

Solubility Correlation and Thermodynamic Analysis of Sorafenib Free Base and Sorafenib Tosylate in Mono-solvents and Binary Solvent Mixtures

*Shuang Jiang^{a,b}, Yujia Qin^{a,b}, Songgu Wu^{a,b}, Shijie Xu^{a,b}, Kangli Li^{a,b}, Peng Yang^{a,b},
Kaifei Zhao^{a,b}, Lanlan Lin^{a,b}, Junbo Gong^{a,b,*}*

^a School of Chemical Engineering and Technology, State Key Laboratory of Chemical Engineering, Tianjin University, Tianjin 300072, China

^b The Co-Innovation Center of Chemistry and Chemical Engineering of Tianjin, Tianjin 300072, China

AUTHOR INFORMATION

Corresponding Author

*Tel.: 86-22-27405754. Fax: +86-22-27374971. E-mail: junbo_gong@tju.edu.cn

Table S1. Parameters and *ARD* of the Apelblat Model in Mono-solvents.

Parameters	1-propanol	Isopropanol	1-butanol	2-methyl-1-propanol	1-pentanol
			SFB		
<i>A</i>	-152.81	-108.79	-123.98	193.85	-221.54
<i>B</i>	3472.78	1519.22	2205.93	-12727.66	6775.66
<i>C</i>	23.59	16.96	19.26	-27.85	33.68
<i>ARD</i> %	2.88	3.36	3.13	3.69	1.89
			ST		
<i>A</i>	-102.44	-95.93	-18.63	-69.81	39.98
<i>B</i>	1857.83	1197.13	-1888.10	-179.51	-5220.85
<i>C</i>	15.40	14.57	2.89	10.77	-5.54
<i>ARD</i> %	2.18	1.33	2.27	3.46	4.29

Table S2. Parameters and *ARD* of the CNIBS/R–K Model for Solubility in the (2-Propanol + 1, 4-Dioxane) Binary Solvents.

<i>T/K</i>	<i>B</i> ₀	<i>B</i> ₁	<i>B</i> ₂	<i>B</i> ₃	<i>B</i> ₄	<i>ARD</i> %
SFB						
283.15	-7.71	10.18	-17.80	15.57	-7.83	1.06
293.15	-7.42	9.75	-18.32	18.15	-9.50	1.67
303.15	-6.98	7.83	-12.15	9.08	-4.64	0.86
313.15	-6.64	7.00	-9.73	5.46	-2.58	1.35
323.15	-6.30	6.25	-7.10	1.19	-0.14	1.86
333.15	-5.94	6.35	-9.82	6.72	-3.03	1.48
ST						
283.15	-12.24	14.64	-29.01	30.60	-13.46	1.87
293.15	-11.82	13.09	-24.80	25.28	-10.90	1.93
303.15	-11.01	7.65	-7.12	2.19	-0.46	2.02
313.15	-10.42	4.82	0.82	-6.62	3.02	2.23
323.15	-9.98	3.92	2.05	-6.79	2.73	1.56
333.15	-9.49	3.55	2.49	-7.72	3.45	1.04

Table S3. Calculated Values of Mixing Thermodynamic Properties of SFB in Different Mono-solvents.^a

T/K	$\Delta_{\text{mix}}H$ J mol ⁻¹	$\Delta_{\text{mix}}S$ J mol ⁻¹ K ⁻¹	$\Delta_{\text{mix}}G$ J mol ⁻¹
1-propanol			
283.15	-2.9305	0.0294	-11.2477
293.15	-3.4171	0.0379	-14.5414
303.15	-4.6570	0.0556	-21.5224
313.15	-6.1116	0.0792	-30.9233
323.15	-8.0994	0.1140	-44.9444
333.15	-10.0817	0.1571	-62.4049
2-propanol			
283.15	-2.9905	0.0194	-8.4854
293.15	-3.3569	0.0245	-10.5305
303.15	-4.8674	0.0376	-16.2768
313.15	-6.3004	0.0529	-22.8802
323.15	-8.2151	0.0749	-32.4310
333.15	-10.2398	0.1028	-44.4713
1-butanol			
283.15	-3.4612	0.0257	-10.7309
293.15	-3.9312	0.0324	-13.4348
303.15	-5.5860	0.0488	-20.3802
313.15	-7.3834	0.0693	-29.0912
323.15	-9.6866	0.0979	-41.3274
333.15	-12.2028	0.1343	-56.9507
2-methyl-1-propanol			
283.15	-1.2682	0.0109	-4.3597
293.15	-1.6682	0.0159	-6.3396
303.15	-2.7279	0.0277	-11.1254
313.15	-3.4065	0.0390	-15.6282
323.15	-4.2582	0.0555	-22.1838
333.15	-4.8684	0.0746	-29.7104
1-pentanol			
283.15	-3.8465	0.0217	-10.0012
293.15	-4.7461	0.0293	-13.3450
303.15	-6.3677	0.0421	-19.1283
313.15	-8.0705	0.0577	-26.1447
323.15	-10.6045	0.0812	-36.8504
333.15	-13.7792	0.1133	-51.5135

^a The expanded uncertainties are $U(\Delta_{\text{mix}}H) = 0.05 \Delta_{\text{mix}}H$, $U(\Delta_{\text{mix}}S) = 0.06 \Delta_{\text{mix}}S$, $U(\Delta_{\text{mix}}G) = 0.06 \Delta_{\text{mix}}G$ (0.95 level of confidence).

Table S4. Calculated Values of Mixing Thermodynamic Properties of ST in Different Mono-solvents.^a

T/K	$\Delta_{\text{mix}}H$ J mol ⁻¹	$\Delta_{\text{mix}}S$ J mol ⁻¹ K ⁻¹	$\Delta_{\text{mix}}G$ J mol ⁻¹
1-propanol			
283.15	-2.5082	0.0014	-2.9168
293.15	-2.9239	0.0023	-3.5952
303.15	-3.9898	0.0036	-5.0887
313.15	-4.9136	0.0053	-6.5797
323.15	-5.9978	0.0076	-8.4417
333.15	-7.5340	0.0107	-11.0954
2-propanol			
283.15	-1.3274	0.0012	-1.6629
293.15	-1.7029	0.0019	-2.2458
303.15	-2.3126	0.0029	-3.1875
313.15	-3.0370	0.0043	-4.3890
323.15	-3.7694	0.0061	-5.7543
333.15	-4.9015	0.0088	-7.8493
1-butanol			
283.15	-2.3708	0.0013	-2.7423
293.15	-2.7084	0.0021	-3.3222
303.15	-3.6622	0.0033	-4.6683
313.15	-4.4922	0.0049	-6.0209
323.15	-5.4868	0.0070	-7.7368
333.15	-6.5103	0.0096	-9.7014
2-methyl-1-propanol			
283.15	-1.0412	0.0011	-1.3392
293.15	-1.5009	0.0017	-2.0087
303.15	-2.1263	0.0028	-2.9609
313.15	-2.8260	0.0041	-4.1221
323.15	-3.4124	0.0058	-5.2816
333.15	-4.6417	0.0085	-7.4861
1-pentanol			
283.15	-0.9642	0.0010	-1.2530
293.15	-1.3452	0.0016	-1.8278
303.15	-2.0921	0.0028	-2.9269
313.15	-2.7054	0.0041	-3.9822
323.15	-3.2203	0.0056	-5.0457
333.15	-4.2660	0.0082	-7.0034

^a The expanded uncertainties are $U(\Delta_{\text{mix}}H) = 0.05 \Delta_{\text{mix}}H$, $U(\Delta_{\text{mix}}S) = 0.06 \Delta_{\text{mix}}S$, $U(\Delta_{\text{mix}}G) = 0.06 \Delta_{\text{mix}}G$ (0.95 level of confidence).