Supporting Information

Solubility of Benzoin in Six Mono-solvents and in Some Binary Solvent Mixtures at Various Temperatures

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Table S1. Parameters of the modified Apelblat equation for benzoin in binary mixed solvents (P=0.1 MPa)

x_2	10^{-3}A	10^{-3}B	10^{-3}C	10^{5}RMSD	ARD%
		acetone +methanol			
0.10	-0.2600	8.4416	0.0399	3.1684	1.5408
0.20	-0.2194	6.6258	0.0338	2.1912	1.4816
0.30	-0.1345	2.7201	0.0212	2.2696	1.7319
0.40	-0.0881	0.6116	0.0145	2.5371	2.0619
0.50	-0.0601	-0.7482	0.0102	2.7491	1.9608
0.60	-0.1703	4.2032	0.0266	2.3289	1.6365
0.70	-0.1042	1.2046	0.0168	2.3289	1.6365
0.80	-0.1915	5.0602	0.0298	1.2512	1.5139
0.90	-0.2141	6.0388	0.0331	1.0674	1.7564
		acetone +ethanol			
0.10	-0.2379	7.5075	0.0366	3.8196	2.2140
0.20	-0.2351	7.3307	0.0362	3.5451	2.1426
0.30	-0.1585	6.3620	0.0332	2.1468	1.4727
0.40	-0.2205	6.5505	0.0341	1.9096	1.3559
0.50	-0.2662	8.4900	0.0409	1.9190	1.7044
0.60	-0.3207	10.8843	0.0490	3.4249	3.1659
0.70	-0.2145	6.1741	0.0331	3.0211	2.4532
0.80	-0.3235	11.0278	0.0494	2.3302	3.6792
0.90	-0.1170	1.5682	0.0186	0.7384	1.3055

Table S2. Parameters of the modified CNIBS/R-K equation for benzoin in binary mixed solvents (P=0.1 MPa)

x_2	b_0	b_1	b_2	b_3	b_4	RMSD	ARD%
			acetone + methanol				
283.15	-5.0458	2.4138	-10.2145	14.2442	-8.0475	0.9543	2.6594
288.15	-4.8531	1.5386	-7.3975	10.9691	-6.7228	0.8577	2.0884
293.15	-4.588	0.8475	-4.3118	6.1206	-4.0699	0.6024	0.6976
298.15	-4.3539	0.2343	-0.0290	-1.8980	0.3289	1.2072	1.4236
303.15	-4.1955	0.7249	-2.6023	2.6362	-2.1572	0.4972	0.4894
308.15	-3.9860	0.7528	-2.8350	3.1139	-2.4043	0.7112	0.3972
313.15	-3.7768	0.5096	-2.0055	2.1128	-1.9854	2.0363	1.1398
318.15	-3.5883	0.4783	-1.4811	0.9962	-1.2904	2.7404	1.2437
323.15	-3.3531	-3.3531	-3.3531	-3.3531	-3.3531	2.3126	0.8962
			acetone + ethanol				
283.15	-5.0392	1.5219	-6.3232	6.8873	-3.7857	0.5329	1.2052
288.15	-4.8428	1.5466	-7.3041	8.9187	-4.8154	0.6296	0.9795
293.15	-4.5862	1.3344	-6.0468	7.1250	-4.0331	0.7054	0.9014
298.15	-4.3537	1.3216	-7.1077	9.7960	-5.6690	0.4602	0.6527
303.15	-4.1936	0.6641	-2.9294	2.5220	-1.8229	0.6933	0.7559
308.15	-3.9861	0.6059	-2.4880	1.5510	-1.2171	0.8564	0.8000
313.15	-3.7734	0.4364	-2.0284	0.9463	-0.8969	1.4286	1.0582
318.15	-3.5843	0.2952	-0.9155	-0.6379	-0.2183	1.6070	0.9360
323.15	-3.3527	0.3343	-1.3617	0.3786	-0.8530	2.5759	1.0495

Table S3. Parameters of the λh equation for benzoin in binary mixed solvents (P=0.1 MPa)

x_2	λ	10^{-3}h	RMSD	ARD%
		acetone + methanol		
0.10	0.3402	10.8182	2.1000	2.5938
0.20	0.3293	11.0165	2.4322	2.1180
0.30	0.3319	11.0445	2.8772	2.1220
0.40	0.3279	11.4503	2.8524	2.2743
0.50	0.3069	12.1702	2.8875	2.0912
0.60	0.2943	13.0366	1.3390	1.9210
0.70	0.2340	16.0120	1.4715	1.8389
0.80	0.1980	19.2716	1.6789	2.1014
0.90	0.1496	25.8941	1.2947	2.5101
		acetone + ethanol		
0.10	0.3117	11.4560	2.8188	2.8709
0.20	0.3279	11.1037	2.2352	2.6730
0.30	0.3267	11.2908	2.6565	2.4439
0.40	0.3265	11.6000	2.4138	2.2363
0.50	0.3420	11.6378	2.5169	2.8401
0.60	0.3229	12.6958	3.2798	3.3913
0.70	0.2187	17.6763	2.0414	2.8650
0.80	0.1950	20.6348	2.7490	3.9773
0.90	0.1380	29.0640	0.9170	1.6655

Table S4. Parameters of the modified Apelblat equation for benzoin in pure solvents (P=0.1 MPa)

solvent	10^{-3}A	10^{-3}B	10^{-3}C	10^{5}RMSD	ARD%
acetone	-0.3390	12.0000	0.0517	2.1582	1.2644
ethyl acetate	-0.1584	3.7219	0.0248	2.7237	1.6779
methanol	0.0701	-7.1985	-0.0091	1.0929	3.7032
ethanol	-0.1017	0.5717	0.0165	0.9809	2.3535
1-propanol	-0.1277	0.8817	0.0208	0.5323	1.8039
1-butanol	0.2480	-16.1233	-0.0351	0.5165	1.2041

Table S5. Parameters of the λh equation for benzoin in pure solvents (P=0.1 MPa)

solvent	λ	10^{-3}h	RMSD	ARD%
acetone	0.4594	8.2564	4.9871	3.8949
ethyl acetate	0.3588	10.05570	2.0335	2.0105
methanol	0.1258	33.7732	1.2165	4.4884
ethanol	0.1204	36.2562	1.0610	2.0230
1-propanol	0.2749	20.0131	0.5604	1.8273
1-butanol	0.1965	26.2087	0.3316	3.6207

Table S6. Parameters of the Jouyban-Acree model for benzoin in binary mixed solvents (P=0.1 MPa)

solvent	A0	A1	A2	ARD%
ethyl acetate + methanol	729.2438	291.3496	177.2939	3.5
ethyl acetate + ethanol	824.4875	432.8073	321.5378	3.5

Table S7. Parameters of the Van't-JA model for benzoin in binary mixed solvents (P=0.1 MPa)

solvent	a_2	b_2	a_3	b_3	A_0	A_1	A_2	ARD%
Ethyl acetate + methanol	7.916	- 3665.698	8.595	-4308.082	743.892	-307.124	330.333	2.9
Ethyl acetate + ethanol	8.015	- 3693.807	8.486	- 4315.187	706.649	- 154.137	214.347	2.7

Table S8. Comparison of solubility data and previous literature at 298.15 K[13]

solvent	Data in this work(10^3x_1)	Data in literature[a]($10^3x_{1,}$)	Relative error
ethanol	2.50	2.40	4.0
1-propanol	2.02	2.34	15.8
1-butanol	1.98	2.36	19.1
Ethyl acetate	12.85	12.85	0

[a]: The result may be caused by instrumental error, measurement error, measurement methods and other error. The instrumental error is determined by instrumental accuracy. For example, accuracy of electric balance is ±0.0001 g, accuracy of shaker is ±0.1 K, these all could bring about instrumental error. Measurement error is determined by experiment process, some operations such as reading indicator and weighing could cause error. Moreover, UVS method could also lead to error.

From Table S8, the experimental solubility data of benzoin in ethyl acetate and ethanol at 298.15 K is well conformed to the literature data, but there are some deviations between the experimental solubility data and literature data in 1-propanol and 1-butanol. So the solubility of benzoin were reperformed by using static analytical method using the same materials in 1-propanol and 1-butanol at 288.15 to 303.15 K to validate the solubility data and measurements in this work.[46-49]

Table S9 Comparison of experimental solubility of benzoin by UV method and static method at 288.15 to 303.15 K (P=0.1 Mpa)[46-49]

T/K	Solubility data by UVs method 10^3x_1	Solubility data by static method 10^3x_1	Relative error	T/K	Solubility data by UVs method 10^3x_1	Solubility data by static method 10^3x_1	Relative error
	1-propanol				1-butanol		
288.15	1.11	1.07	3.60%	288.15	0.99	1.06	7.07%
293.15	1.50	1.40	6.67%	293.15	1.44	1.40	2.78%
298.15	2.02	2.11	4.46%	298.15	1.98	1.96	1.01%
303.15	2.84	2.80	1.41%	303.15	2.67	2.50	6.37%

The standard uncertainty of T is u (T) = 0.1 K. The relative standard uncertainty of pressure is u_r (P) = 0.05. The relative standard uncertainty of the solubility measurement is $u_r(x_1)$ =0.06.

From table S9, the relative error of solubility data obtained by the two methods is less than 7.07%, which indicates the method that used in this work could be validated. And we also have used UV method to measure solubility of other substances (salicylic acid) whose solubility data was investigated by static method in the literature to validate our method.[50] The absorbance of the diluted solutions was recorded at 300 nm. Results are shown in Table S10.

Table S10. Comparison of mole fraction solubility data of salicylic acid and previous literature at 298.15 K (P=0.1 Mpa)[50]

solvent	Data in this work	Data in literature	Relative error/%
methanol	0.119	0.128	7.5
ethyl acetate	0.146	0.136	6.8
acetone	0.178	0.179	0.6
water	0.00024	0.00025	4.2

In this work, the standard uncertainty of T is u (T) = 0.1 K. The relative standard uncertainty of pressure is u_r (P) = 0.05. The relative standard uncertainty of the solubility measurement is $u_r(x_1)$ =0.06.

From table S10, the relative error of solubility data obtained by the two methods is less than 7.5%, which indicates the method that used in this work could be validated.

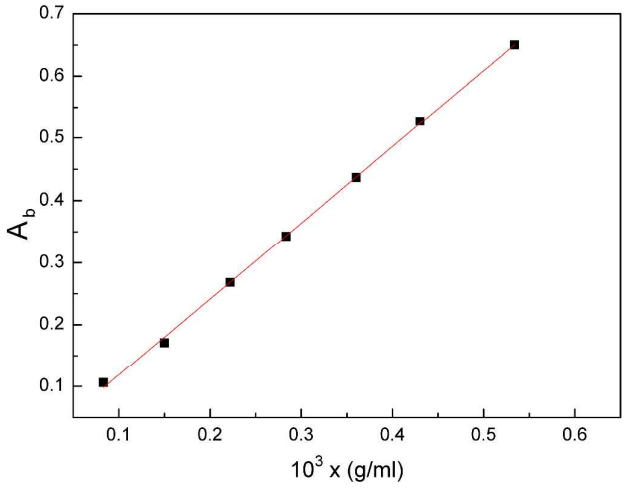

Figure S1. Calibration curve of benzoin

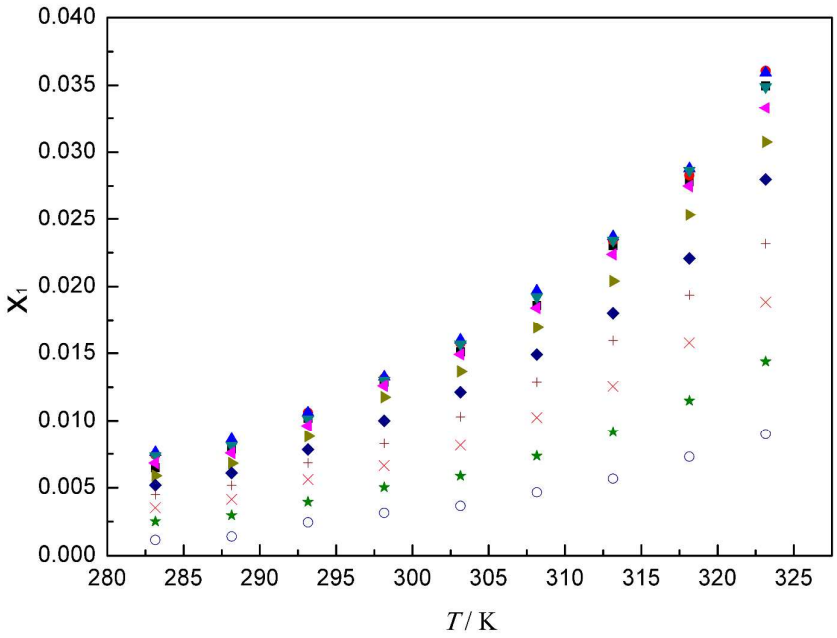

Figure S2. Mole fraction solubility (x_1) of benzoin versus temperature T in ethyl acetate + methanol (x_2) binary solvent mixtures: ■, x_2=0.00; ●, x_2=0.10; ▲, x_2=0.20; ▼, x_2=0.30; ◄, x_2=0.40; ►, x_2=0.50; ◆, x_2=0.60; ┼, x_2=0.70; ×, x_2=0.80; ★, x_2=0.90; ○, x_2=1.00.

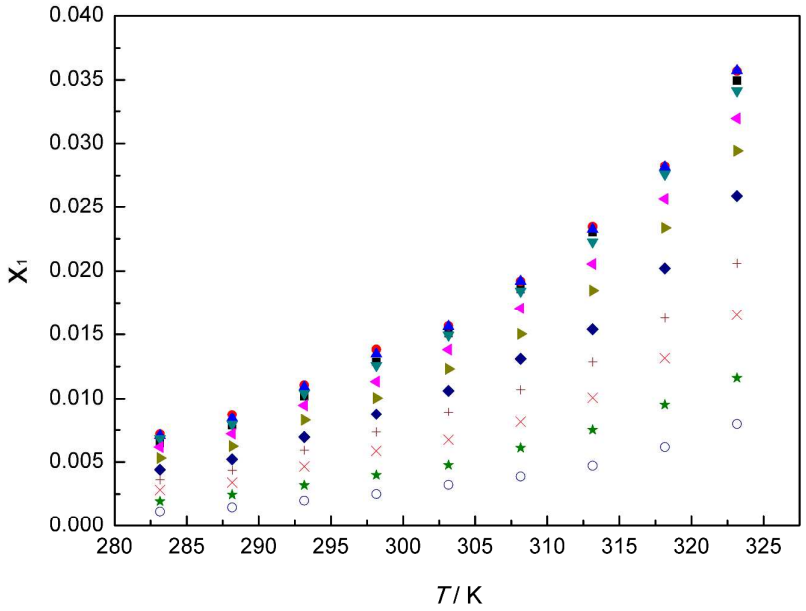

Figure S3. Mole fraction solubility (x_1) of benzoin versus temperature T in ethyl acetate + ethanol (x_2) binary solvent mixtures: ■, x_2=0.00; ●, x_2=0.10; ▲, x_2=0.20; ▼, x_2=0.30; ◄, x_2=0.40; ►, x_2=0.50; ◆, x_2=0.60; ┼, x_2=0.70; ×, x_2=0.80; ★, x_2=0.90; ○, x_2=1.00.

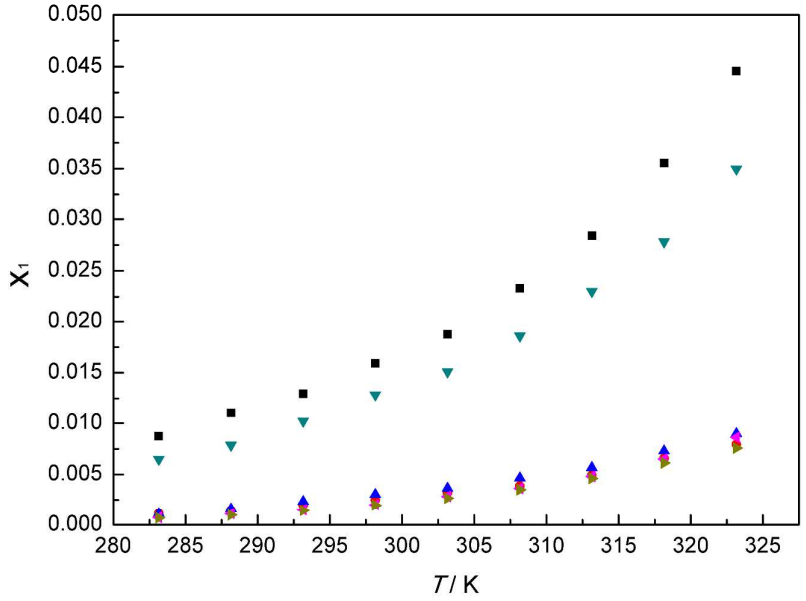

Figure S4. Mole fraction solubility (x_1) of benzoin versus temperature T in mono-solvents: ■, acetone; ▼, ethyl acetate; ▲, methanol; ●, ethanol; ◄, 1-propanol; ►, 1-butanol.

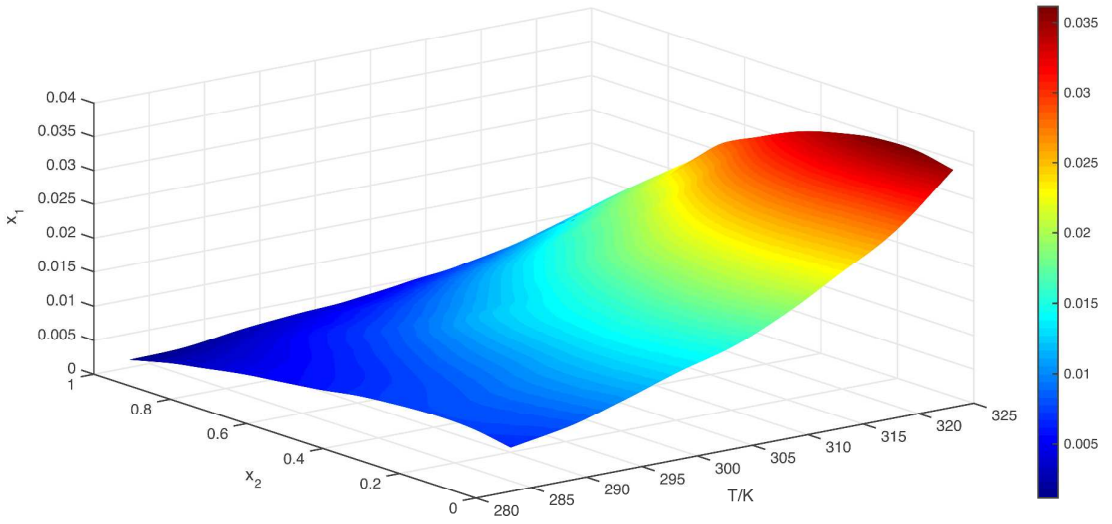

Figure S5. Mole fraction solubility (x_1) of benzoin versus temperature T in ethyl acetate + methanol binary solvent mixtures at various temperatures

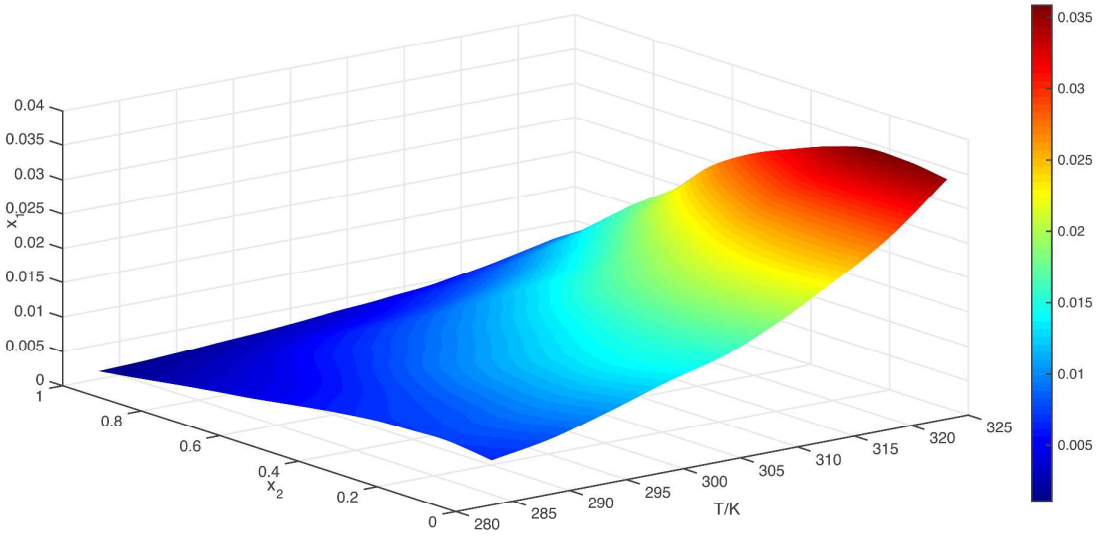

Figure S6. Mole fraction solubility (x_1) of benzoin versus temperature T in ethyl acetate + ethanol binary solvent mixtures at various temperatures