

## Supporting Information

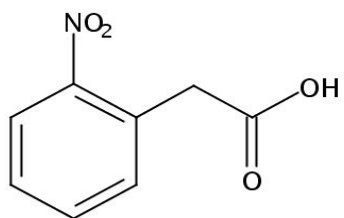
# Equilibrium Solubility and Dissolution Property Analysis of 2-Nitrophenylacetic Acid in Thirteen Pure Solvents at Elevated Temperatures

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**FIGURE S1.** Structure of 2-nitrophenylacetic acid.

**Table S1**

The values of  $\alpha$ ,  $\beta$  and  $\pi^*$  and Hildebrand solubility parameters ( $\delta_H$ ) of the solvents studied.<sup>a</sup>

Solvent	$\alpha$	$\beta$	$\pi$	$\delta_H(\text{J}/\text{cm}^3)^{1/2}$
methanol	0.98	0.66	0.60	29.61
ethanol	0.86	0.75	0.54	26.52
isopropanol	0.76	0.84	0.48	23.58
<i>n</i> -propanol	0.84	0.90	0.52	24.60
EG	0.90	0.52	0.92	33.11
acetonitrile	0.19	0.40	0.75	24.40
DMF	0	0.69	0.88	24.86
1,4-dioxane	0	0.37	0.55	20.48
<i>n</i> -butanol	0.84	0.84	0.47	23.20
ethyl acetate	0	0.45	0.55	18.48
isobutanol	0.79	0.84	0.40	22.66
water	1.17	0.47	1.09	47.81
cyclohexane	0	0	0	16.77

<sup>a</sup> Taken from the Refs. (S1-S4).

**Table S2**Dissolution thermodynamic properties of of 2-nitrophenylacetic acid dissolved in different solvents.<sup>a</sup>

$T / \text{K}$	$\Delta_d G^\circ$	$\Delta_d H^\circ$	$\Delta_d S^\circ$	$\% \zeta_{\text{H}}$	$\% \zeta_{\text{TS}}$	$\ln \gamma_1^\infty$	$H_1^{E,\infty}$
	$\text{J}\cdot\text{mol}^{-1}$	$\text{J}\cdot\text{mol}^{-1}$	$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$				$\text{kJ}\cdot\text{mol}^{-1}$
methanol							
283.15	-435.3	862.3	4.582	39.92	60.08	-0.351	
288.15	-476.0	958.8	4.982	40.06	59.94	-0.308	
293.15	-531.2	1099	5.561	40.27	59.73	-0.266	
298.15	-582.7	1233	6.091	40.44	59.56	-0.226	
303.15	-650.8	1422	6.838	40.69	59.31	-0.187	-5.837
308.15	-721.1	1628	7.622	40.93	59.07	-0.150	
313.15	-802.7	1882	8.575	41.21	58.79	-0.113	
318.15	-889.2	2172	9.623	41.51	58.49	-0.078	
323.15	-978.5	2495	10.75	41.80	58.20	-0.044	
328.15	-1071	2857	11.97	42.11	57.89	-0.011	
ethanol							
283.15	-290.0	701.5	3.502	41.44	58.56	0.073	
288.15	-330.8	817.0	3.983	41.58	58.42	0.082	
293.15	-375.9	948.8	4.519	41.73	58.27	0.090	
298.15	-430.7	1116	5.189	41.92	58.08	0.097	
303.15	-498.9	1337	6.056	42.14	57.86	0.104	-0.977
308.15	-583.1	1628	7.174	42.40	57.60	0.110	
313.15	-667.7	1935	8.310	42.64	57.36	0.116	
318.15	-760.2	2291	9.589	42.88	57.12	0.121	
323.15	-862.8	2714	11.07	43.14	56.86	0.126	
328.15	-976.6	3220	12.79	43.42	56.58	0.130	
<i>n</i> -propanol							
283.15	-193.9	486.9	2.404	41.70	58.30	0.466	
288.15	-228.2	588.1	2.833	41.88	58.12	0.466	
293.15	-267.3	708.4	3.328	42.06	57.94	0.466	
298.15	-308.7	839.4	3.851	42.23	57.77	0.465	
303.15	-356.7	998.1	4.469	42.42	57.58	0.465	0.116
308.15	-412.3	1191	5.204	42.62	57.38	0.464	
313.15	-480.4	1443	6.142	42.87	57.13	0.463	
318.15	-552.8	1725	7.160	43.09	56.91	0.462	
323.15	-637.9	2081	8.412	43.35	56.65	0.461	
328.15	-738.2	2537	9.979	43.65	56.35	0.459	
isopropanol							
283.15	-164.8	381.1	1.928	41.11	58.89	0.621	
288.15	-190.7	452.1	2.231	41.29	58.71	0.637	-2.109

293.15	-219.7	534.7	2.573	41.48	58.52	0.652	
298.15	-250.9	626.5	2.943	41.66	58.34	0.666	
303.15	-290.2	749.2	3.429	41.89	58.11	0.680	
308.15	-327.2	868.0	3.879	42.07	57.93	0.694	
313.15	-373.4	1026	4.469	42.30	57.70	0.707	
318.15	-420.9	1197	5.084	42.52	57.48	0.720	
323.15	-474.3	1401	5.804	42.76	57.24	0.732	
328.15	-535.4	1653	6.669	43.03	56.97	0.744	
EG							
283.15	-158.2	367.5	1.856	41.14	58.86	0.454	
288.15	-182.8	435.6	2.146	41.33	58.67	0.516	
293.15	-211.3	517.7	2.487	41.53	58.47	0.585	
298.15	-243.1	613.4	2.873	41.73	58.27	0.662	
303.15	-277.0	719.5	3.287	41.93	58.07	0.742	
308.15	-315.5	845.9	3.769	42.14	57.86	0.831	-1.867
313.15	-361.0	1004	4.359	42.38	57.62	0.934	
318.15	-411.9	1193	5.044	42.64	57.36	1.049	
323.15	-468.8	1418	5.837	42.91	57.09	1.174	
328.15	-531.1	1683	6.746	43.18	56.82	1.310	
acetonitrile							
283.15	-150.9	352.1	1.776	41.18	58.82	0.753	
288.15	-167.0	394.8	1.950	41.27	58.73	0.769	
293.15	-188.9	456.1	2.200	41.42	58.58	0.784	
298.15	-217.9	542.1	2.549	41.63	58.37	0.799	
303.15	-247.9	634.4	2.911	41.83	58.17	0.813	
308.15	-285.4	756.5	3.381	42.07	57.93	0.826	-2.064
313.15	-329.6	910.4	3.960	42.34	57.66	0.839	
318.15	-378.7	1092	4.623	42.61	57.39	0.851	
323.15	-429.2	1291	5.323	42.87	57.13	0.862	
328.15	-482.6	1516	6.091	43.13	56.87	0.873	
cyclohexane							
283.15	-0.095	0.375	0.00166	44.38	55.62	8.098	
288.15	-0.127	0.516	0.00223	44.52	55.48	7.983	
293.15	-0.167	0.696	0.00294	44.65	55.35	7.872	
298.15	-0.219	0.942	0.00389	44.79	55.21	7.765	
303.15	-0.282	1.240	0.00502	44.89	55.11	7.661	
308.15	-0.354	1.594	0.00632	45.00	55.00	7.561	15.60
313.15	-0.446	2.059	0.00800	45.11	54.89	7.463	
318.15	-0.560	2.663	0.01013	45.24	54.76	7.369	
323.15	-0.708	3.487	0.01298	45.39	54.61	7.278	
328.15	-0.885	4.522	0.01648	45.54	54.46	7.189	
<i>n</i> -butanol							

283.15	-179.1	420.1	2.116	41.21	58.79	0.543	
288.15	-206.9	497.0	2.443	41.39	58.61	0.556	
293.15	-237.7	585.3	2.807	41.56	58.44	0.569	
298.15	-270.1	680.7	3.189	41.72	58.28	0.581	
303.15	-311.6	810.6	3.702	41.94	58.06	0.593	
308.15	-356.8	959.1	4.270	42.16	57.84	0.605	-1.786
313.15	-407.3	1134	4.921	42.39	57.61	0.616	
318.15	-463.8	1342	5.675	42.63	57.37	0.626	
323.15	-519.3	1556	6.421	42.85	57.15	0.637	
328.15	-593.9	1872	7.514	43.15	56.85	0.647	
ethyl acetate							
283.15	-304.7	685.1	3.496	40.90	59.10	-0.004	
288.15	-340.2	778.2	3.881	41.03	58.97	0.017	
293.15	-392.3	924.4	4.492	41.25	58.75	0.037	
298.15	-450.6	1096	5.186	41.47	58.53	0.056	
303.15	-526.0	1333	6.131	41.76	58.24	0.074	
308.15	-601.3	1582	7.085	42.02	57.98	0.091	-2.700
313.15	-680.4	1859	8.110	42.27	57.73	0.108	
318.15	-756.9	2141	9.107	42.49	57.51	0.124	
323.15	-823.9	2395	9.960	42.66	57.34	0.139	
328.15	-899.0	2697	10.96	42.86	57.14	0.153	
isobutanol							
283.15	-92.75	256.9	1.235	42.35	57.65	1.211	
288.15	-111.3	315.1	1.480	42.50	57.50	1.190	
293.15	-136.3	398.0	1.823	42.69	57.31	1.169	
298.15	-166.0	500.5	2.236	42.89	57.11	1.149	
303.15	-205.7	646.8	2.812	43.14	56.86	1.129	
308.15	-246.1	800.5	3.396	43.34	56.66	1.110	2.946
313.15	-290.0	973.7	4.036	43.52	56.48	1.092	
318.15	-336.0	1161	4.705	43.68	56.32	1.074	
323.15	-385.4	1368	5.425	43.83	56.17	1.056	
328.15	-454.2	1681	6.508	44.05	55.95	1.040	
water							
283.15	-0.580	2.099	0.0095	43.93	56.07	6.235	
288.15	-0.811	3.079	0.0135	44.18	55.82	6.141	
293.15	-1.059	4.150	0.0178	44.34	55.66	6.048	
298.15	-1.378	5.587	0.0234	44.51	55.49	5.958	
303.15	-1.759	7.355	0.0301	44.66	55.34	5.870	13.39
308.15	-2.276	9.884	0.0395	44.84	55.16	5.784	
313.15	-2.860	12.81	0.0500	44.98	55.02	5.699	
318.15	-3.648	16.99	0.0649	45.15	54.85	5.616	
323.15	-4.579	22.09	0.0825	45.30	54.70	5.535	
328.15	-5.771	28.95	0.1058	45.47	54.53	5.455	

DMF							
283.15	-1935	3628	19.65	39.47	60.53	-2.044	
288.15	-2118	4084	21.52	39.70	60.30	-1.994	
293.15	-2280	4502	23.14	39.90	60.10	-1.947	
298.15	-2477	5050	25.25	40.15	59.85	-1.901	
303.15	-2674	5638	27.42	40.42	59.58	-1.857	
308.15	-2874	6290	29.74	40.70	59.30	-1.814	-6.589
313.15	-3052	6922	31.85	40.97	59.03	-1.774	
318.15	-3230	7632	34.14	41.27	58.73	-1.734	
323.15	-3392	8370	36.40	41.58	58.42	-1.697	
328.15	-3548	9224	38.92	41.94	58.06	-1.660	
1,4-dioxane							
288.15	-478.7	1164	5.702	41.47	58.53	-0.289	
293.15	-543.7	1353	6.470	41.63	58.37	-0.278	
298.15	-614.1	1565	7.307	41.80	58.20	-0.267	
303.15	-705.3	1857	8.452	42.02	57.98	-0.256	
308.15	-797.6	2165	9.614	42.22	57.78	-0.246	-1.538
313.15	-906.6	2553	11.05	42.46	57.54	-0.237	
318.15	-1027	3010	12.69	42.71	57.29	-0.228	
323.15	-1155	3535	14.51	42.98	57.02	-0.219	
328.15	-1292	4141	16.56	43.25	56.75	-0.211	

<sup>a</sup> $\Delta_d G^\circ$ ,  $\Delta_d H^\circ$  and  $\Delta_d S^\circ$  refers to, respectively, the dissolution Gibbs energy change, dissolution enthalpy and dissolution entropy;  $\gamma_1^\infty$  denotes the activity coefficient under infinitesimal concentration; and  $H_1^{E,\infty}$  denotes reduced excess enthalpy;  $\% \zeta_H$  and  $\% \zeta_{TS}$  stand for the contributions of dissolution enthalpy and dissolution entropy to the dissolution Gibbs energy change, respectively.

## References

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