889
313.15	1.93	−1.01	0.35	0.6458
318.15	2.09	−1.16	0.43	0.7169
323.15	2.23	−1.28	0.50	0.7806
328.15	2.31	−1.35	0.55	0.8199
333.15	2.43	−1.45	0.61	0.8768
				M) = 8.9131

$$x = X_B + (X_A - X_B)x_A + \frac{(J_0 - J_1 + J_2)x_A}{T} + \frac{(-J_0 + 3J_1 - 5J_2)x_A^2}{T} + \frac{(-2J_1 + 8J_2)x_A^3}{T} + \frac{(-4J_2)x_A^4}{T} \quad (19)$$

:

$$T \quad x = A_0 + A_1T + A_2Tx_A + A_3x_A + A_4x_A^2 + A_5x_A^3 + A_6x_A^4 \quad (20)$$

$A_0, A_1, A_2, A_3, A_4, A_5$ A_6
y T x $T, Tx_A, x_A, x_A{}^2, x_A{}^3, x_A{}^4$
y - y , 10.

3.2.5. Mean deviation

M) 24 -
.

$$MD = 100\frac{\frac{|x - x^{cal}|}{x}}{N} \quad (21)$$

N , x x
y . -
M 3 5, .

3.2.6. Thermodynamic parameters

, y
y 3.1 11.

3.3. Chart analysis

3.3.1. Pure solvents

A 2 2, y
,
y .
A 3 5, A
A , λh ,
13.29, 22.60 18.60, y.

TABLE 10

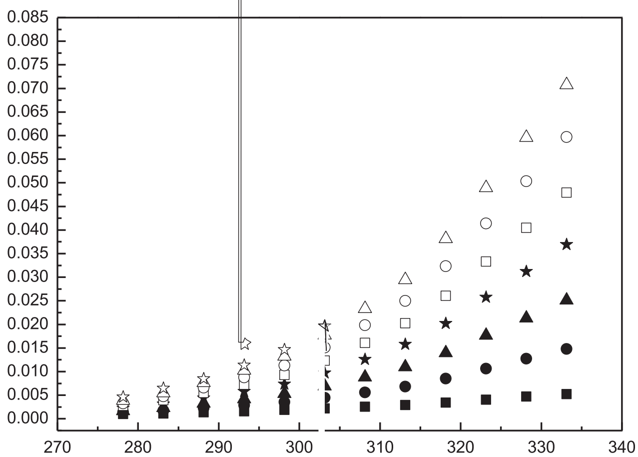
∫ y A y
.

$T/$	M		
278.15	2.2186	A_0	−4520.05
283.15	1.5718	A_1	8.51
288.15	2.3076	A_2	3.16
293.15	2.3877	A_3	970.35
298.15	2.3449	A_4	−2430.06
303.15	3.0637	A_5	1783.14
308.15	1.7529	A_6	–

A
λh , .
A 6, y ΔH_m^0
ΔG_m^0 .M ,
y y
, $\%\xi_H$ ⩾56.51%. -
, -
y- . A 6,
ΔG_m^0 y
. -
. W y
. -
, y -
. , y , y
, y
y . y
. , -
y y .

3.3.2. Binary solvent mixtures

A 7 3, y
(y + y) y -
, y -
. A
. y
. W y
y .
A 8 10, M
A , B / ∫ y A
20.2248, 8.9131 28.9011, y.
B / -
A ∫ y A . A y,
A
∫ y A



y . ,
A ʃ y A
y B /
A 11, y
Δ H_m^0 Δ G_m^0 .
y
- .M ,
y y
, $\%\xi_H$ ⩾56.51%.

4. Conclusions

W 2 11 2 3: (1)
278.15 333.15 , y
,
. y , y
y . y
y
y - ; (2)
y y
(' , A , λ) ,
A , -
y (A
, B / ʃ y A) y

, B /
M , A
ʃ y A
y B / ; (3) y-
, y ,
-
.
,
y.

Acknowledgments

y y ʃ -
y
((14)2057), ʃ y
(B 2014386).

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