TABLE 10 Comparison Between the Estimated pK_a Values by Different Methods with Experimental Dissociation Constants

Amine	SHE Method		Theoretical Method			Cosmo-RS Method	Experimental Values
	pK_a without correction	pK_a with correction	DFT/B3LYP 6-31G(d)	DFT/B3LYP 6-311G++(d,p)	MP2 6-31G(d)		
3-(Diethylamino) propylamine[V1]	8.81	8.11	6.95	3.69	6.60	10.36	10.44
3-(Diethylamino) propylamine[V2]	10.27	9.57	8.74	6.81	8.23	9.89	
1,3-Diaminopentane[V1]	9.47	8.77	5.01	3.21	5.38	10.65	10.38
1,3-Diaminopentane[V2]	8.42	7.72	7.99	4.11	7.16	9.39	
3-Butoxypropylamine	8.18	7.48	7.88	4.94	6.24	10.02	9.90
2-(methylamino) ethanol	8.32	7.62	6.51	3.80	6.07	9.50	9.84
Bis(2-methoxyethyl) amine	6.65	5.95	4.45	1.70	3.76	7.07	8.62
α-Methylbenzylamine	7.69	6.49	5.20	2.13	4.74	9.29	9.37
2-Aminoheptane	8.78	8.08	7.21	4.30	6.31	10.43	10.53
3-Amino-1-phenylbutane	8.30	7.10	6.20	3.34	5.47	9.83	10.19