

Data from Article:  
**A Unified View to Brønsted Acidity Scales: Do we need Solvated Protons?**

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[Chem. Sci. 2017](#), DOI: [10.1039/c7sc01424d](#)

**Table 2. Acidity scale in 1,2-dichloroethane; see the text for in-depth explanations of the data.**

No	Acid	$pK_{ip,rel}$	$pK_{a,rel}$	$pK_{a,DCE}$	$pH_{abs}^{H_2O}$ (BP) <sup>a</sup>	Directly measured $\Delta pK_{ip}$ values in DCE
1	9-COOMe-fluorene	13.2	13.1	58.1	15.4	
2	(4-Me-C <sub>6</sub> F <sub>4</sub> ) <sub>2</sub> CHCN	12.9	12.8	57.8	15.1	0.24, 1.38
3	(4-Me-C <sub>6</sub> F <sub>4</sub> )(C <sub>6</sub> F <sub>5</sub> )CHCN	11.9	11.7	56.7	14.0	1.03, 1.95
4	9-CN-fluorene	11.0	10.9	55.9	13.2	1.03, 0.99
5	(4-H-C <sub>6</sub> F <sub>4</sub> )(C <sub>6</sub> F <sub>5</sub> )CHCN	10.8	10.7	55.7	13.0	0.20, 1.12
6	(4-Cl-C <sub>6</sub> F <sub>4</sub> )(C <sub>6</sub> F <sub>5</sub> )CHCN	9.9	9.7	54.7	12.0	1.22, 0.42
7	(2-C <sub>10</sub> F <sub>7</sub> )(C <sub>6</sub> F <sub>5</sub> )CHCN	9.5	9.4	54.4	11.7	0.55, 0.93
8	9-C <sub>6</sub> F <sub>5</sub> -octafluorofluorene	9.0	8.8	53.8	11.1	0.37, 1.29
9	(2-C <sub>10</sub> F <sub>7</sub> ) <sub>2</sub> CHCN	8.6	8.4	53.4	10.7	1.13, 1.54
10	(4-CF <sub>3</sub> -C <sub>6</sub> F <sub>4</sub> )(C <sub>6</sub> F <sub>5</sub> )CHCN	7.5	7.3	52.3	9.6	1.03, 0.22
11	(C <sub>6</sub> F <sub>5</sub> )CH(CN)COOEt	7.5	7.5	52.5	9.8	0.04, 0.38
12	(4-Cl-C <sub>6</sub> F <sub>4</sub> )CH(CN)COOEt	7.3	7.2	52.2	9.5	-0.30, 0.22
13	(2-C <sub>10</sub> F <sub>7</sub> )CH(CN)COOEt	7.1	7.0	52.0	9.3	1.47, 1.62
14	(4-CF <sub>3</sub> -C <sub>6</sub> F <sub>4</sub> )CH(CN)COOEt	5.7	5.6	50.6	7.9	1.46, 0.03
15	(4-NC <sub>5</sub> F <sub>4</sub> )(C <sub>6</sub> F <sub>5</sub> )CHCN	5.7	5.5	50.5	7.8	1.24, 1.75
16	(4-NC <sub>5</sub> F <sub>4</sub> )CH(CN)COOEt	4.4	4.4	49.4	6.7	0.37, 1.40
17	3-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CH(CN) <sub>2</sub>	4.0	4.0	49.0	6.3	1.00, 1.55
18	(CF <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> CH(CN)COOEt	3.0	2.8	47.8	5.1	0.62, 0.56
19	4-H-C <sub>6</sub> F <sub>4</sub> CH(CN) <sub>2</sub>	2.5	2.5	47.5	4.8	0.01, 0.11
20	(4-NC <sub>5</sub> F <sub>4</sub> ) <sub>2</sub> CHCN	2.4	2.3	47.3	4.6	1.02, 0.97
21	2-C <sub>10</sub> F <sub>7</sub> CH(CN) <sub>2</sub>	1.4	1.3	46.3	3.6	1.02, 1.07
22	Bromothymol blue	1.4	1.1	46.1	3.4	0.06, 1.00
23	Bromocresol green	0.5	0.2	45.2	2.5	-1.35, 1.47
24	Picric acid <sup>b</sup>	0.0	0.0	45.0	2.3	
25	HCl	-0.4	0.2	45.2	2.5	-0.69, -1.25, -0.73, 1.32, 0.71, 0.73, 0.90, 0.36
26	2,3,4,6-(CF <sub>3</sub> ) <sub>4</sub> -C <sub>6</sub> HCH(CN) <sub>2</sub>	-0.7	-0.8	44.2	1.5	0.09, 1.48, 1.09
27	4-CF <sub>3</sub> -C <sub>6</sub> F <sub>4</sub> CH(CN) <sub>2</sub>	-0.8	-0.8	44.2	1.5	0.04, 0.77, 0.74, 1.00, 2.08, 1.78
28	Styphnic acid	-0.9	-0.9	44.1	1.4	
29	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> SO <sub>2</sub> NHTos <sup>c</sup>	-1.5	-1.7	43.3	0.6	
30	HNO <sub>3</sub>	-1.7	-1.4	43.6	0.9	0.28, 1.01, 1.13
31	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> SO <sub>2</sub> NHSO <sub>2</sub> C <sub>6</sub> H <sub>4</sub> -4-Cl	-2.4	-2.6	42.4	-0.3	0.88, 0.08, 0.24, 1.26
32	H <sub>2</sub> SO <sub>4</sub>	-2.5	-2.2	42.8	0.1	0.12, 1.02, 1.05, 1.48
33	C <sub>6</sub> (CF <sub>3</sub> ) <sub>5</sub> CH(CN) <sub>2</sub>	-2.6	-2.8	42.2	-0.5	1.02, 1.02, 1.05, 1.48
34	(4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -SO <sub>2</sub> ) <sub>2</sub> NH	-3.7	-3.9	41.1	-1.6	0.47, 0.80, 1.35, 0.93
35	3-NO <sub>2</sub> -4-Cl-C <sub>6</sub> H <sub>3</sub> SO <sub>2</sub> NHSO <sub>2</sub> C <sub>6</sub> H <sub>4</sub> -4-NO <sub>2</sub>	-4.1	-4.3	40.7	-2.0	0.36, 0.62, 0.39, 0.93
36	(3-NO <sub>2</sub> -4-Cl-C <sub>6</sub> H <sub>3</sub> SO <sub>2</sub> ) <sub>2</sub> NH	-4.5	-4.6	40.4	-2.3	0.19, 0.62, 0.39, 0.93
37	HBr	-4.9	-4.4	40.6	-2.1	
38	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> SO <sub>2</sub> CH(CN) <sub>2</sub>	-5.1	-5.1	39.9	-2.8	0.80, 1.33, 1.03
39	2,4,6-(SO <sub>2</sub> F) <sub>3</sub> -Phenol	-5.9	-6.0	39.0	-3.7	
40	2,4,6-IF <sub>3</sub> -Phenol <sup>d</sup>	-6.4	-6.6	38.4	-4.3	-0.64

No	Acid	$pK_{ip,rel}$	$pK_{a,rel}$	$pK_{a,DCE}$	$pH_{abs}^{H_2O}$ (BP) <sup>a</sup>	Directly measured $\Delta pK_{ip}$ values in DCE
41	CH(CN) <sub>3</sub>	-6.5	-6.4	38.6	-4.1	
42	4-Cl-C <sub>6</sub> H <sub>4</sub> SO(=NTf)NHTos	-6.8	-7.0	38.0	-4.7	0.42 0.94 1.14 1.12
43	NH <sub>2</sub> -TCNP <sup>c</sup>	-6.8	-6.8	38.2	-4.5	0.33 0.42 1.14 1.12 0.65 0.51 0.05 0.24
44	2,3,5-tricyanocyclopentadiene	-7.0	-7.0	38.0	-4.7	0.20
45	Pentacyanophenol	-7.6	-7.5	37.5	-5.2	0.67 0.84
46	4-Cl-C <sub>6</sub> H <sub>4</sub> SO(=NTf)NHSO <sub>2</sub> C <sub>6</sub> H <sub>4</sub> -4-Cl	-7.6	-7.9	37.1	-5.6	1.77
47	HI	-7.7	-7.3	37.7	-5.0	0.98 1.56 1.64 1.00 1.13 1.10 1.04 1.01 0.96 0.81 0.90
48	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> SO <sub>2</sub> NHTf	-7.8	-7.9	37.1	-5.6	0.93
49	Me-TCNP	-8.6	-8.6	36.4	-6.3	0.09 0.13 0.12 1.42 0.96 0.81 0.90
50	3,4-(MeO) <sub>2</sub> -C <sub>6</sub> H <sub>3</sub> -TCNP	-8.7	-8.9	36.1	-6.6	-0.02 0.12 0.24 0.28 0.59 0.74 0.67 0.60 1.61
51	4-MeO-C <sub>6</sub> H <sub>4</sub> -TCNP	-8.7	-8.9	36.1	-6.6	0.12 0.46 0.24 0.28 0.59 0.74 0.67 0.60 1.61
52	C(CN) <sub>2</sub> =C(CN)OH	-8.8	-8.7	36.3	-6.4	0.22 0.46 0.24 0.28 0.59 0.74 0.67 0.60 1.61
53	4-Cl-C <sub>6</sub> H <sub>4</sub> SO(=NTf)NHSO <sub>2</sub> C <sub>6</sub> H <sub>4</sub> -NO <sub>2</sub>	-8.8	-9.1	35.9	-6.8	0.22 0.46 0.24 0.28 0.59 0.74 0.67 0.60 1.61
54	2,4-(NO <sub>2</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>3</sub> SO <sub>2</sub> OH	-8.9	-9.0	36.0	-6.7	0.59 0.06 0.52 0.13 0.60 1.62 1.23
55	C <sub>6</sub> F <sub>3</sub> CH(Tf) <sub>2</sub>	-9.0	-9.1	35.9	-6.8	0.47 0.44 1.33 1.56 1.57 1.62 1.23
56	HB(CN)(CF <sub>3</sub> ) <sub>3</sub>	-9.3	-9.3	35.7	-7.0	0.47 0.44 1.33 1.56 1.57 1.62 1.23
57	Ph-TCNP	-9.4	-9.5	35.5	-7.2	0.83 1.06 1.34 0.01 0.21 0.60 0.84 0.84 0.89 0.91 0.93
58	HBF <sub>4</sub>	-10.3	-10.0	35.0	-7.7	0.26 1.06 1.34 0.01 0.21 0.60 0.84 0.84 0.89 0.91 0.93
59	FSO <sub>2</sub> OH	-10.5	-10.3	34.7	-8.0	0.22 0.58 0.78 0.73 0.84 0.84 0.89 0.91 0.93
60	3-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -TCNP	-10.5	-10.7	34.3	-8.4	0.22 0.58 0.78 0.73 0.84 0.84 0.89 0.91 0.93
61	H-TCNP	-10.7	-10.7	34.3	-8.4	0.46 0.78 0.73 0.84 0.84 0.89 0.91 0.93
62	[C <sub>6</sub> H <sub>5</sub> SO(=NTf)] <sub>2</sub> NH	-11.1	-11.4	33.6	-9.1	0.29 0.28 0.44 0.21 0.47 0.49 0.47 0.40 0.32 0.73 0.75 0.67 0.63
63	[(C <sub>2</sub> F <sub>5</sub> ) <sub>2</sub> PO] <sub>2</sub> NH	-11.3	-11.5	33.5	-9.2	0.29 0.28 0.44 0.21 0.47 0.49 0.47 0.40 0.32 0.73 0.75 0.67 0.63
64	2,4,6-(NO <sub>2</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>2</sub> SO <sub>2</sub> OH	-11.3	-11.4	33.6	-9.1	0.29 0.28 0.44 0.21 0.47 0.49 0.47 0.40 0.32 0.73 0.75 0.67 0.63
65	[C(CN) <sub>2</sub> =C(CN)] <sub>2</sub> CH <sub>2</sub>	-11.4	-11.5	33.5	-9.2	0.10 0.44 0.21 0.47 0.49 0.47 0.40 0.32 0.73 0.75 0.67 0.63
66	TfOH	-11.4	-11.3	33.7	-9.0	0.04 0.09 0.47 0.49 0.47 0.40 0.32 0.73 0.75 0.67 0.63
67	C <sub>6</sub> H <sub>5</sub> SO(=NTf)NHTf	-11.5	-11.7	33.3	-9.4	0.36 0.25 0.20 0.10 0.06 0.19 0.21 0.42 0.46 0.43 0.40 0.69 0.93 1.04 1.05 0.96
68	TfCH(CN) <sub>2</sub>	-11.6	-11.5	33.5	-9.2	0.36 0.25 0.20 0.10 0.06 0.19 0.21 0.42 0.46 0.43 0.40 0.69 0.93 1.04 1.05 0.96
69	Br-TCNP	-11.8	-11.8	33.2	-9.5	0.10 0.06 0.19 0.21 0.42 0.46 0.43 0.40 0.69 0.93 1.04 1.05 0.96
70	[C(CN) <sub>2</sub> =C(CN)] <sub>2</sub> NH	-11.8	-12.0	33.0	-9.7	0.10 0.06 0.19 0.21 0.42 0.46 0.43 0.40 0.69 0.93 1.04 1.05 0.96
71	3,5-(CF <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>3</sub> -TCNP	-11.8	-12.0	33.0	-9.7	0.19 0.31 0.30 0.45 0.19 0.21 0.42 0.46 0.43 0.40 0.69 0.93 1.04 1.05 0.96
72	TfNH <sup>f</sup>	-11.9	-12.0	33.0	-9.7	0.19 0.31 0.30 0.45 0.19 0.21 0.42 0.46 0.43 0.40 0.69 0.93 1.04 1.05 0.96
73	4-Cl-C <sub>6</sub> H <sub>4</sub> SO(=NTf)NHTf	-12.1	-12.3	32.7	-10.0	0.01 0.13 0.21 0.29 0.27 1.29 0.69 0.93 1.04 1.05 0.96
74	Cl-TCNP	-12.1	-12.1	32.9	-9.8	0.10 0.13 0.21 0.29 0.27 1.29 0.69 0.93 1.04 1.05 0.96
75	(C <sub>3</sub> F <sub>7</sub> SO <sub>2</sub> ) <sub>2</sub> NH	-12.1	-12.3	32.7	-10.0	0.10 0.13 0.21 0.29 0.27 1.29 0.69 0.93 1.04 1.05 0.96
76	(C <sub>4</sub> F <sub>9</sub> SO <sub>2</sub> ) <sub>2</sub> NH	-12.2	-12.4	32.6	-10.1	-0.19 0.10 0.29 0.27 1.29 0.69 0.93 1.04 1.05 0.96
77	CN-CH <sub>2</sub> -TCNP	-12.3	-12.4	32.6	-10.1	0.02 0.44 0.47 0.72 1.06 0.77 0.80 1.04 1.05 0.96
78	(C <sub>2</sub> F <sub>5</sub> SO <sub>2</sub> ) <sub>2</sub> NH	-12.3	-12.4	32.6	-10.1	0.02 0.44 0.47 0.72 1.06 0.77 0.80 1.04 1.05 0.96
79	CF <sub>3</sub> -TCNP	-12.7	-12.8	32.2	-10.5	0.40 0.56 0.11 0.69 0.07 0.86
80	HClO <sub>4</sub>	-13.0	-12.8	32.2	-10.5	0.40 0.56 0.11 0.69 0.07 0.86
81	CF <sub>2</sub> (CF <sub>2</sub> SO <sub>2</sub> ) <sub>2</sub> NH	-13.1	-13.1	31.9	-10.8	0.19 0.44 1.76 1.92 2.16
82	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> SO(=NTf)NHTf	-13.1	-13.3	31.7	-11.0	0.19 0.44 1.76 1.92 2.16
83	HB(CN) <sub>4</sub>	-13.3	-13.3	31.7	-11.0	0.19 0.44 1.76 1.92 2.16
84	(FSO <sub>2</sub> ) <sub>3</sub> CH	-13.6	-13.6	31.4	-11.3	1.76 1.92 2.16
85	Tf <sub>2</sub> CH(CN)	-14.9	-15.0	30.0	-12.7	1.76 1.92 2.16
86	2,3,4,5-tetracyanocyclopentadiene	-15.1	-15.1	29.9	-12.8	1.73 0.22 0.40 0.23 0.21
87	CN-TCNP	-15.3	-15.3	29.7	-13.0	1.73 0.22 0.40 0.23 0.21

<sup>a</sup> Estimates of absolute acidities in terms of aqueous pH of 1:1 HA/A<sup>-</sup> buffer solution in DCE of the respective acid. <sup>b</sup>  $pK_{ip,rel}$  value of picric acid is arbitrarily set to 0. <sup>c</sup> Tos represents the 4-Me-C<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>-group. <sup>d</sup> Tf represents the CF<sub>3</sub>SO<sub>2</sub>-group. <sup>e</sup> X-TCNP represents 2-X-1,1,3,3-tetracyanopropene. <sup>f</sup> Reference acid for the  $pK_{a,DCE}$  values with computational  $pK_{a,DCE}$  value 33.