

TABLE 9 The Estimated pK_a Values of the Eight Amines with Three Different Methods at T = 298.15 K

Solvent	$pK_{a,PDS}^{19}$	$pK_{a,Sumon}^{20}$	$pK_{a,QSSR}^{21}$	$pK_a^{Exp.}$
3-(Diethylamino) propylamine ^{V1}	10.63	10.44	10.24	10.44
3-(Diethylamino) propylamine ^{V2}	10.37	10.46	10.28	
1,3-Diaminopentane ^{V1}	10.64	10.46	10.28	10.38
1,3-Diaminopentane ^{V2}	10.64	10.46	10.28	
3-Butoxypropylamine	10.58	10.38	10.13	9.90
2-(Methylamino) ethanol	10.51	10.50	10.20	9.84
Bis(2-methoxyethyl) Amine	10.19	9.98	9.24	8.62
α -Methylbenzylamine	10.77	10.60	10.60	9.37
2-Aminoheptane	10.77	10.60	10.60	10.53
3-Amino-1-phenylbutane	10.77	10.60	10.60	10.19