

Table 1. Fit Data Set for COSMO-RS Acid pK_a Calculations in Acetonitrile.^a

Compound ^b	CAS-RN	Type	Class	Delocalized ^c	ΔG_{diss}	pK _a ^{Exp}	pK _a ^{Calc}	pK _a ^{Calc} _(corr)
(C ₆ F ₅)CH(CN)COOEt	2340-87-6	CH	Methane	Yes	27.93	17.75	16.15	19.20
(4-CF ₃ -C ₆ F ₄)CH(CN)COOEt	32251-53-9	CH	Methane	Yes	24.47	16.08	13.46	16.73
4-Me-C ₆ H ₄ CH(CN) ₂	33534-88-2	CH	Methane	Yes	23.89	17.59	13.01	16.31
(C ₆ H ₅)(C ₆ F ₅)CHCN	42238-33-5	CH	Methane	Yes	37.30	26.14	23.44	25.90
(C ₆ F ₅) ₂ CHCN	42238-34-6	CH	Methane	Yes	31.22	21.10	18.72	21.56
(4-CF ₃ -C ₆ F ₄)(C ₆ F ₅)CHCN	42238-35-7	CH	Methane	Yes	26.33	18.14	14.91	18.06
(4-Cl-C ₆ F ₄)(C ₆ F ₅)CHCN	42238-36-8	CH	Methane	Yes	30.00	20.36	17.76	20.68
(4-H-C ₆ F ₄)(C ₆ F ₅)CHCN	42254-09-1	CH	Methane	Yes	31.34	21.11	18.80	21.64
(4-Me-C ₆ F ₄)(C ₆ F ₅)CHCN	52345-34-3	CH	Methane	Yes	32.60	21.94	19.78	22.54
(4-Cl-C ₆ F ₄)CH(CN)COOEt	55810-56-5	CH	Methane	Yes	27.16	17.39	15.55	18.65
(4-NC ₃ F ₄)CH(CN)COOEt	55810-61-2	CH	Methane	Yes	23.29	14.90	12.54	15.88
4-H-C ₆ F ₄ CH(CN) ₂	55810-63-4	CH	Methane	Yes	19.79	12.98	9.82	13.38
(4-H-C ₆ F ₄)CH(CN)COOEt	55852-22-7	CH	Methane	Yes	28.48	18.08	16.58	19.60
4-CF ₃ -C ₆ F ₄ CH(CN) ₂	55852-24-9	CH	Methane	Yes	14.75	10.19	5.90	9.77
(4-Me-C ₆ F ₄) ₂ CHCN	58432-44-3	CH	Methane	Yes	33.96	22.80	20.85	23.52
(4-CF ₃ -C ₆ F ₄) ₂ CHCN	58432-55-6	CH	Methane	Yes	22.27	16.13	11.75	15.15
(4-Me-C ₆ F ₄)(C ₆ H ₅)CHCN	58432-62-5	CH	Methane	Yes	38.99	26.96	24.76	27.11
(2-C ₁₀ F ₇)CH(CN)COOEt	62325-34-2	CH	Methane	Yes	27.14	17.50	15.54	18.64
2-C ₁₀ F ₇ CH(CN) ₂	62325-35-3	CH	Methane	Yes	18.55	12.23	8.85	12.49
(4-NC ₃ F ₄)(2-C ₁₀ F ₇)CHCN	62325-37-5	CH	Methane	Yes	23.98	16.02	13.08	16.38
(2-C ₁₀ F ₇) ₂ CHCN	62325-38-6	CH	Methane	Yes	28.08	19.32	16.27	19.31
(4-NC ₃ F ₄)(C ₆ F ₅)CHCN	62325-51-3	CH	methane	Yes	23.44	16.40	12.66	15.99
(2-C ₁₀ F ₇)(C ₆ F ₅)CHCN	64934-68-5	CH	Methane	Yes	29.47	20.08	17.35	20.30
(2,4,6-Cl ₃ -C ₆ F ₂)(C ₆ F ₅)CHCN	64934-69-6	CH	Methane	Yes	29.76	20.13	17.58	20.51
4-Me-C ₆ F ₄ CH(CN) ₂	64934-71-0	CH	methane	Yes	21.14	13.87	10.87	14.34
(4-NC ₃ F ₄) ₂ CHCN	64934-72-1	CH	Methane	Yes	19.79	13.46	9.82	13.38
C ₆ F ₅ CH(CN) ₂	719-38-0	CH	Methane	Yes	19.88	13.01	9.89	13.44
3-CF ₃ -C ₆ H ₄ CH(CN) ₂	99726-60-0	CH	Methane	Yes	20.10	14.72	10.06	13.60
4-NO ₂ -C ₆ H ₄ CH(CN) ₂	7077-65-8	CH	Methane	Yes	16.09	11.61	6.94	10.73
C ₆ H ₅ CHTf ₂	40906-82-9	CH	Methane	Yes	13.78	7.85	5.14	9.08
(C ₆ F ₅)CH(COOEt) ₂	1582-05-4	CH/OH ^d	Methane	Yes	35.12	22.85	21.75	24.34
2,3,5-Tricyanocyclopentadiene	215395-09-8	CH	Cyclopentadiene	Yes	8.88	4.16	1.33	5.57
9-C ₆ F ₅ -Fluorene	73482-93-6	CH	Fluorene	Yes	42.17	28.11	27.24	29.39
Fluoradene	205-94-7	CH	Fluorene	Yes	36.15	23.90	22.55	25.08
9-COOMe-Fluorene	3002-30-0	CH	Fluorene	Yes	35.04	23.53	21.68	24.28
9-CN-Fluorene	1529-40-4	CH	Fluorene	Yes	30.80	21.36	18.39	21.25
9-C ₆ F ₅ -Octafluorofluorene	63264-80-2	CH	Fluorene	Yes	31.41	18.88	18.86	21.69
Octafluorofluorene	27053-34-5	CH	Fluorene	Yes	40.09	24.49	25.62	27.90
2,4,6-Br ₃ -Phenol	118-79-6	OH	Phenol	No	33.18	20.35	20.24	17.59
4-NC ₃ F ₄ -OH	2693-66-5	OH	Phenol	No	27.42	15.40	15.75	13.47
4-CF ₃ -2,3,5,6-F ₄ -Phenol	2787-79-3	OH	Phenol	No	28.39	16.62	16.51	14.16
4-C ₆ F ₅ -2,3,5,6-F ₄ -Phenol	2894-87-3	OH	Phenol	No	31.29	18.11	18.76	16.24
1-C ₁₀ F ₇ OH	5386-30-1	OH	Phenol	No	33.08	19.72	20.16	17.52
2,3,4,5,6-Br ₅ -Phenol	608-71-9	OH	Phenol	No	28.95	17.83	16.95	14.56
2-C ₁₀ F ₇ OH	727-49-1	OH	Phenol	No	31.68	18.50	19.07	16.52
2,3,5,6-F ₄ -Phenol	769-39-1	OH	Phenol	No	34.44	20.12	21.22	18.49
2,3,4,5,6-F ₅ -Phenol	771-61-9	OH	Phenol	No	33.84	20.11	20.75	18.06
2,3,4,5,6-Cl ₅ -Phenol	87-86-5	OH	Phenol	No	29.71	18.02	17.53	15.11
2,4,6-(SO ₂ F) ₃ -Phenol	882492-01-5	OH	Phenol	No	11.33	5.53	3.23	1.96
2-NO ₂ -Phenol	88-75-5	OH	Phenol	No	39.41	22.85	25.09	22.05
2,4-(NO ₂) ₂ -Phenol	51-28-5	OH	Phenol	No	29.54	16.66	17.41	14.99
Picric acid	88-89-1	OH	Phenol	No	20.30	11.00	10.21	8.37
2,4,6-Tf ₃ -Phenol	71571-37-4	OH	Phenol	No	13.50	4.80	4.92	3.51
(CF ₃) ₃ COH	2378-02-01	OH	Alcohol	No	32.71	20.55	19.88	17.26
Acetic acid	64-19-7	OH	Carboxylic acid	No	41.89	23.51	27.01	23.82
Benzoic acid	65-85-0	OH	Carboxylic acid	No	38.28	21.51	24.20	21.24
TosOH	104-15-4	OH	Sulfonic acid	No	21.71	8.45	11.31	9.38
4-NO ₂ -C ₆ H ₄ SO ₃ H	138-42-1	OH	Sulfonic acid	No	17.26	6.60	7.85	6.20

(continued)

Table 1. (Continued)

Compound ^b	CAS-RN	Type	Class	Delocalized ^c	ΔG_{diss}	$pK_{\text{a}}^{\text{Exp}}$	$pK_{\text{a}}^{\text{Calc}}$	$pK_{\text{a}}^{\text{Calc}}(\text{corr})$
1-C ₁₀ H ₇ SO ₃ H	85-47-2	OH	Sulfonic acid	No	20.23	7.89	10.16	8.33
3-NO ₂ -C ₆ H ₄ SO ₃ H	98-47-5	OH	Sulfonic acid	No	17.77	6.65	8.25	6.57
4-Cl-C ₆ H ₄ SO ₃ H	98-66-8	OH	Sulfonic acid	No	19.60	7.16	9.67	7.88
4-Me-C ₆ H ₄ C(=O)NHTf	343337-70-2	NH	Carbonylsulfonamide	No	23.78	11.46	12.92	10.87
C ₆ H ₅ C(=O)NHTf	39062-91-4	NH	Carbonylsulfonamide	No	23.62	11.06	12.80	10.75
4-NO ₂ -C ₆ H ₄ C(=O)NHTf	39062-98-1	NH	Carbonylsulfonamide	No	20.90	9.49	10.68	8.80
4-Cl-C ₆ H ₄ C(=O)NHTf	39062-99-2	NH	Carbonylsulfonamide	No	22.57	10.36	11.98	10.00
4-F-C ₆ H ₄ C(=O)NHTf	39063-00-8	NH	Carbonylsulfonamide	No	23.57	10.65	12.76	10.71
4-MeO-C ₆ H ₄ C(=O)NHTf	39063-05-3	NH	Carbonylsulfonamide	No	24.57	11.60	13.54	11.43
Saccharin	81-07-2	NH	Carbonylsulfonamide	No	29.83	14.57	17.63	15.19
4-NO ₂ -C ₆ H ₄ SO ₂ NHTos	100724-78-5	NH	Sulfonimide	No	24.20	10.04	13.25	11.16
C ₆ H ₅ SO ₂ NHTf	174788-87-5	NH	Sulfonimide	No	18.24	5.89	8.61	6.90
4-Cl-C ₆ H ₄ SO ₂ NHTf	174788-89-7	NH	Sulfonimide	No	17.93	5.34	8.37	6.68
4-NO ₂ -C ₆ H ₄ SO ₂ NHTf	174788-91-1	NH	Sulfonimide	No	16.49	4.39	7.25	5.65
4-Cl-C ₆ H ₄ SO(=NTf)NHTos	174788-93-3	NH	Sulfonimide	No	17.43	5.14	7.98	6.32
4-Cl-C ₆ H ₄ SO(=NTf)NHSO ₂ C ₆ H ₄ -4-Cl	174788-95-5	NH	Sulfonimide	No	16.69	4.34	7.40	5.79
4-Cl-C ₆ H ₄ SO(=NTf)NHSO ₂ C ₆ H ₄ -4-NO ₂	174788-97-7	NH	Sulfonimide	No	13.51	3.62	4.93	3.52
4-Cl-3-NO ₂ -C ₆ H ₃ SO ₂ NHTos	215395-06-5	NH	Sulfonimide	No	24.02	9.71	13.11	11.04
TosNHTf	215395-07-6	NH	Sulfonimide	No	18.94	6.17	9.16	7.40
(C ₆ H ₅ SO ₂) ₂ NH	2618-96-4	NH	Sulfonimide	No	26.40	11.34	14.96	12.74
(4-Cl-C ₆ H ₄ SO ₂) ₂ NH	2725-55-5	NH	Sulfonimide	No	24.80	10.20	13.72	11.60
Tos ₂ NH	3695-00-9	NH	Sulfonimide	No	27.22	11.97	15.60	13.32
(4-NO ₂ -C ₆ H ₄ SO ₂) ₂ NH	4009-06-7	NH	Sulfonimide	No	21.46	8.19	11.11	9.20
4-MeO-C ₆ H ₄ C(=NTf)NHTf	500721-87-9	NH	Sulfonimide	No	17.75	6.41	8.23	6.55
4-Me-C ₆ H ₄ C(=NTf)NHTf	500721-89-1	NH	Sulfonimide	No	18.79	6.19	9.04	7.30
C ₆ H ₅ C(=NTf)NHTf	500721-91-5	NH	Sulfonimide	No	18.25	6.04	8.62	6.91
4-F-C ₆ H ₄ C(=NTf)NHTf	500721-93-7	NH	Sulfonimide	No	18.14	5.66	8.54	6.83
4-Cl-C ₆ H ₄ C(=NTf)NHTf	500721-95-9	NH	Sulfonimide	No	17.24	5.56	7.84	6.19
4-NO ₂ -C ₆ H ₄ C(=NTf)NHTf	500721-97-1	NH	Sulfonimide	no	16.88	5.13	7.55	5.93
4-Cl-C ₆ H ₄ SO ₂ NHTos	69173-28-0	NH	Sulfonimide	No	25.77	11.10	14.47	12.29
4-NO ₂ -C ₆ H ₄ SO ₂ NHSO ₂ C ₆ H ₄ -4-Cl	95468-16-9	NH	Sulfonimide	No	23.02	9.17	12.33	10.32
(4-NC ₅ F ₄)(C ₆ H ₅)NH	39077-43-5	NH	Amine(sec)	No	42.88	26.34	27.79	24.53
(4-Me ₂ N-C ₆ F ₄)(C ₆ F ₅)NH	80588-34-7	NH	Amine(sec)	No	41.52	25.12	26.73	23.56
(4-Me-C ₆ F ₄)(C ₆ F ₅)NH	80588-36-9	NH	Amine(sec)	No	40.77	24.94	26.15	23.02
2,4,6-(SO ₂ F) ₃ -Aniline	133213-11-3	NH	Aniline	No	34.85	19.66	21.54	18.79

^a ΔG_{diss} : Gibbs free energies of dissociation calculated from eq. (3) in kcal mol⁻¹; $pK_{\text{a}}^{\text{Exp}}$: Experimental pK_{a} value in acetonitrile, taken from ref. 7; $pK_{\text{a}}^{\text{Calc}}$: pK_{a} value calculated by eq. (4); $pK_{\text{a}}^{\text{Calc}}(\text{corr})$: pK_{a} value calculated by eq. (7).

^bTf denotes CF₃-SO₂⁻; Tos denotes 4-Me-C₆H₄-SO₂⁻.

^cFormal notation, see text.

^dTautomeric equilibrium, see text.

Table 2. Test Data Set for COSMO-RS Acid pK_a Calculations in Acetonitrile.^a

Compound	Type	Class	Delocalized	ΔG_{diss}	pK _a ^{Exp}	Ref.	pK _a ^{Calc}	pK _a ^{Calc} _(corr)
Trinitromethane	CH	Aliphatic	Yes	15.59	7.3	7	6.55	10.37
1-(4-Nitrophenyl)-1-nitropropane	CH	Aliphatic	Yes	32.85	23.9	44	19.98	22.72
1-(4-Nitrophenyl)-2-methyl-1-nitropropane	CH	Aliphatic	Yes	36.34	25.9	44	22.70	25.22
1,2-Dicyanocyclopentadiene	CH	Cyclopentadiene	Yes	17.63	10.17	45	8.14	11.83
1,2,3-Tricyanocyclopentadiene	CH	Cyclopentadiene	Yes	7.22	1.44	45	0.04	4.38
1,2,4-Tricyano-3-methylcyclopentadiene	CH	Cyclopentadiene	Yes	6.30	3.4	45	-0.68	3.73
9-Cyanofluorene	CH	Fluorene	Yes	30.84	20.8	44	18.42	21.28
Pentakis(trifluoromethyl)-phenylmalonitrile	CH	Methane	Yes	10.79	8.86	29	2.82	6.94
2,3,4,6-Tetrakis(trifluoromethyl)-phenylmalonitrile	CH	Methane	Yes	12.98	10.45	29	4.52	8.50
Pentakis(trifluoromethyl)-toluene	CH	Methane	Yes	43.37	28.7	29	28.17	30.25
Pentacyanotoluene	CH	Methane	Yes	29.74	20.14	Present study	17.56	20.50
2,4,6-Trinitrotoluene	CH	Methane	Yes	32.15	23.2	44	19.44	22.22
4-Nitrophenylacetone	CH	Methane	Yes	33.35	25.4	44	20.37	23.07
4-Nitrophenylphenylacetone	CH	Methane	Yes	28.57	22.7	44	16.65	19.66
4-Bromophenyl-4-nitrophenylacetone	CH	Methane	Yes	27.52	21.3	44	15.83	18.91
4-Nitrophenyl-4-methoxyphenylacetone	CH	Methane	Yes	29.35	23.1	44	17.26	20.22
Bis(4-nitrophenyl)acetone	CH	Methane	Yes	21.70	19	44	11.31	14.74
Bis(4-nitrophenyl)ethylacetate	CH	Methane	Yes	31.40	25.1	44	18.85	21.68
4-Nitrophenylnitromethane	CH	Methane	Yes	29.51	20.7	44	17.38	20.33
Phthalic acid	OH	Carboxylic acid	Yes	24.86	14.3	7	13.77	17.01
2,2-Diphenic acid	OH	Carboxylic acid	Yes	27.08	15.7	7	15.49	18.59
3-Methylphthalic acid	OH	Carboxylic acid	Yes	27.93	17	7	16.15	19.20
Propanedioic acid	OH	Carboxylic acid	Yes	26.42	15.3	7	14.98	18.12
Succinic acid	OH	Carboxylic acid	Yes	29.70	17.6	7	17.53	20.47
Tetrahydroxysuccinic acid	OH	Carboxylic acid	Yes	24.26	13.7	7	13.30	16.58
Tartronic acid	OH	Carboxylic acid	Yes	24.19	13.8	7	13.24	16.52
2,6-Dihydroxybenzoic acid	OH	Carboxylic acid	Yes	23.00	12.6	7	12.32	15.67
Perchloric acid	OH	Perchloric acid	Yes	7.05	1.57	7	-0.10	4.26
Fluorosulfuric acid	OH	Sulfuric acid	Yes	3.73	3.38	7	-2.68	1.89
2,4,6-Trinitrothiophenol	SH	Thiophenol	Yes	15.67	11	7	6.61	10.43
<i>o</i> -Mercaptophenol	SH	Thiophenol	Yes	29.20	19.34	7	17.14	20.11
1,1,3,3-Tetranitrobutane	CH	Aliphatic	No	20.42	8	7	10.31	8.46
Pentakis(trifluoromethyl)-aniline	NH	Aniline	No	40.54	24.59	29	25.96	22.85
1,3,7,9-Tetranitrophenoxazine	NH	Phenoxazine	No	34.15	18.8	7	20.99	18.29
1,3,7-Trinitrophenoxazine	NH	Phenoxazine	No	33.52	20.3	7	20.50	17.84
1,3,9-Trinitrophenoxazine	NH	Phenoxazine	No	39.23	21.9	7	24.95	21.92
1,3-Dinitrophenoxazine	NH	Phenoxazine	No	37.92	22.4	7	23.93	20.98
1,7-Dimethyl-3-nitrophenoxazine	NH	Phenoxazine	No	39.79	25.9	7	25.38	22.32
1-Methyl-3-nitrophenoxazine	NH	Phenoxazine	No	39.45	25.8	7	25.12	22.08
1-Nitrophenoxazine	NH	Phenoxazine	No	46.83	28.4	7	30.86	27.36
3,7-Dinitrophenoxazine	NH	Phenoxazine	No	35.46	22.8	7	22.01	19.22
3-Nitrophenoxazine	NH	Phenoxazine	No	40.29	25.7	7	25.77	22.68
3,4-Dichlorobenzenesulfonamide	NH	Sulfonamide	No	44.35	23.29	7	28.93	25.58
4-Methylbenzenesulfonamide	NH	Sulfonamide	No	48.12	24.82	7	31.86	28.28
Benzenesulfonamide	NH	Sulfonamide	No	47.29	24.61	7	31.21	27.68
<i>m</i> -Chlorobenzenesulfonamide	NH	Sulfonamide	No	45.49	23.8	7	29.82	26.40
<i>m</i> -Cyanobenzenesulfonamide	NH	Sulfonamide	No	44.42	23.23	7	28.98	25.63
<i>m</i> -Methoxybenzenesulfonamide	NH	Sulfonamide	No	47.35	24.48	7	31.26	27.73
<i>m</i> -Nitrobenzenesulfonamide	NH	Sulfonamide	No	43.97	22.95	7	28.63	25.31
<i>m</i> -Toluenesulfonamide	NH	Sulfonamide	No	47.59	24.67	7	31.45	27.90
<i>m</i> -Trifluoromethylbenzenesulfonamide	NH	Sulfonamide	No	44.97	23.53	7	29.41	26.02
<i>o</i> -Xylene-4-sulfonamide	NH	Sulfonamide	No	47.46	25.01	7	31.35	27.81
<i>p</i> -Bromobenzenesulfonamide	NH	Sulfonamide	No	45.99	24.04	7	30.21	26.76
<i>p</i> -Fluorobenzenesulfonamide	NH	Sulfonamide	No	47.11	24.19	7	31.08	27.56
<i>p</i> -Methoxybenzenesulfonamide	NH	Sulfonamide	No	48.42	25.09	7	32.10	28.49
<i>p</i> -Nitrobenzenesulfonamide	NH	Sulfonamide	No	43.47	22.91	7	28.25	24.95
4-Bromobenzoic acid	OH	Carboxylic acid	No	37.07	20.3	7	23.27	20.37
4-Hydroxybenzoic acid	OH	Carboxylic acid	No	40.29	20.8	7	25.77	22.68

(continued)

Table 2. (Continued)

Compound	Type	Class	Delocalized	ΔG_{diss}	$\text{p}K_{\text{a}}^{\text{Exp}}$	Ref.	$\text{p}K_{\text{a}}^{\text{Calc}}$	$\text{p}K_{\text{a}}^{\text{Calc}}(\text{corr})$
Chloroaceticacid	OH	Carboxylic acid	No	34.01	18.8	7	20.88	18.18
Cyanoaceticacid	OH	Carboxylic acid	No	32.99	18	7	20.09	17.45
Dichloroaceticacid	OH	Carboxylic acid	No	28.78	13.2	7	16.82	14.44
Fumaricacid	OH	Carboxylic acid	No	35.85	19.2	7	22.31	19.50
Oxalicacid	OH	Carboxylic acid	No	29.18	14.5	7	17.12	14.73
Salicylicacid	OH	Carboxylic acid	No	31.13	16.7	7	18.64	16.13
Trichloroaceticacid	OH	Carboxylic acid	No	23.86	10.75	7	12.99	10.93
Trifluoroaceticacid	OH	Carboxylic acid	No	25.37	12.65	7	14.16	12.00
1,3-Benzenedicarboxylicacid	OH	Carboxylic acid	No	36.59	19.3	7	22.89	20.03
1,4-Benzenedicarboxylicacid	OH	Carboxylic acid	No	36.29	19.7	7	22.66	19.81
1,8-Naphthalicacid	OH	Carboxylic acid	No	37.36	21.8	7	23.49	20.58
2,3-Dibromopropionicacid	OH	Carboxylic acid	No	33.09	17.1	7	20.17	17.53
2,4,6-Trimethylbenzoicacid	OH	Carboxylic acid	No	37.85	20.5	7	23.87	20.93
2,4-Dichlorobenzoicacid	OH	Carboxylic acid	No	34.54	18.4	7	21.30	18.56
2,4-Dinitrobenzoicacid	OH	Carboxylic acid	No	28.30	16.1	7	16.44	14.10
2,5-Dichlorobenzenesulfonicacid	OH	Carboxylic acid	No	16.80	6.2	7	7.49	5.87
2,6-Dichlorobenzoicacid	OH	Carboxylic acid	No	31.88	17.6	7	19.23	16.66
2,6-Dinitrobenzoicacid	OH	Carboxylic acid	No	27.69	15.8	7	15.96	13.66
2-Chloro-benzoicacid	OH	Carboxylic acid	No	34.97	19	7	21.63	18.87
3,4-Dichlorobenzoicacid	OH	Carboxylic acid	No	35.42	19	7	21.98	19.19
3,4-Dimethylbenzoicacid	OH	Carboxylic acid	No	39.69	19	7	25.30	22.25
3,5-Dichlorobenzoicacid	OH	Carboxylic acid	No	34.24	18.7	7	21.07	18.35
3,5-Dinitrobenzoicacid	OH	Carboxylic acid	No	31.33	17	7	18.79	16.26
3-Bromobenzoicacid	OH	Carboxylic acid	No	36.14	19.5	7	22.54	19.71
3-Nitrobenzoicacid	OH	Carboxylic acid	No	34.62	19.2	7	21.36	18.62
4-Chloro-3-nitrobenzoicacid	OH	Carboxylic acid	No	32.68	18.5	7	19.85	17.24
4-Dimethylaminobenzoicacid	OH	Carboxylic acid	No	42.81	23	7	27.73	24.48
4-Nitrobenzoicacid	OH	Carboxylic acid	No	34.49	18.7	7	21.26	18.53
Butyricacid	OH	Carboxylic acid	No	42.30	22.7	7	27.34	24.12
Hexanedioicacid	OH	Carboxylic acid	No	42.01	20.3	7	27.11	23.91
Hydracrylicacid	OH	Carboxylic acid	No	36.41	21	7	22.75	19.90
Hydroxy-aceticacid	OH	Carboxylic acid	No	34.24	19.3	7	21.06	18.35
Nonanedioicacid	OH	Carboxylic acid	No	42.38	20.9	7	27.40	24.17
<i>o</i> -Nitrobenzoicacid	OH	Carboxylic acid	No	32.97	18.2	7	20.08	17.44
Pentanedioicacid	OH	Carboxylic acid	No	41.64	19.2	7	26.82	23.64
Tartaricacid	OH	Carboxylic acid	No	30.44	15.1	7	18.11	15.63
Nitricacid	OH	Nitric acid	No	23.02	8.8	7	12.33	10.32
2-Bromophenol	OH	Phenol	No	41.33	23.92	7	26.58	23.42
3,4,5-Trichlorophenol	OH	Phenol	No	38.37	22.5	7	24.28	21.31
3,4-Dichlorophenol	OH	Phenol	No	41.46	24	7	26.68	23.51
3,5-Dichlorophenol	OH	Phenol	No	39.53	23.3	7	25.18	22.13
3-Chlorophenol	OH	Phenol	No	43.27	25	7	28.09	24.81
4-Bromophenol	OH	Phenol	No	44.63	25.53	7	29.15	25.79
4-Chlorophenol	OH	Phenol	No	45.04	25.44	7	29.47	26.07
4-Nitrophenol	OH	Phenol	No	33.95	20.7	7	20.83	18.14
<i>p</i> -Cresole	OH	Phenol	No	48.85	27.45	7	32.43	28.80
Phenol	OH	Phenol	No	47.49	29.14	29	31.37	27.83
2-Methylphenol	OH	Phenol	No	47.88	27.5	7	31.67	28.11
3,4-Dinitrophenol	OH	Phenol	No	28.51	17.9	7	16.60	14.25
3-Chloro-4-nitrophenol	OH	Phenol	No	31.87	19.9	7	19.22	16.65
3-Nitrophenol	OH	phenol	No	40.75	23.8	7	26.13	23.01
3-Trifluoromethyl-4-nitrophenol	OH	Phenol	No	31.31	19.3	7	18.78	16.26
4-Chloro-2,6-dinitrophenol	OH	Phenol	No	27.75	15.3	7	16.01	13.71
4-Cyanophenol	OH	Phenol	No	38.50	22.7	7	24.38	21.39
<i>m</i> -Trifluoromethylphenol	OH	Phenol	No	43.31	24.9	7	28.12	24.84
4-(1,1-Dimethylethyl)-phenol	OH	Phenol	No	48.90	27.48	7	32.47	28.84
3,5-Dinitrophenol	OH	Phenol	No	34.55	20.5	46	21.31	18.57
2,3,5,6-Tetrafluoro-4-methylphenol	OH	Phenol	No	36.08	20.3	47	22.49	19.66

(continued)

Table 2. (Continued)

Compound	Type	Class	Delocalized	ΔG_{diss}	$\text{p}K_{\text{a}}^{\text{Exp}}$	Ref.	$\text{p}K_{\text{a}}^{\text{Calc}}$	$\text{p}K_{\text{a}}^{\text{Calc}}(\text{corr})$
2,4,6-Trichlorophenol	OH	Phenol	No	40.29	22.5	46	25.77	22.68
2-Trifluoromethylphenol	OH	Phenol	No	40.55	24.88	29	25.97	22.86
3-Trifluoromethylphenol	OH	Phenol	No	43.37	26.5	29	28.17	24.88
4-Trifluoromethylphenol	OH	Phenol	No	41.69	25.54	29	26.86	23.68
3,5-Bis(trifluoromethyl)-phenol	OH	Phenol	No	38.83	23.78	29	24.63	21.63
2,6-Bis(1,1-dimethylethyl)-4-nitrophenol	OH	Phenol	No	29.44	19	46	17.33	14.92
Pentakis(trifluoromethyl)-phenol	OH	Phenol	No	17.00	10.46	29	7.65	6.02
4-Methylbenzenesulfonic acid	OH	Sulfonic acid	No	21.40	8.01	7	11.07	9.16
Methanesulfonic acid	OH	Sulfonic acid	No	23.19	9.97	7	12.47	10.45
Trifluoromethanesulfonic acid	OH	Sulfonic acid	No	9.13	2.6	7	1.52	0.38
H ₂ SO ₄	OH	Sulfuric acid	No	15.81	7.2	7	6.72	5.16
HBr	BrH	Atom	No	10.01	5.5	7	2.20	0.14
HCl	ClH	Atom	No	19.24	8.9	7	9.39	7.50

^a ΔG_{diss} : Gibbs free energies of dissociation calculated from eq. (3) in kcal mol⁻¹; $\text{p}K_{\text{a}}^{\text{Exp}}$: Experimental $\text{p}K_{\text{a}}$ value in acetonitrile; Ref.: Experimental $\text{p}K_{\text{a}}$ value data source reference; $\text{p}K_{\text{a}}^{\text{Calc}}$: $\text{p}K_{\text{a}}$ value calculated by eq. (4); $\text{p}K_{\text{a}}^{\text{Calc}}(\text{corr})$: $\text{p}K_{\text{a}}$ value calculated by eq. (7).