TABLE 12 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 Protonated 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}	10.45	7.13	10.09	10.19	6.93	9.85	9.95	6.74	9.61	9.71	6.56	9.38	9.48	6.38	9.16	9.04	6.03	8.73
3-(Diethylamino) propylamine^{V2}	12.27	10.31	11.75	11.99	10.06	11.48	11.72	9.82	11.22	11.45	9.59	10.96	11.20	9.36	10.72	10.71	8.93	10.24
1,3-Diaminopentane^{V1}	11.51	7.56	10.66	11.24	7.35	10.40	10.98	7.16	10.15	10.73	6.96	9.91	10.48	6.78	9.68	10.01	6.42	9.24
1,3-Diaminopentane^{V2}	8.45	6.64	8.84	8.26	6.46	8.62	8.07	6.28	8.41	7.89	6.11	8.20	7.71	5.94	7.99	7.37	5.62	7.61
3-Butoxypropylamine	11.42	8.42	9.72	11.13	8.18	9.48	10.85	7.95	9.25	10.58	7.73	9.03	10.31	7.52	8.81	9.81	7.11	8.40
2-(methylamino) ethanol	10.00	7.24	9.55	9.76	7.04	9.32	9.52	6.85	9.09	9.29	6.66	8.87	9.07	6.48	8.65	8.65	6.14	8.24
Bis(2-methoxyethyl) amine	7.90	5.11	7.20	7.70	4.95	7.01	7.50	4.80	6.82	7.31	4.65	6.64	7.12	4.51	6.47	6.77	4.23	6.14
α-Methylbenzylamine	8.67	5.54	8.19	8.45	5.38	7.98	8.24	5.21	7.78	8.03	5.06	7.58	7.83	4.90	7.39	7.46	4.61	7.03
2-Aminoheptane	10.71	7.75	9.80	10.46	7.54	9.56	10.22	7.35	9.33	9.98	7.16	9.10	9.75	6.97	8.89	9.32	6.62	8.47
3-Amino-1-phenylbutane	9.69	6.77	8.94	9.45	6.58	8.71	9.22	6.40	8.49	9.00	6.22	8.28	8.78	6.05	8.08	8.37	5.72	7.68