TABLE 11 Dissociation Constant Values of the Studied Amines at Various Temperatures (K) for DFT1 (DFT/B3LYP/6-31G(d)), DFT2 (DFT/B3LYP/6-311G++(d,p)), and MP2 (MP2/6-31G(d)) Calculations by Hydronium Thermodynamic Cycle

Amine	Temperature /K																	
	293.15			298.15			303.15			308.15			313.15			323.15		
	DFT1	DFT2	MP2	DFT1	DFT2	MP2	DFT1	DFT2	MP2	DFT1	DFT2	MP2	DFT1	DFT2	MP2	DFT1	DFT2	MP2
3-(Diethylamino) propylamine^{V1}	7.34	7.43	7.87	7.24	7.32	7.77	7.14	7.23	7.66	7.05	7.13	7.56	6.96	7.04	7.47	6.79	6.87	7.28
3-(Diethylamino) propylamine^{V2}	9.16	10.61	9.53	9.03	10.45	9.40	8.91	10.31	9.27	8.79	10.16	9.15	8.68	10.02	9.03	8.46	9.76	8.80
1,3-Diaminopentane^{V1}	8.41	7.85	8.44	8.29	7.75	8.32	8.17	7.64	8.21	8.06	7.54	8.10	7.96	7.44	7.99	7.76	7.25	7.79
1,3-Diaminopentane^{V2}	5.34	6.94	6.62	5.30	6.94	6.63	5.26	6.77	6.46	5.23	6.69	6.38	5.19	6.61	6.30	5.12	6.45	6.16
3-Butoxypropylamine	8.32	8.71	7.50	8.18	8.57	7.40	8.04	8.44	7.31	7.91	8.31	7.21	7.79	8.18	7.12	7.55	7.94	6.95
2-(Methylamino) ethanol	6.90	7.54	7.33	6.81	7.43	7.24	6.72	7.33	7.14	6.63	7.24	7.05	6.55	7.15	6.96	6.40	6.97	6.79
Bis(2-methoxyethyl) amine	4.79	5.40	4.98	4.74	5.34	4.93	4.69	5.28	4.88	4.65	5.22	4.83	4.60	5.17	4.78	4.51	5.06	4.69
α-Methylbenzylamine	5.56	5.84	5.97	5.49	5.77	5.90	5.43	5.70	5.84	5.37	5.63	5.77	5.31	5.57	5.71	5.20	5.44	5.58
2-Aminoheptane	7.60	8.04	7.58	7.50	7.93	7.48	7.41	7.83	7.38	7.32	7.73	7.29	7.23	7.64	7.20	7.06	7.45	7.02
3-Amino-1-phenylbutane	6.58	7.07	6.72	6.49	6.98	6.63	6.41	6.88	6.55	6.33	6.80	6.47	6.26	6.71	6.39	6.11	6.55	6.24