

No	Acid	pK <sub>a,rel</sub>	pK <sub>a,DCE</sub>	pH <sup>H<sub>2</sub>O</sup> <sub>obs</sub> (BP)	Directly measured ΔpK <sub>ip</sub> values in DCE
1	9-COOMe-fluorene	13.1	58.1	15.4	
2	(4-Me-C <sub>6</sub> F <sub>4</sub> ) <sub>2</sub> CHCN	12.8	57.8	15.1	0.24
3	(4-Me-C <sub>6</sub> F <sub>4</sub> )(C <sub>6</sub> F <sub>5</sub> )CHCN	11.7	56.7	14.0	1.03, 1.38, 1.95
4	9-CN-fluorene	10.9	55.9	13.2	0.99
5	(4-H-C <sub>6</sub> F <sub>4</sub> )(C <sub>6</sub> F <sub>5</sub> )CHCN	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	9.7	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	9.4	54.4	11.7	0.55, 0.93, 1.29
9	9-C <sub>6</sub> F <sub>5</sub> -octafluorofluorene	8.8	53.8	11.1	0.37, 0.93
9	(2-C <sub>10</sub> F <sub>7</sub> ) <sub>2</sub> CHCN	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	7.3	52.3	9.6	0.04, 1.03, 0.22, 0.38
11	(C <sub>6</sub> F <sub>5</sub> )CH(CN)COOEt	7.5	52.5	9.8	
12	(4-Cl-C <sub>6</sub> F <sub>4</sub> )CH(CN)COOEt	7.2	52.2	9.5	-0.30, 0.22, 0.38
13	(2-C <sub>10</sub> F <sub>7</sub> )CH(CN)COOEt	7.0	52.0	9.3	1.47, 1.46, 1.62
14	(4-CF <sub>3</sub> -C <sub>6</sub> F <sub>4</sub> )CH(CN)COOEt	5.6	50.6	7.9	0.03, 1.24, 1.75
15	(4-NC <sub>6</sub> F <sub>4</sub> )(C <sub>6</sub> F <sub>5</sub> )CHCN	5.5	50.5	7.8	
16	(4-NC <sub>6</sub> F <sub>4</sub> )CH(CN)COOEt	4.4	49.4	6.7	0.37, 1.40, 1.75
17	3-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CH(CN) <sub>2</sub>	4.0	49.0	6.3	1.00, 1.40
18	(CF <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> CH(CN)COOEt	2.8	47.8	5.1	0.62, 1.55
19	4-H-C <sub>6</sub> F <sub>4</sub> CH(CN) <sub>2</sub>	2.5	47.5	4.8	0.01, 0.56, 0.11, 0.97, 1.07
20	(4-NC <sub>6</sub> F <sub>4</sub> ) <sub>2</sub> CHCN	2.3	47.3	4.6	1.02, 0.06, 1.00, 1.47
21	2-C <sub>10</sub> F <sub>7</sub> CH(CN) <sub>2</sub>	1.3	46.3	3.6	
22	Bromothymol blue	1.1	46.1	3.4	-1.35, 1.00, 1.47
23	Bromocresol green	0.2	45.2	2.5	
24	Picric acid	0.0	45.0	2.3	
25	HCl	0.2	45.2	2.5	-0.69, -1.25, -0.73, 1.32, 0.71, 0.73, 0.90, 0.36, 1.09
26	2,3,4,6-(CF <sub>3</sub> ) <sub>4</sub> -C <sub>6</sub> HCH(CN) <sub>2</sub>	-0.8	44.2	1.5	0.09, 0.04, 0.77, 0.74, 1.00, 2.08, 1.78
27	4-CF <sub>3</sub> -C <sub>6</sub> F <sub>4</sub> CH(CN) <sub>2</sub>	-0.8	44.2	1.5	
28	Styphnic acid	-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	-1.7	43.3	0.6	
30	HNO <sub>3</sub>	-1.4	43.6	0.9	0.28, 1.01, 1.13, 0.08, 0.24, 1.26
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	-2.6	42.4	-0.3	0.88, 0.12, 1.02, 1.02, 1.05, 1.48
32	H <sub>2</sub> SO <sub>4</sub>	-2.2	42.8	0.1	0.47, 0.80, 0.36, 1.35, 0.93
33	C <sub>6</sub> (CF <sub>3</sub> ) <sub>3</sub> CH(CN) <sub>2</sub>	-2.8	42.2	-0.5	0.39, 0.19, 0.62, 0.93, 1.03
34	(4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -SO <sub>2</sub> ) <sub>2</sub> NH	-3.9	41.1	-1.6	0.80, 1.33, 0.64, 0.42, 0.94, 1.14, 1.12, 0.65, 0.51, 0.05, 0.24
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>	-4.3	40.7	-2.0	0.20, 0.42, 0.94, 1.14, 1.12, 0.65, 0.51, 0.05, 0.24
36	(3-NO <sub>2</sub> -4-Cl-C <sub>6</sub> H <sub>3</sub> SO <sub>2</sub> ) <sub>2</sub> NH	-4.6	40.4	-2.3	
37	HBr	-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	39.9	-2.8	0.80, 1.33, 0.64, 0.42, 0.94, 1.14, 1.12, 0.65, 0.51, 0.05, 0.24
39	2,4,6-(SO <sub>2</sub> F) <sub>3</sub> -Phenol	-6.0	39.0	-3.7	
40	2,4,6-Tf <sub>3</sub> -Phenol	-6.6	38.4	-4.3	
41	CH(CN) <sub>3</sub>	-6.4	38.6	-4.1	
42	4-Cl-C <sub>6</sub> H <sub>4</sub> SO(=NTf) <sub>2</sub> NHTos	-7.0	38.0	-4.7	
43	NH <sub>2</sub> -TCNP	-6.8	38.2	-4.5	
44	2,3,5-tricyanocyclopentadiene	-7.0	38.0	-4.7	
45	Pentacyanophenol	-7.5	37.5	-5.2	
46	4-Cl-C <sub>6</sub> H <sub>4</sub> SO(=NTf) <sub>2</sub> NHSO <sub>2</sub> C <sub>6</sub> H <sub>4</sub> -4-Cl	-7.9	37.1	-5.6	
47	HI	-7.3	37.7	-5.0	
48	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> SO <sub>2</sub> NHTf	-7.9	37.1	-5.6	0.98, 0.93, 1.56, 1.64, 1.00, 1.13, 1.10, 1.04, 1.01, 0.96, 0.81, 0.90
49	Me-TCNP	-8.6	36.4	-6.3	0.09, 0.13, 0.42, 0.94, 1.14, 1.12, 0.65, 0.51, 0.05, 0.24
50	3,4-(MeO) <sub>2</sub> -C <sub>6</sub> H <sub>3</sub> -TCNP	-8.9	36.1	-6.6	
51	4-MeO-C <sub>6</sub> H <sub>4</sub> -TCNP	-8.9	36.1	-6.6	
52	C(CN) <sub>2</sub> =C(CN)OH	-8.7	36.3	-6.4	0.12, 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) <sub>2</sub> NHSO <sub>2</sub> C <sub>6</sub> H <sub>4</sub> -NO <sub>2</sub>	-9.1	35.9	-6.8	
54	2,4-(NO <sub>2</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>3</sub> SO <sub>2</sub> OH	-9.0	36.0	-6.7	0.59, 0.06, 0.52, 0.74, 0.67, 0.60, 1.61
55	C <sub>6</sub> F <sub>4</sub> CH(Tf) <sub>2</sub>	-9.1	35.9	-6.8	
56	HB(CN)(CF <sub>3</sub> ) <sub>3</sub>	-9.3	35.7	-7.0	0.47, 0.44, 1.33, 1.56, 1.57, 1.62, 1.23
57	Ph-TCNP	-9.5	35.5	-7.2	
58	HBFA	-10.0	35.0	-7.7	0.83, 1.06, 1.34, 0.01, 0.21, 0.60, 0.73, 0.84, 0.84, 0.89, 0.91, 0.93
59	FSO <sub>2</sub> OH	-10.3	34.7	-8.0	
60	3-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -TCNP	-10.7	34.3	-8.4	0.22, 0.58, 0.46, 0.78, 0.73, 0.84, 0.84, 0.89, 0.91, 0.93
61	H-TCNP	-10.7	34.3	-8.4	
62	[C <sub>6</sub> H <sub>4</sub> SO(=NTf)] <sub>2</sub> NH	-11.4	33.6	-9.1	
63	[(C <sub>6</sub> F <sub>5</sub> ) <sub>2</sub> PO] <sub>2</sub> NH	-11.5	33.5	-9.2	0.29, 0.28, 0.44, 0.21, 0.10, 0.47, 0.49, 0.12, 0.40, 0.07, 0.32
64	2,4,6-(NO <sub>2</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>2</sub> SO <sub>2</sub> OH	-11.4	33.6	-9.1	
65	[C(CN) <sub>2</sub> =C(CN)] <sub>2</sub> CH <sub>2</sub>	-11.5	33.5	-9.2	
66	TfOH	-11.3	33.7	-9.0	
67	C <sub>6</sub> H <sub>4</sub> SO(=NTf) <sub>2</sub> NHTf	-11.7	33.3	-9.4	0.04, 0.09, 0.36, 0.25, 0.20, 0.10, 0.47, 0.49, 0.12, 0.40, 0.07, 0.32
68	TfCH(CN) <sub>2</sub>	-11.5	33.5	-9.2	
69	Br-TCNP	-11.8	33.2	-9.5	
70	[C(CN) <sub>2</sub> =C(CN)] <sub>2</sub> NH	-12.0	33.0	-9.7	0.10, 0.06, 0.45, 0.19, 0.21, 0.73, 0.75, 0.67, 0.63
71	3,5-(CF <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>3</sub> -TCNP	-12.0	33.0	-9.7	
72	Tf <sub>2</sub> NH	-12.0	33.0	-9.7	0.19, 0.31, 0.30, 0.15, 0.42, 0.46
73	4-Cl-C <sub>6</sub> H <sub>4</sub> SO(=NTf) <sub>2</sub> NHTf	-12.3	32.7	-10.0	
74	Cl-TCNP	-12.1	32.9	-9.8	0.01, 0.10, 0.13, 0.21, 0.29, 0.27, 1.29, 0.43, 0.40
75	(C <sub>2</sub> F <sub>5</sub> SO <sub>2</sub> ) <sub>2</sub> NH	-12.3	32.7	-10.0	
76	(C <sub>2</sub> F <sub>5</sub> SO <sub>2</sub> ) <sub>2</sub> NH	-12.4	32.6	-10.1	0.19, 0.10, 0.02, 0.44, 0.47, 0.72, 1.06, 0.77, 0.69, 0.93, 1.04, 1.05, 0.96
77	CN-CH <sub>2</sub> -TCNP	-12.4	32.6	-10.1	
78	(C <sub>2</sub> F <sub>5</sub> SO <sub>2</sub> ) <sub>2</sub> NH	-12.4	32.6	-10.1	
79	CF <sub>3</sub> -TCNP	-12.8	32.2	-10.5	
80	HClO <sub>4</sub>	-12.8	32.2	-10.5	-0.80, 0.40, 0.56, 0.11, 0.89, 0.07, 0.86, 1.04
81	CF <sub>3</sub> (CF <sub>2</sub> SO <sub>2</sub> ) <sub>2</sub> NH	-13.1	31.9	-10.8	
82	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> SO(=NTf) <sub>2</sub> NHTf	-13.3	31.7	-11.0	0.19, 0.44, 1.76, 1.92, 2.16
83	HB(CN) <sub>4</sub>	-13.3	31.7	-11.0	
84	(FSO <sub>2</sub> ) <sub>3</sub> CH	-13.6	31.4	-11.3	
85	Tf <sub>2</sub> CH(CN)	-15.0	30.0	-12.7	-1.46, 1.73, 0.22, 0.40
86	2,3,4,5-tetracyanocyclopentadiene	-15.1	29.9	-12.8	0.23, 0.21
87	CN-TCNP	-15.3	29.7	-13.0	