

Supporting Information

Solubility and dissolution behavior analysis of 7-azaindole in pure and binary mixture solvents at temperatures ranging from 278.15 to 323.15K

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Table S1. Vendor of the instrument, software used for data analysis of FTIR and DSC.

Instruments	Vendor	Wavenumber range	Resolution	Exposure time	Software
FTIR	NICOLET	4000-350cm ⁻¹ sample mass	≥ 0.4cm ⁻¹ type of pan	3s temperature	OMNIC
DSC	TA	4.4 mg	Aluminium	313.15-473.15K	Origin

Table S2. Parameters and RMSD values of the Modified Apelblat equation for 7-azaindole in acetone + n-hexane at Temperature Range from 278.15 to 323.15 K^a

n	Modified Apelblat equation				
	A	B	C	100ARD	100RMSD
0.1	-3.90	32.16	-3548.75	1.28	0.19
0.2	-15.58	110.12	-6926.63	0.88	0.16
0.3	-22.50	156.34	-8944.40	0.99	0.16
0.4	-20.55	142.49	-8088.60	0.92	0.18
0.5	-20.06	138.77	-7773.75	0.56	0.12
0.6	-13.11	91.75	-5539.13	0.33	0.11
0.7	-11.95	83.38	-4980.59	0.20	0.06
0.8	-1.57	13.35	-1688.22	0.63	0.21
0.9	-5.17	37.30	-2680.50	0.06	0.03

^a A, B, and C are Parameters of Modified Apelblat equation.

^b ARD and RMSD stand for average relative deviation and root mean square deviation, respectively.

Table S3. Parameters and RMSD values of the Modified Apelblat equation for 7-azaindole in isopropanol + n-hexane at Temperature Range from 278.15 to 323.15 K^a

n	Modified Apelblat equation				
	A	B	C	100ARD	100RMSD
0.1	3.60	-16.94	-1792.42	1.00	0.08
0.2	-4.86	39.30	-4144.95	1.28	0.16
0.3	-3.37	28.71	-3459.58	1.17	0.21
0.4	-2.62	23.15	-3039.03	0.49	0.10
0.5	-1.56	15.49	-2502.92	1.12	0.28
0.6	2.51	-12.51	-1045.30	0.96	0.29

0.7	1.71	-7.74	-1069.86	0.98	0.28
0.8	2.367	-12.749	-664.918	0.75	0.25
0.9	11.001	-71.286	2145.292	0.34	0.12

^a A, B, and C are Parameters of Modified Apelblat equation.

^b ARD and RMSD stand for average relative deviation and root mean square deviation, respectively.

Table S4. Parameters and RMSD values of the Modified Jouyban-Acree Model for 7-azaindole in acetone + n-hexane at Temperature Range from 278.15 to 323.15 K ^a

T/K	Modified Jouyban-Acree Model		
	100ARD	Parameters	
278.15	0.57	A ₁	2.03
283.15	0.98	B ₁	-932.96
288.15	0.79	A ₂	6.30
293.15	0.59	B ₂	-2488.35
298.15	0.86	J ₀	-85.97
303.15	0.39	J ₁	106.82
308.15	0.30	J ₂	116.72
313.15	0.29		
318.15	0.46		
323.15	0.13		

^aA₁, A₂, B₁, B₂, J₀, J₁, and J₂ are prarmeters of Modified Jouyban-Acree Model;

^b ARD is average relative deviation.

Table S5. Parameters and RMSD values of the Modified Jouyban-Acree Model for 7-azaindole in Isopropanol + n-hexane at Temperature Range from 278.15 to 323.15 K ^a

T/K	Modified Jouyban-Acree Model		
	100ARD	Parameters	
278.15	0.67	A ₁	1.96
283.15	0.72	B ₁	-973.14
288.15	0.74	A ₂	7.89
293.15	0.62	B ₂	-3151.17

298.15	0.87	J_0	201.31
303.15	0.62	J_1	-58.06
308.15	0.72	J_2	-1.06
313.15	0.34		
318.15	0.50		
323.15	0.71		

^aA₁, A₂, B₁, B₂, J₀, J₁, and J₂ are prarmeters of Modified Jouyban-Acree Model;

^b ARD is average relative deviation

Table S6. Parameters and RMSD values of the CNIBS/R-K Model for 7-azaindole in acetone + n-hexane at Temperature Range from 278.15 to 323.15 K

T/K	B0	B1	B2	B3	B4	100ARD	100RMSD
278.15	-2.54829	0.05733	0.82766	2.82512	-2.57631	1.02	0.51
283.15	-2.51165	1.06598	-1.65064	4.93198	-3.17039	1.23	0.26
288.15	-2.38175	0.94092	-0.37541	2.03675	-1.45222	1.17	0.21
293.15	-2.20016	0.98667	-1.16392	3.02289	-1.80772	0.79	0.13
298.15	-1.98430	-0.03426	2.31388	-1.83798	0.47501	1.00	0.24
303.15	-1.96618	1.34147	-2.55926	4.40410	-2.26627	0.93	0.36
308.15	-1.80051	0.87826	-1.29976	2.72691	-1.48585	1.16	0.30
313.15	-1.60598	0.15985	0.40069	0.99044	-0.88048	0.76	0.21
318.15	-1.50556	0.21733	-0.21587	2.00042	-1.39231	0.73	0.18
323.15	-1.40013	0.30120	-0.65477	2.27944	-1.36207	1.00	0.44

^aB0 to B4 are parameters

^bThe ARD represent average relative deviation, RMSD is root mean square deviation

Table S7. Parameters and RMSD values of the CNIBS/R-K Model in isopropanol + n-hexane binary mixture solvents

T/K	B0	B1	B2	B3	B4	100ARD	100RMSD
278.15	-3.22334	0.91505	4.52959	-7.18224	3.53005	1.02	0.13
283.15	-3.30975	3.53726	-4.32542	4.37518	-1.77760	0.68	0.08
288.15	-3.02178	2.11613	0.31613	-1.84092	1.01956	0.58	0.10
293.15	-2.84211	2.06066	-0.22889	-0.72384	0.36125	0.49	0.07
298.15	-2.72039	2.84568	-3.46663	3.41359	-1.41384	0.76	0.12
303.15	-2.52891	2.64330	-3.63231	4.13790	-1.94139	0.30	0.06
308.15	-2.31159	1.63441	0.15549	-1.76146	1.09136	0.17	0.04
313.15	-2.20365	2.39527	-3.34830	3.42254	-1.43899	0.28	0.06
318.15	-2.02548	1.93748	-1.83290	1.09579	-0.27480	0.18	0.04
323.15	-1.84881	1.45851	-0.86410	0.19847	0.01833	0.28	0.09

^aB0 to B4 are parameters

^bThe ARD represent average relative deviation, RMSD is root mean square deviation