

Table 1. Experimental basicities in MeCN, H₂O, gas phase, and calculated GB values. Bases measured in this work are given in bold. The rest are reference bases.

Base	ΔpK_a	$pK_a(\text{MeCN})^a$	$pK_a(\text{H}_2\text{O})$	GB(exp) ^b	GB(calc) ^c
1 2-Cl-C ₆ H ₄ P ₁ (pyrr)		20.17			
2 Quino[7,8-h]quinoline	0.58	19.61	12.0 ^c	-	244.1
3 2,5-Cl ₂ -C ₆ H ₃ P ₁ (pyrr)	1.10	18.52			
4 4-NO ₂ -C ₆ H ₄ P ₁ (pyrr)	1.10	18.51			
5 2,3-(NH ₂) ₂ -Pyridine		15.24			
6 Imidazole		15.05	6.95 ^d	217.3	218.1
7 2,4-(NO ₂) ₂ -C ₆ H ₃ P ₁ (pyrr)	0.19	14.88			
8 2,6-(NH ₂) ₂ -Pyridine	0.25	14.77			
9 2,6-Cl ₂ -4-NO ₂ -C ₆ H ₂ P ₁ (pyrr)	0.62	14.43			
10 2,6-(CH ₃) ₂ -Pyridine	1.60	14.13			
11 2,6-NO ₂ -C ₆ H ₃ P ₁ (pyrr)	0.45	14.12			
12 Phenanthroline	0.63	13.68	5.12 ^p	>217	230.9
13 Benzimidazole	-0.41	13.52	5.56 ^q	220.0	219.8
14 2-CH ₃ -Pyridine		13.32			
15 Isoquinoline	0.57	12.69	5.46 ^f	219.9	220.4
16 Acridine	1.02	12.67	5.62 ^f	224.8	225.8
17 Pyridine	0.59	12.53	5.23 ^f	214.7	214.7
18 Thiabendazole	-0.18	12.42	4.64 ^g	-	223.8
19 2,2'-Bipyridine	0.25	12.26	4.54 ^h	223.1	225.0
20 Carbazim	0.69	12.24	4.53 ⁱ	-	221.9
21 Quinoline	0.79	11.96	4.93 ^f	220.2	219.8
22 5,6-Benzoquinoline	1.10	11.96	5.15 ^h	-	222.6
23 4-CH ₃ O-Aniline	0.56	11.86			
24 2-CH ₃ -Quinoline-8-amine	0.36	11.54			
25 Phthalazine	0.44	11.55	3.47 ^f	-	219.5
26 N,N-Me ₂ -Aniline	0.12	11.43			
27 2,2'-Biquinoline	0.74	11.28	3.66 ⁿ	-	230.0
28 7,8-Benzoquinoline	1.00	10.84	4.25 ^h	-	221.3
29 Aniline	-0.65	10.62			
30 Cinnoline	0.79	10.5 ^e	2.29 ^f	216.2	217.4
31 2-CH ₃ -Aniline	0.37	10.50			
32 Pyridazine	0.41	10.07	2.33 ^f	209.6	210.5
33 2-CH ₃ O-Pyridine	0.13	9.93			
34 1-Naphthylamine		9.77			
35 3-Cl-Pyridine	-0.73	9.55			
36 4-Br-Aniline	0.59	9.43			
37 Quinazoline	0.37	9.19	1.95 ^j	-	212.3
38 Pyrazole	0.85	9.1	2.48 ^g	205.7	206.0
39 Pyrimidine	0.72	8.72	1.3 ^f	204.5	204.6
40 2,4-F ₂ -Aniline	-0.77	8.39			
41 4-CF ₃ -Aniline	1.21	8.03			
42 1,2,3-Triazole	-0.66	7.9	1.17 ^q	202.5	202.4
43 2-Cl-Aniline	0.30	7.86			
44 Pyrazine	0.11	7.74	0.6 ^f	202.4	202.0
45 4-F-3-NO ₂ -Aniline	0.86	7.67			
46 2,6-(CH ₃ O) ₂ -Pyridine	0.42	7.64			
47 Indazole	0.37	7.61	1.25 ^j	207.7	208.3
48 Caffeine	0.05	7.51	0.60 ^k	-	210.0
49 Quinoxaline	0.23	7.40	0.56 ^f	208.8	208.9
50 Benzotriazole	1.48	6.88	0.42 ^l	-	210.2
51 2-Cl-Pyridine	0.77	6.79			
52 N,N-Ph ₂ -N-CH ₃ -Amine	-0.58	6.52			
53 4-NO₂-Imidazole	0.53	6.34	-0.16 ^m	-	201.6
54 4-NO ₂ -Aniline	0.06	6.22			
55 2,5-Cl ₂ -Aniline	0.86	6.21			
56 2-NO₂-Imidazole	-0.68	5.54	-0.81 ^d	-	200.4
57 2,6-Cl ₂ -Aniline	0.48	5.06			
58 5-NO₂-Indazole	0.22	4.91	-0.96 ^e	-	197.8
59 6-NO₂-Indazole	-0.13	4.88	-0.97 ^e	-	197.7
60 2-NO ₂ -Aniline	1.16	4.80			
61 4-Cl-2-NO ₂ -Aniline	0.06	3.80			
62 2-Cl-4-NO ₂ -Aniline	1.11	3.66			
63 Uracil	0.24	3.38	-0.5 ^o	201.2	200.2
64 Thymine	0.67	2.70	-0 ^o	203.2	203.1
65 2,3,4,5,6-Cl ₅ -Aniline	0.36	2.35			

^a pK_a values measured in this work are bold and the rest are reference bases.^[17,27] ^b Reference [22]. ^c GB or pK_a values calculated in this work. ^d Reference [4]. ^e Reference [5]. ^f Reference [6]. ^g Reference [7]. ^h Reference [8]. ⁱ Reference [16]. ^j Reference [9]. ^k Reference [10]. ^l Reference [11]. ^m Reference [12]. ⁿ Reference [13]. ^o Reference [28]. ^p Reference [14]. ^q Reference [15].