Supporting Information

Solubility Modelling and Mixing Thermodynamics of Thiamphenicol in Water and Twelve Neat Organic Solvents from T = (278.15 to 318.15) K

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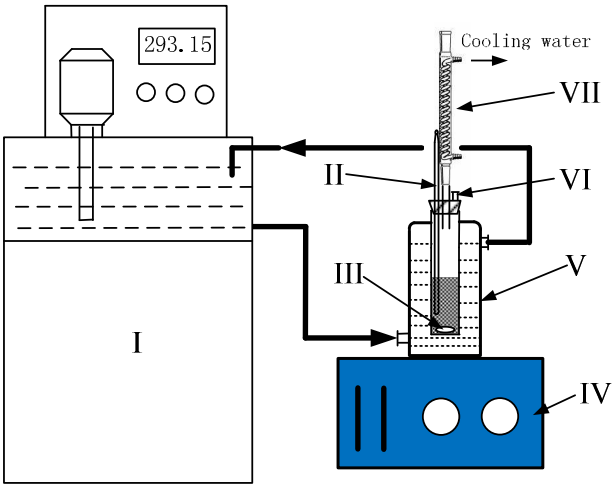

Figure S1. Schematic diagram of experimental apparatus: I, smart thermostatic water bath; II, mercury-in-glass thermometer; III, magnetic stirrer; IV, stirrer controller; V, jacketed glass vessel; VI, sampling port; VII, condenser.

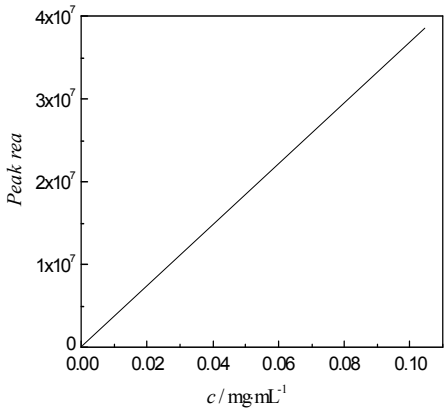

Figure S2. Relationship between peak area and concentration of thiamphenicol.

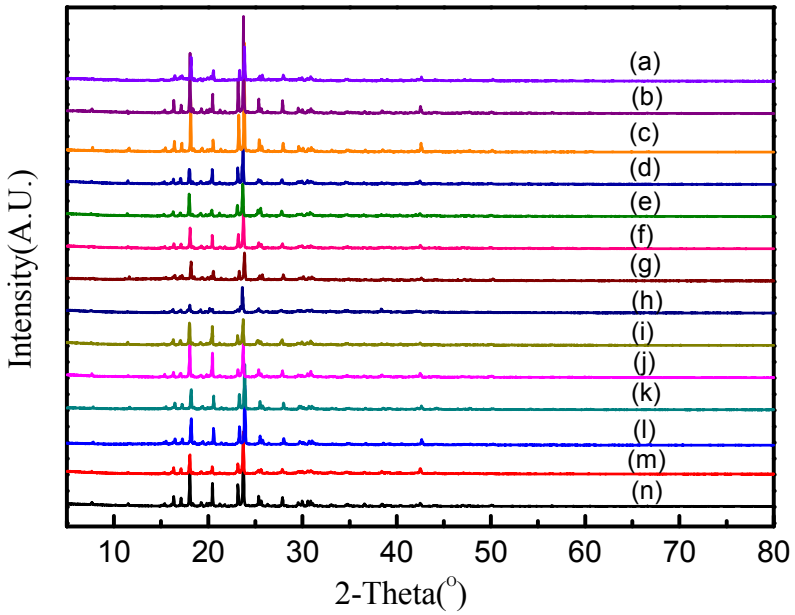

Figure S3. XPRD patterns of thiamphenicol crystallized in different solvents: (a) raw material thiamphenicol; (b) methanol; (c) ethanol; (d) *n*-propanol; (e) isopropanol; (f) *n*-butanol; (g) acetone; (h) acetonitrile; (i) ethyl acetate; (j) 2-butanone; (k) toluene; (l) water; (m) DMF; (n) 1,4-dioxane.

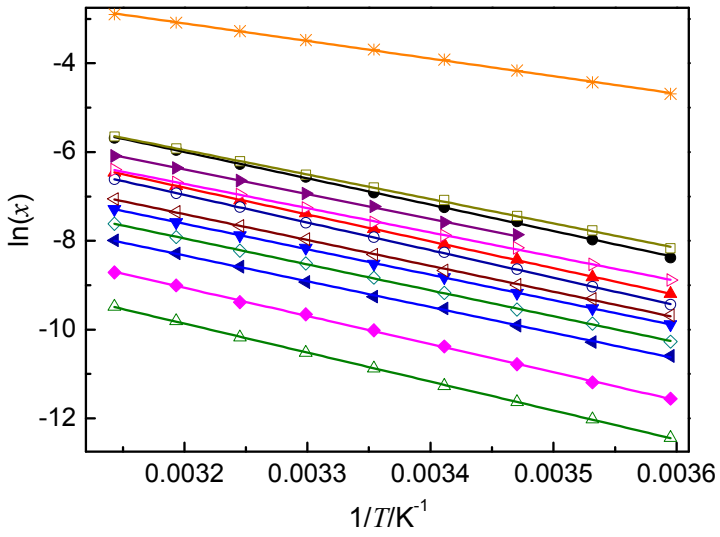

Figure S4. The van't Hoff plots of ln(x) versus 1/T in different solvents: ✳, DMF; ●, methanol; ▲, ethanol; ►, 1,4-dioxane; ▼, *n*-propanol; ◄, water; ◆, *n*-butanol; □, acetone; ▷, 2-butanone; ○, acetonitrile; ◁, ethyl acetate; ◇, isopropanol; ∆, toluene.

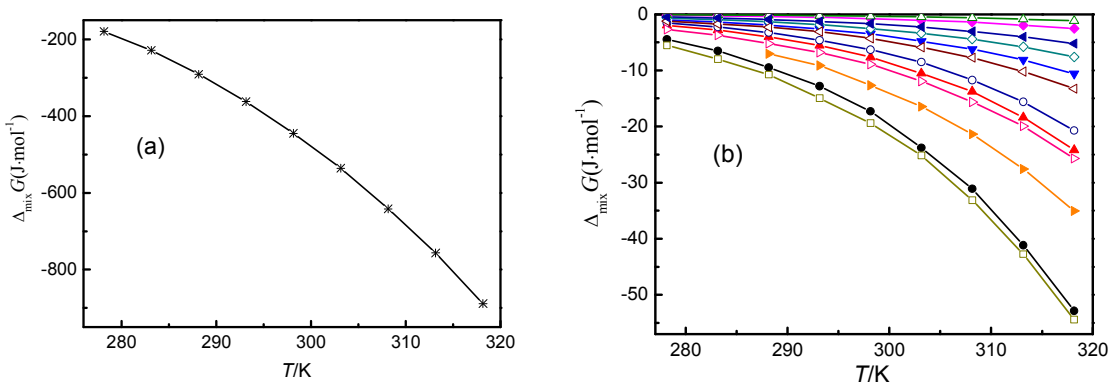

Figure S5. Calculated the change of mixing Gibbs energy at measured solubility points: (a) ✳, DMF; (b) ●, methanol; ▲, ethanol; ►, 1,4-dioxane; ▼, *n*-propanol; ◄, water; ◆, *n*-butanol; □, acetone; ▷, 2-butanone; ○, acetonitrile; ◁, ethyl acetate; ◇, isopropanol; ▵, toluene.

Table S1 Source and purity of the materials used in the work.

Chemicals	Molar mass $g \cdot mol^{-1}$	Melting point K	Melting enthalpy $kJ \cdot mol^{-1}$	molar volume $mL \cdot mol^{-1}$ (295 K)	Source	Initial mass fraction purity	Purification method	Final mass fraction purity	Analysis method
thiamphenicol	356.22	437.76[a] 436.15-438.15[b] 437.15-438.15[c,d] 437.45-439.45[e]	46.91[a]	229.82[f]	Beijing HWRK Chemical Co., Ltd	0.975	Crystallization	0.996	HPLC[h]
2-butanone	72.11			89.98[g]		0.994	None	0.994	GC[i]
n-propanol	60.06			74.58[g]		0.994	None	0.994	GC
n-butanol	74.12			91.40[g]		0.993	None	0.993	GC
isopropanol	60.06			74.75[g]		0.995	None	0.995	GC
ethanol	46.07			58.37[g]	Sinopharm Chemical Reagent Co., Ltd., China.	0.995	None	0.995	GC
methanol	32.04			40.74[g]		0.997	None	0.997	GC
toluene	92.14			105.79[g]		0.996	None	0.996	GC
ethyl acetate	88.11			97.87[g]		0.995	None	0.995	GC
acetonitrile	41.05			52.85[g]		0.994	None	0.994	GC
1,4-dioxane	88.11			85.24[g]		0.996	None	0.996	GC
DMF	73.09			77.38[g]		0.996	None	0.996	GC
acetone	58.05			74.00[g]		0.995	None	0.995	GC
water	18.02			18.05	Our lab		Distillation	Conductivity < 2 $\mu S \cdot cm^{-1}$	Conductivity meter

[a] This work. Determined at 101.2 kPa. The standard uncertainties u are $u(T) = 0.5$ K, $u(p) = 0.45$ kPa and $u(\Delta_{fus}H) = 0.40$ $kJ \cdot mol^{-1}$.

[b,c,d,e,f,g] Take from Refs. (S1,S2,S3,S4 and S5), respectively.

[h] High-performance liquid phase chromatograph.

[i] Gas chromatography.

Table S2 Parameters of the equations and *RMSD* values for thiamphenicol in different solvents.

Solvent	Modified Apelblat equation				λh equation			Wilson model			NRTL model			
	A	*B*	*C*	10^4 *RMSD*	λ	*h*	10^4 *RMSD*	g_{12}	g_{21}	10^4 *RMSD*	λ_{12}	λ_{21}	α	10^4 *RMSD*
ethanol	5.61	-5715.5	1.02	0.05	0.2758	21893.2	0.06	180.36	4184.5	0.07	372.77	284.35	0.40	0.06
n-propanol	-2.64	-5148.8	2.00	0.08	0.0928	61815.7	0.03	874.96	57425.8	0.03	1748.5	197.93	0.20	0.03
1,4-dioxane	34.83	-6547.6	-3.53	0.07	0.2442	22375.9	0.08	-1830.3	10759.8	0.08	1450.5	-185.05	0.20	0.08
n-butanol	48.84	-7991.4	-5.63	0.01	0.0376	168334.6	0.02	5289.1	10254.9	0.02	1523.2	867.83	0.30	0.02
acetonitrile	-5.92	-5356.7	2.80	0.04	0.2752	22581.7	0.04	1027.7	3703.6	0.05	17.461	550.39	0.25	0.04
ethyl acetate	5.95	-5651.4	0.83	0.03	0.1256	46404.0	0.04	1126.9	10542.5	0.04	1630.5	437.37	0.35	0.03
isopropanol	-4.88	-5109.7	2.31	0.02	0.0722	80713.1	0.02	1741.4	56831.3	0.03	2611.0	549.68	0.25	0.02
DMF	119.21	-8822.9	-16.38	0.98	1.7666	2262.1	4.08	-1858.0	-744.43	2.92	-575.61	97.728	0.20	1.15
toluene	-36.06	-4468.5	7.05	0.003	0.0203	322185.2	0.0004	7619.6	87219.9	0.004	1517.2	897.68	0.20	0.005
methanol	106.74	-10096.5	-14.00	0.12	0.5554	10667.2	0.25	-1996.1	4216.1	0.34	6.218	259.79	0.47	0.25
2-butanone	-35.15	-3411.4	6.85	0.06	0.1755	31069.2	0.07	-996.30	59891.1	0.10	1752.3	-82.644	0.20	0.07
water	-34.32	-3857.6	6.67	0.02	0.0486	119568.2	0.02	-436.56	10817.7	0.02	2499.9	487.68	0.20	0.02
acetone	10.80	-5431.4	0.11	0.12	0.3907	14062.9	0.15	-2715.4	6197.2	0.18	1077.4	-21.044	0.40	0.16

Table S3 Experimental mole fraction solubility (x) of thiamphenicol in different solvents at the temperature range from T= (278.15 To 318.15) K under 101.2 kPa.[a]

T / K	100 x	100 *RD*			
		Modified Apelblat equation	λh equation	Wilson model	NRTL model
Acetonitrile					
278.15	0.007958	-2.83	-1.45	-1.79	-1.46
283.15	0.01192	-1.39	-0.50	-0.54	-0.49
288.15	0.01771	0.48	0.98	1.16	1.01
293.15	0.02587	1.83	2.05	2.34	2.09
298.15	0.03633	0.42	0.44	0.76	0.48
303.15	0.05023	-1.48	-1.60	-1.34	-1.56
308.15	0.07158	0.69	0.51	0.60	0.52
313.15	0.09796	-0.20	-0.39	-0.58	-0.42
318.15	0.1343	0.04	-0.13	-0.71	-0.22
100 *RAD*		1.04	0.89	1.09	0.92
Ethyl acetate					
278.15	0.006238	3.83	2.12	1.78	2.71
283.15	0.009090	4.12	2.73	2.51	3.14
288.15	0.01244	-0.50	-1.62	-1.74	-1.37
293.15	0.01715	-3.32	-4.13	-4.16	-4.04
298.15	0.02457	-1.04	-1.51	-1.47	-1.58
303.15	0.03481	1.16	1.02	1.11	0.81
308.15	0.04709	-0.22	-0.05	0.08	-0.40
313.15	0.06432	0.35	0.81	0.96	0.32
318.15	0.08611	-0.15	0.57	0.74	-0.02
100 *RAD*		1.63	1.62	1.62	1.60
Ethanol					
278.15	0.01017	-1.27	-0.32	-0.61	-0.33
283.15	0.01480	-1.87	-1.15	-1.18	-1.11
288.15	0.02195	0.74	1.24	1.39	1.31
293.15	0.03090	-0.65	-0.32	-0.07	-0.24
298.15	0.04383	-0.11	0.06	0.33	0.13
303.15	0.06246	1.97	2.01	2.22	2.05
308.15	0.08374	-0.96	-1.03	-0.96	-1.05
313.15	0.1153	-0.24	-0.42	-0.56	-0.50
318.15	0.1567	0.14	-0.15	-0.60	-0.31
100 *RAD*		0.88	0.74	0.88	0.78

n-Propanol					
278.15	0.005106	-0.06	0.34	0.51	0.13
283.15	0.007345	0.05	0.25	0.37	0.19
288.15	0.01035	-0.71	-0.65	-0.58	-0.61
293.15	0.01473	0.66	0.64	0.65	0.73
298.15	0.01991	-2.07	-2.13	-2.16	-2.02
303.15	0.02853	2.09	2.03	1.97	2.12
308.15	0.03799	-0.08	-0.12	-0.22	-0.08
313.15	0.05095	-0.63	-0.63	-0.75	-0.65
318.15	0.06866	0.19	0.24	0.11	0.14
100 *RAD*		0.73	0.78	0.81	0.74
Isopropanol					
278.15	0.003460	-3.34	-1.70	-1.17	-1.34
283.15	0.005196	0.81	1.94	2.30	2.14
288.15	0.007131	-2.93	-2.15	-1.92	-2.07
293.15	0.01037	0.34	0.78	0.87	0.76
298.15	0.01458	1.26	1.45	1.42	1.37
303.15	0.02015	1.50	1.50	1.34	1.37
308.15	0.02689	-0.76	-0.92	-1.20	-1.08
313.15	0.03642	-0.62	-0.91	-1.29	-1.06
318.15	0.04926	0.27	-0.11	-0.58	-0.22
100 *RAD*		1.32	1.27	1.34	1.27
1,4-Dioxane					
288.15	0.03844	1.60	1.37	1.35	1.34
293.15	0.05082	-3.20	-3.14	-3.13	-3.09
298.15	0.07285	1.36	1.59	1.61	1.67
303.15	0.09734	0	0.28	0.31	0.36
308.15	0.1302	-0.19	0.02	0.04	0.07
313.15	0.1732	0.10	0.12	0.13	0.11
318.15	0.2272	-0.03	-0.33	-0.33	-0.40
100 *RAD*		0.89	0.86	0.87	0.90
Toluene					
278.15	0.0003958	0.83	0.84	1.47	0.40
283.15	0.0006031	2.00	1.46	1.92	1.25
288.15	0.0008894	1.13	0.27	0.57	0.23
293.15	0.001281	-0.96	-1.95	-1.82	-1.88
298.15	0.001893	0.61	-0.29	-0.32	-0.15
303.15	0.002696	-0.47	-1.11	-1.32	-0.95

308.15	0.003805	-1.47	-1.69	-2.07	-1.55
313.15	0.005528	1.38	1.73	1.20	1.83
318.15	0.007604	-0.32	0.74	0.04	0.77
100 *RAD*		1.02	1.12	1.19	1.00
DMF					
278.15	0.9203	-0.37	-2.33	1.62	-0.35
283.15	1.197	-0.92	-1.28	-0.26	-0.69
288.15	1.561	0.24	0.93	-0.08	0.51
293.15	1.987	0.32	1.58	-0.58	0.54
298.15	2.501	0.55	1.93	-0.53	0.68
303.15	3.082	-0.13	0.99	-1.03	-0.11
308.15	3.786	0.02	0.49	-0.40	-0.06
313.15	4.575	-0.41	-0.91	-0.10	-0.55
318.15	5.529	0.20	-1.59	1.39	0.01
100 *RAD*		0.35	1.34	0.67	0.39
Methanol					
278.15	0.02297	-1.77	-3.80	-4.02	-3.98
283.15	0.03451	-0.20	-0.65	-0.54	-0.74
288.15	0.05181	3.02	3.60	3.89	3.59
293.15	0.07155	-0.33	0.86	1.25	0.90
298.15	0.09933	-1.61	-0.24	0.13	-0.16
303.15	0.1411	0.93	2.04	2.27	2.14
308.15	0.1893	-0.82	-0.31	-0.30	-0.19
313.15	0.2586	0.60	0.13	-0.20	0.23
318.15	0.3413	-0.15	-1.94	-2.75	-1.89
100 *RAD*		1.05	1.51	1.71	1.54
2-Butanone					
278.15	0.01385	-2.28	-0.85	0.62	-1.06
283.15	0.01970	-0.88	-0.26	0.78	-0.32
288.15	0.02858	3.38	3.43	4.04	3.46
293.15	0.03792	-0.26	-0.56	-0.31	-0.48
298.15	0.05096	-1.82	-2.29	-2.41	-2.19
303.15	0.07043	0.29	-0.16	-0.62	-0.08
308.15	0.09521	0.97	0.69	-0.09	0.73
313.15	0.1248	-0.67	-0.65	-1.74	-0.66
318.15	0.1664	0.13	0.56	-0.78	0.49
100 *RAD*		1.19	1.05	1.27	1.05
n-Butanol					

278.15	0.0009545	0.57	0.42	0.36	0.39
283.15	0.001382	-3.18	-2.80	-2.79	-2.78
288.15	0.002079	-1.43	-0.74	-0.67	-0.69
293.15	0.003104	1.04	1.84	1.93	1.90
298.15	0.004461	1.10	1.87	1.95	1.92
303.15	0.006393	2.22	2.77	2.83	2.80
308.15	0.008424	-3.81	-3.60	-3.59	-3.60
313.15	0.01228	1.59	1.26	1.20	1.22
318.15	0.01647	-0.23	-1.26	-1.41	-1.35
100 *RAD*		1.68	1.84	1.86	1.85
Acetone					
278.15	0.02832	-5.27	-3.99	-4.00	-3.89
283.15	0.04248	0.73	1.72	1.81	1.81
288.15	0.05851	-0.73	0.06	0.21	0.13
293.15	0.08403	3.09	3.63	3.79	3.68
298.15	0.1116	0.25	0.59	0.73	0.62
303.15	0.1486	-1.35	-1.24	-1.17	-1.25
308.15	0.2018	0.01	-0.12	-0.15	-0.17
313.15	0.2683	0.18	-0.21	-0.38	-0.30
318.15	0.3523	-0.01	-0.69	-1.03	-0.80
100 *RAD*		1.29	1.36	1.47	1.41
Water					
278.15	0.002501	3.06	3.22	2.56	3.00
283.15	0.003423	-1.90	-2.28	-2.58	-2.43
288.15	0.004959	-0.14	-0.84	-0.84	-0.91
293.15	0.007300	4.12	3.34	3.52	3.31
298.15	0.009523	-2.60	-3.37	-3.08	-3.36
303.15	0.01325	-1.99	-2.54	-2.23	-2.50
308.15	0.01872	1.01	0.85	1.06	0.91
313.15	0.02532	0.49	0.81	0.86	0.90
318.15	0.03391	-0.23	0.69	0.50	0.81
100 *RAD*		1.73	1.99	1.92	2.02

[a] Standard uncertainties u are $u(T) = 0.05$ K, $u(p) = 0.45$ kPa; Relative standard uncertainty u_r is $u_r(x) = 0.026$. *RD* denotes the relative deviation; and *RAD*, relative average deviation.

Table S4 Activity coefficients (γ) of thiamphenicol in different neat solvents at the temperature range from T= (278.15 To 318.15) K.

T / K	γ						
	Acetonitrile	*Ethyl acetate*	*Ethanol*	*n-Propanol*	*Isopropanol*	*1,4-Dioxane*	*Toluene*
278.15	36.36	46.38	28.45	56.67	83.63	---	731.05
283.15	30.54	40.05	24.60	49.56	70.06	---	603.61
288.15	25.76	36.67	20.78	44.07	63.97	11.87	512.90
293.15	22.01	33.20	18.43	38.66	54.91	11.20	444.51
298.15	19.49	28.82	16.16	35.57	48.57	9.72	374.07
303.15	17.47	25.21	14.05	30.75	43.54	9.01	325.44
308.15	15.13	23.01	12.94	28.52	40.29	8.32	284.71
313.15	13.61	20.73	11.56	26.16	36.60	7.70	241.15
318.15	12.17	18.99	10.43	23.81	33.19	7.20	215.02
	DMF	*Methanol*	*2-Butanone*	*n-Butanol*	*Acetone*	*Water*	
278.15	0.314	12.60	20.89	303.14	10.22	115.69	
283.15	0.304	10.55	18.48	263.42	8.57	106.35	
288.15	0.292	8.80	15.96	219.42	7.80	91.99	
293.15	0.287	7.96	15.02	183.45	6.78	78.00	
298.15	0.283	7.13	13.90	158.73	6.35	74.36	
303.15	0.285	6.22	12.46	137.24	5.90	66.22	
308.15	0.286	5.72	11.38	128.60	5.37	57.87	
313.15	0.291	5.16	10.68	108.56	4.97	52.65	
318.15	0.300	4.79	9.83	99.27	4.64	48.22	

Table S5 The calculated values for $\Delta_{mix}G$, $\Delta_{mix}H$, $\Delta_{mix}S$, $\ln\gamma_1^{\infty}$, and $H_1^{E,\infty}$: $\Delta_{mix}G$, $\Delta_{mix}S$ and $\Delta_{mix}S$ denote the mixing Gibbs energy, mixing enthalpy, and mixing entropy, respectively; γ_1^{∞} denotes the infinitesimal concentration activity coefficient, and $H_1^{E,\infty}$ denotes infinitesimal concentration reduced excess enthalpy.[a]

T / K	$\Delta_{mix}G$ J·mol^{-1}	$\Delta_{mix}H$ J·mol^{-1}	$\Delta_{mix}S$ J· K^{-1}·mol^{-1}	$\ln\gamma_1^{\infty}$	$H_1^{E,\infty}$ kJ·mol^{-1}
Acetonitrile					
278.15	-1.546	0.340	0.007	2.038	
283.15	-2.253	0.521	0.010	2.005	
288.15	-3.253	0.790	0.014	1.972	
293.15	-4.616	1.177	0.020	1.940	
298.15	-6.316	1.685	0.027	1.908	4.637
303.15	-8.509	2.375	0.036	1.877	
308.15	-11.74	3.447	0.049	1.846	
313.15	-15.60	4.801	0.065	1.816	
318.15	-20.72	6.694	0.086	1.786	
Ethyl acetate					
278.15	-1.207	0.086	0.005	2.316	
283.15	-1.712	0.128	0.007	2.306	
288.15	-2.294	0.178	0.009	2.295	
293.15	-3.087	0.249	0.011	2.285	
298.15	-4.286	0.363	0.016	2.275	1.472
303.15	-5.877	0.523	0.021	2.265	
308.15	-7.729	0.720	0.027	2.255	
313.15	-10.22	1.001	0.036	2.246	
318.15	-13.26	1.363	0.046	2.236	
Ethanol					

278.15	-1.973	0.293	0.008	1.804	
283.15	-2.800	0.439	0.011	1.782	
288.15	-4.031	0.670	0.016	1.759	
293.15	-5.532	0.970	0.022	1.737	
298.15	-7.625	1.414	0.030	1.715	3.213
303.15	-10.53	2.068	0.042	1.694	
308.15	-13.76	2.843	0.054	1.672	
313.15	-18.37	4.011	0.071	1.651	
318.15	-24.18	5.581	0.094	1.629	
n-Propanol					
278.15	-0.989	0.045	0.004	2.504	
283.15	-1.387	0.064	0.005	2.497	
288.15	-1.906	0.091	0.007	2.491	
293.15	-2.635	0.129	0.009	2.484	
298.15	-3.476	0.174	0.012	2.478	0.882
303.15	-4.811	0.249	0.017	2.473	
308.15	-6.239	0.332	0.021	2.467	
313.15	-8.121	0.445	0.027	2.461	
318.15	-10.59	0.599	0.035	2.456	
Isopropanol					
278.15	-0.672	0.060	0.003	2.876	
283.15	-0.979	0.090	0.004	2.863	
288.15	-1.315	0.124	0.005	2.850	
293.15	-1.854	0.180	0.007	2.838	1.736
298.15	-2.533	0.254	0.009	2.826	
303.15	-3.401	0.350	0.012	2.814	
308.15	-4.423	0.467	0.016	2.803	
313.15	-5.810	0.633	0.021	2.792	

318.15	-7.605	0.855	0.027	2.782	
DMF					
278.15	-179.4	-43.93	0.487	-2.813	
283.15	-228.5	-56.48	0.607	-2.775	
288.15	-290.9	-72.63	0.758	-2.739	
293.15	-361.9	-91.03	0.924	-2.705	
298.15	-444.9	-112.6	1.115	-2.671	-4.850
303.15	-535.8	-136.0	1.319	-2.639	
308.15	-641.8	-163.4	1.553	-2.608	
313.15	-756.4	-192.6	1.800	-2.578	
318.15	-888.6	-226.2	2.082	-2.549	
Toluene					
278.15	-0.077	0.030	0.0004	5.071	
283.15	-0.114	0.046	0.0006	5.013	
288.15	-0.164	0.068	0.0008	4.956	
293.15	-0.230	0.098	0.0011	4.902	
298.15	-0.330	0.144	0.0016	4.850	7.615
303.15	-0.457	0.205	0.0022	4.799	
308.15	-0.627	0.289	0.0030	4.750	
313.15	-0.878	0.420	0.0041	4.703	
318.15	-1.173	0.578	0.0055	4.657	
1,4-Dioxane					
288.15	-7.060	-0.578	0.022	1.198	
293.15	-9.137	-0.751	0.029	1.208	
298.15	-12.65	-1.057	0.039	1.218	-1.452
303.15	-16.46	-1.384	0.050	1.228	
308.15	-21.37	-1.812	0.063	1.237	
313.15	-27.57	-2.357	0.081	1.246	

318.15	-35.06	-3.018	0.101	1.254	
Methanol					
278.15	-4.474	0.424	0.018	0.956	
283.15	-6.524	0.680	0.025	0.941	
288.15	-9.482	1.086	0.037	0.926	
293.15	-12.79	1.590	0.049	0.911	
298.15	-17.29	2.330	0.066	0.895	2.320
303.15	-23.78	3.484	0.090	0.879	
308.15	-31.08	4.907	0.117	0.863	
313.15	-41.16	7.018	0.154	0.846	
318.15	-52.85	9.674	0.197	0.830	
2-Butanone					
278.15	-2.683	-0.138	0.009	1.507	
283.15	-3.718	-0.196	0.012	1.514	
288.15	-5.230	-0.285	0.017	1.522	
293.15	-6.792	-0.378	0.022	1.529	
298.15	-8.901	-0.507	0.028	1.536	-0.997
303.15	-11.92	-0.701	0.037	1.542	
308.15	-15.63	-0.947	0.048	1.549	
313.15	-19.92	-1.241	0.060	1.555	
318.15	-25.69	-1.653	0.076	1.561	
n-Butanol					
278.15	-0.185	0.053	0.0009	4.179	
283.15	-0.262	0.078	0.0012	4.136	
288.15	-0.383	0.117	0.0017	4.095	5.690
293.15	-0.554	0.176	0.0025	4.055	
298.15	-0.774	0.254	0.0034	4.016	
303.15	-1.077	0.366	0.0048	3.978	

308.15	-1.391	0.484	0.0061	3.941	
313.15	-1.951	0.710	0.0085	3.905	
318.15	-2.546	0.956	0.0110	3.869	
Water					
278.15	-0.483	0.021	0.0018	3.238	
283.15	-0.649	0.033	0.0024	3.232	
288.15	-0.913	0.053	0.0034	3.224	
293.15	-1.301	0.087	0.0047	3.216	
298.15	-1.665	0.126	0.0060	3.207	1.311
303.15	-2.248	0.192	0.0080	3.198	
308.15	-3.068	0.297	0.0109	3.188	
313.15	-4.025	0.438	0.0143	3.178	
318.15	-5.225	0.636	0.0184	3.167	
Acetone					
278.15	-5.516	-0.395	0.018	0.746	
283.15	-8.008	-0.565	0.026	0.756	
288.15	-10.76	-0.740	0.035	0.766	
293.15	-14.96	-1.008	0.048	0.775	
298.15	-19.41	-1.264	0.061	0.783	-1.147
303.15	-25.17	-1.583	0.078	0.790	
308.15	-33.13	-2.012	0.101	0.797	
313.15	-42.74	-2.490	0.129	0.803	
318.15	-54.42	-3.023	0.162	0.808	

[a] Expanded uncertainties U are U ($\Delta_{mix}G^o$) = 0.005 J·mol^{-1}; U ($\Delta_{mix}S^o$) = 0.001 J· K^{-1}·mol^{-1}; U ($\Delta_{mix}H^o$) =0.003 J·mol^{-1} (0.95 level of confidence).

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