

Solute Descriptors for Phenoxide Anions

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Supplementary Material

TABLE S1. Values of pKa(w), pKa(s) for Substituted Phenols, together with Log *P* for transfer from Water to the Given Solvent for H⁺, the Neutral form of the Phenol and the Corresponding Phenoxide Anion. The Reference is to the Source of pKa(s).

Compound	Ref	Solvent	pKa(w)	pKa(s)	Log <i>P</i>		
					H ⁺	Neutral	Anion
Phenol	31	Methanol	9.99	14.33	-1.82	1.81	-0.71
	20	DMF	9.99	15.40	2.52	2.19	-5.74
	28	DMA	9.99	13.45	4.90	2.56	-5.80
	28	NMP	9.99	15.50	3.33	2.69	-6.15
2-Methylphenol	21	Methanol	10.31	14.86	-1.82	2.32	-0.41
3-Methylphenol	21	Methanol	10.10	14.43	-1.82	2.18	-0.33
4-Methylphenol	21	Methanol	10.28	14.54	-1.82	2.29	-0.15
2,3-Dimethylphenol	21	Methanol	10.54	15.08	-1.82	2.62	-0.10
2,4-Dimethylphenol	21	Methanol	10.60	15.04	-1.82	2.54	-0.08
2,5-Dimethylphenol	21	Methanol	10.41	14.91	-1.82	2.58	-0.10

2,6-Dimethylphenol	21	Methanol	10.59	15.26	-1.82	2.58	-0.27
3,4-Dimethylphenol	21	Methanol	10.36	14.63	-1.82	2.53	0.08
3,5-Dimethylphenol	21	Methanol	10.20	14.57	-1.82	2.60	0.05
4-t-Butylphenol	21	Methanol	10.31	14.52	-1.82	3.46	1.07
2-Fluorophenol	21	Methanol	8.73	12.94	-1.82	2.10	-0.29
	20	Methanol	8.73	12.48	-1.82	2.10	0.17
2-Chlorophenol	21	Methanol	8.48	12.97	-1.82	2.17	-0.50
	28	DMF	8.48	13.91	2.52	2.58	-5.37
3-Chlorophenol	21	Methanol	9.02	13.10	-1.82	2.68	0.42
	28	DMF	9.02	16.29	2.52	3.55	-6.24
4-Chlorophenol	21	Methanol	9.38	13.59	-1.82	2.50	0.11
	28	MeCN	9.38	25.44	-7.85	1.93	-6.28
	28	DMF	9.38	16.78	2.52	3.30	-6.62
	28	NMP	9.38	16.50	3.33	3.78	-6.67
2,4-Dichlorophenol	28	DMSO	7.85	13.25	3.40	4.57	-4.23
	22	Isopropanol	7.85	14.48	-1.93	3.25	-1.45
2,5-Dichlorophenol	28	DMF	7.51	13.85	2.52	3.81	-5.05
2,6-Dichlorophenol	28	DMF	6.79	12.55	2.52	3.47	-4.81
	28	DMSO	6.79	11.54	3.40	3.92	-4.23
	22	Isopropanol	6.79	13.58	-1.93	2.85	-2.01
3,4-Dichlorophenol	28	MeCN	8.63	24.06	-7.85	2.87	-4.71
3,5-Dichlorophenol	21	Methanol	8.18	12.11	-1.82	3.73	1.62
	24	MeCN	8.18	23.31	-7.85	2.81	-4.47
	22	t-Butanol	8.18	17.04	-3.30	3.92	-1.64
2-Bromophenol	28	MeCN	8.41	23.92	-7.85	2.07	-5.59

	28	DMF	8.41	13.85	2.52	2.82	-5.14
3-Bromophenol	21	Methanol	9.01	13.30	-1.82	2.83	0.36
4-Bromophenol	21	Methanol	9.36	13.63	-1.82	2.67	0.22
	28	MeCN	9.36	25.53	-7.85	2.15	-6.17
	28	DMSO	9.36	15.50	3.40	4.75	-4.79
	28	NMP	9.36	16.50	3.33	4.08	-6.39
2,4,6-Tribromophenol	21	Methanol	6.10	10.10	-1.82	4.06	1.88
	28	Propanone	6.10	21.10	-2.56	4.72	-7.72
3-CF ₃ -phenol	28	DMF	8.95	15.70	2.52	3.77	-5.50
	24	t-Butanol	8.95	18.62	-3.30	3.45	-2.92
3-Cyanophenol	28	DMSO	8.61	14.76	3.40	4.96	-4.59
4-Cyanophenol	28	MeCN	7.80	22.77	-7.85	1.62	-5.50
	28	DMSO	7.80	13.05	3.40	4.77	-3.88
2-Methoxyphenol	21	Methanol	9.90	14.48	-1.82	1.69	-1.07
Salicylaldehyde	21	Methanol	8.25	12.82	-1.82	2.09	-0.66
2-Nitrophenol	21	Methanol	7.23	11.53	-1.82	2.02	-0.46
	28	MeCN	7.23	22.00	-7.85	2.32	-4.60
	28	DMF	7.23	12.20	2.52	2.47	-5.02
	28	DMSO	7.23	11.00	3.40	2.72	-4.45
	22	Isopropanol	7.23	13.30	-1.93	1.78	-2.36
3-Nitrophenol	21, 24	Methanol	8.36	12.24	-1.82	2.30	0.24
	28	DMF	8.36	14.64	2.52	3.60	-5.20
	28	DMSO	8.36	14.00	3.40	5.11	-3.93
	28	NMP	8.36	14.30	3.33	4.11	-5.16
	22	Isopropanol	8.36	13.92	-1.93	2.08	-1.55
	22	t-Butanol	8.36	16.99	-3.30	2.13	-3.20
4-Nitrophenol	20	Methanol	7.18	11.09	-1.82	2.11	0.02

	20	MeCN	7.18	20.70	-7.85	1.82	-3.85
	20	DMF	7.18	11.84	2.52	3.51	-3.67
	20	DMA	7.18	10.85	4.90	3.95	-4.62
	20	DMSO	7.18	11.00	3.40	5.15	-2.07
	20	NMP	7.18	12.15	3.33	4.03	-4.27
	22	t-butanol	7.18	14.60	-3.30	1.88	-2.24
2,3-Dinitrophenol	20	Methanol	5.24	9.43	-1.82	2.38	0.01
2,4-Dinitrophenol	21	Methanol	4.10	7.83	-1.82	1.76	-0.15
	28	DMSO	4.10	5.00	3.40	2.93	-1.37
	28	DMF	4.10	6.36	2.52	2.48	-2.30
	28	MeCN	4.10	17.20	-7.85	2.17	-3.08
	28	Propanone	4.10	15.70	-2.56	2.22	-6.82
	28	NMP	4.10	6.80	3.33	2.64	-3.39
2,5-Dinitrophenol	21	Methanol	5.22	8.94	-1.82	1.88	-0.02
	28	DMSO	5.22	6.88	3.40	3.06	-2.00
	28	DMF	5.22	8.78	2.52	2.57	-3.51
	28	Propanone	5.22	19.80	-2.56	2.33	-9.69
	28	NMP	5.22	9.00	3.33	2.78	-4.33
2,6-Dinitrophenol	21	Methanol	3.74	7.64	-1.82	1.66	-0.42
	28	DMSO	3.74	4.82	3.40	3.87	-0.61
	28	DMF	3.74	6.07	2.52	3.09	-1.76
	28	MeCN	3.74	16.45	-7.85	2.58	-2.28
	28	Propanone	3.74	13.78	-2.56	2.49	-4.99
	28	MeNO ₂	3.74	16.00	-0.99	3.07	-8.20
3,4-Dinitrophenol	20	Methanol	5.42	9.46	-1.82	2.84	0.62
3,5-Dinitrophenol	24	MeCN	6.66	20.50	-7.85	2.66	-3.33
	28	DMF	6.66	11.36	2.52	5.00	-2.22
	28	DMSO	6.66	10.60	3.40	7.10	-0.24
	24	t-Butanol	6.66	13.40	-3.30	2.68	-0.76
Picric acid	28	Ethanol	0.43	4.10	-1.60	1.79	-0.28
	20	Acetone	0.43	9.20	-2.56	3.28	-2.93
	20	DMSO	0.43	-0.30	3.40	5.85	3.18
	28	NMP	0.43	2.00	3.33	4.65	-0.25
2,6-Di-t-butyl-4-nitrophenol	20	Methanol	6.62	10.89	-1.82	5.16	2.71
	28	MeCN	6.62	19.10	-7.85	5.11	0.48
Thiophenol	28	DMF	6.61	10.70	2.52	3.08	-3.53
	25	Methanol	6.61	8.65	-1.82	2.63	2.41

4-Methylthiophenol	25	Methanol	6.82	8.96	-1.82	2.95	2.63
2,6-Dibromo-4-nitro	21	Methanol	3.97	7.31	-1.82	3.83	2.31
2-Methyl-4,6-dinitro	28	DMSO	4.35	4.59	3.40	3.58	-0.06
	26	Methanol	4.35	8.19	-1.82	2.31	0.29
1-Naphthol	21	Methanol	9.40	13.91	-1.82	3.09	0.40