DISSOCIATION CONSTANTS OF ORGANIC ACIDS AND BASES

This table lists the dissociation (ionization) constants of over 1070 organic acids, bases, and amphoteric compounds. All data apply to dilute aqueous solutions and are presented as values of pK_a, which is defined as the negative of the logarithm of the equilibrium constant K_a for the reaction

$$HA \rightleftharpoons H^+ + A^-$$

i.e.,

$$K_a = [H^+][A^-]/[HA]$$

where $[H^+]$, etc. represent the concentrations of the respective species in mol/L. It follows that $pK_a = pH + \log[HA] - \log[A^-]$, so that a solution with 50% dissociation has pH equal to the pK_a of the acid.

Data for bases are presented as pK_a values for the conjugate acid, i.e., for the reaction

$$BH^+ \rightleftharpoons H^+ + B$$

In older literature, an ionization constant K_b was used for the reaction $B + H_2O \rightleftharpoons BH^+ + OH^-$. This is related to K_a by

$$pK_a + pK_b = pK_{water} = 14.00 \quad (\text{at } 25°C)$$

Compounds are listed by molecular formula in Hill order.

References

1. Perrin, D. D., *Dissociation Constants of Organic Bases in Aqueous Solution*, Butterworths, London, 1965; Supplement, 1972.
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5. Perrin, D. D., Dempsey, B., and Serjeant, E. P., pK_a *Prediction for Organic Acids and Bases*, Chapman and Hall, London, 1981.
6. Albert, A., and Serjeant, E. P., *The Determination of Ionization Constants, Third Edition*, Chapman and Hall, London, 1984.
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Mol. form.	Name	Step	t/°C	pK_a
CHNO	Cyanic acid		25	3.7
CH_2N_2	Cyanamide		29	1.1
CH_2O	Formaldehyde		25	13.27
CH_2O_2	Formic acid		25	3.75
CH_3NO_2	Nitromethane		25	10.21
CH_3NS_2	Carbamodithioic acid		25	2.95
CH_4N_2O	Urea		25	0.10
CH_4N_2S	Thiourea		25	-1
CH_4O	Methanol		25	15.5
CH_4S	Methanethiol		25	10.33
CH_5N	Methylamine		25	10.66
CH_5NO	*O*-Methylhydroxylamine			12.5
CH_5N_3	Guanidine		25	13.6
C_2HCl_3O	Trichloroacetaldehyde		25	10.04
$C_2HCl_3O_2$	Trichloroacetic acid		20	0.66
$C_2HF_3O_2$	Trifluoroacetic acid		25	0.52
$C_2H_2Cl_2O_2$	Dichloroacetic acid		25	1.35
$C_2H_2O_3$	Glyoxylic acid		25	3.18
$C_2H_2O_4$	Oxalic acid	1	25	1.25
		2	25	3.81
$C_2H_3BrO_2$	Bromoacetic acid		25	2.90
$C_2H_3ClO_2$	Chloroacetic acid		25	2.87
$C_2H_3Cl_3O$	2,2,2-Trichloroethanol		25	12.24
$C_2H_3FO_2$	Fluoroacetic acid		25	2.59
$C_2H_3F_3O$	2,2,2-Trifluoroethanol		25	12.37
$C_2H_3IO_2$	Iodoacetic acid		25	3.18
$C_2H_3NO_4$	Nitroacetic acid		24	1.48
$C_2H_3N_3$	1H-1,2,3-Triazole		20	1.17
$C_2H_3N_3$	1H-1,2,4-Triazole		20	2.27
$C_2H_4N_2$	Aminoacetonitrile		25	5.34
C_2H_4O	Acetaldehyde		25	13.57
C_2H_4OS	Thioacetic acid		25	3.33
$C_2H_4O_2$	Acetic acid		25	4.756
$C_2H_4O_2S$	Thioglycolic acid		25	3.68
$C_2H_4O_3$	Glycolic acid		25	3.83
C_2H_5N	Ethyleneimine		25	8.04
C_2H_5NO	Acetamide		25	15.1
$C_2H_5NO_2$	Acetohydroxamic acid			8.70
$C_2H_5NO_2$	Nitroethane		25	8.46
$C_2H_5NO_2$	Glycine	1	25	2.35
		2	25	9.78
$C_2H_6N_2$	Ethanimidamide		25	12.1
C_2H_6O	Ethanol		25	15.5
C_2H_6OS	2-Mercaptoethanol		25	9.72
$C_2H_6O_2$	Ethyleneglycol		25	15.1
$C_2H_7AsO_2$	Dimethylarsinic acid	1	25	1.57
		2	25	6.27
C_2H_7N	Ethylamine		25	10.65
C_2H_7N	Dimethylamine		25	10.73
C_2H_7NO	Ethanolamine		25	9.50
$C_2H_7NO_3S$	2-Aminoethanesulfonic acid	1	25	1.5
		2	25	9.06
C_2H_7NS	Cysteamine	1	25	8.27
		2	25	10.53
$C_2H_7N_5$	Biguanide	1		11.52
		2		2.93
$C_2H_8N_2$	1,2-Ethanediamine	1	25	9.92
		2	25	6.86
$C_2H_8O_7P_2$	1-Hydroxy-1,1-diphosphonoethane	1		1.35
		2		2.87
		3		7.03
		4		11.3
$C_3H_2O_2$	2-Propynoic acid		25	1.84
C_3H_3NO	Oxazole		33	0.8
C_3H_3NO	Isoxazole		25	-2.0
$C_3H_3NO_2$	Cyanoacetic acid		25	2.47
C_3H_3NS	Thiazole		25	2.52
$C_3H_3N_3O_3$	Cyanuric acid	1		6.88
		2		11.40
		3		13.5
$C_3H_4N_2$	1*H*-Pyrazole		25	2.49
$C_3H_4N_2$	Imidazole		25	6.99

Mol. form.	Name	Step	t/°C	pK_a
$C_3H_4N_2S$	2-Thiazolamine		20	5.36
C_3H_4O	Propargyl alcohol		25	13.6
$C_3H_4O_2$	Acrylic acid		25	4.25
$C_3H_4O_3$	Pyruvic acid		25	2.39
$C_3H_4O_4$	Malonic acid	1	25	2.85
		2	25	5.70
$C_3H_4O_5$	Hydroxypropanedioic acid	1		2.42
		2		4.54
$C_3H_5BrO_2$	3-Bromopropanoic acid		25	4.00
$C_3H_5ClO_2$	2-Chloropropanoic acid		25	2.83
$C_3H_5ClO_2$	3-Chloropropanoic acid		25	3.98
$C_3H_6N_2$	3-Aminopropanenitrile		20	7.80
$C_3H_6N_6$	1,3,5-Triazine-2,4,6-triamine		25	5.00
C_3H_6O	Allyl alcohol		25	15.5
$C_3H_6O_2$	Propanoic acid		25	4.87
$C_3H_6O_2S$	(Methylthio)acetic acid		25	3.66
$C_3H_6O_3$	Lactic acid		25	3.86
$C_3H_6O_3$	3-Hydroxypropanoic acid		25	4.51
$C_3H_6O_4$	Glyceric acid		25	3.52
C_3H_7N	Allylamine		25	9.49
C_3H_7N	Azetidine		25	11.29
C_3H_7NO	2-Propanone oxime		25	12.42
$C_3H_7NO_2$	*L*-Alanine	1	25	2.34
		2	25	9.87
$C_3H_7NO_2$	β-Alanine	1	25	3.55
		2	25	10.24
$C_3H_7NO_2$	Sarcosine	1	25	2.21
		2	25	10.1
$C_3H_7NO_2S$	*L*-Cysteine	1	25	1.5
		2	25	8.7
		3	25	10.2
$C_3H_7NO_3$	*L*-Serine	1	25	2.19
		2	25	9.21
$C_3H_7NO_5S$	*DL*-Cysteic acid	1	25	1.3
		2	25	1.9
		3	25	8.70
$C_3H_7N_3O_2$	Glycocyamine		25	2.82
$C_3H_8O_2$	Ethylene glycol monomethyl ether		25	14.8
$C_3H_8O_3$	Glycerol		25	14.15
C_3H_9N	Propylamine		25	10.54
C_3H_9N	Isopropylamine		25	10.63
C_3H_9N	Trimethylamine		25	9.80
C_3H_9NO	2-Methoxyethylamine		25	9.40
C_3H_9NO	Trimethylamine oxide		20	4.65
$C_3H_{10}N_2$	1,2-Propanediamine, (±)	1	25	9.82
		2	25	6.61
$C_3H_{10}N_2$	1,3-Propanediamine	1	25	10.55
		2	25	8.88
$C_3H_{10}N_2O$	1,3-Diamino-2-propanol	1	20	9.69
		2	20	7.93
$C_3H_{11}N_3$	1,2,3-Triaminopropane	1	20	9.59
		2	20	7.95
$C_4H_4FN_3O$	Flucytosine			3.26
$C_4H_4N_2$	Pyrazine		20	0.65
$C_4H_4N_2$	Pyrimidine		20	1.23
$C_4H_4N_2$	Pyridazine		20	2.24
$C_4H_4N_2O_2$	Uracil		25	9.45
$C_4H_4N_2O_3$	Barbituric acid		25	4.01
$C_4H_4N_2O_5$	Alloxanic acid		25	6.64
$C_4H_4N_4O_2$	5-Nitropyrimidinamine		20	0.35
$C_4H_4O_2$	2-Butynoic acid		25	2.62
$C_4H_4O_4$	Maleic acid	1	25	1.92
		2	25	6.23
$C_4H_4O_4$	Fumaric acid	1	25	3.02
		2	25	4.38
$C_4H_4O_5$	Oxaloacetic acid	1	25	2.55
		2	25	4.37
		3	25	13.03
C_4H_5N	Pyrrole		25	-3.8
$C_4H_5NO_2$	Succinimide		25	9.62
$C_4H_5N_3$	2-Pyrimidinamine		20	3.45
$C_4H_5N_3$	4-Pyrimidinamine		20	5.71
$C_4H_5N_3O$	Cytosine	1		4.60
		2		12.16
$C_4H_5N_3O_2$	6-Methyl-1,2,4-triazine-3,5(2H,4H)-dione			7.6
$C_4H_6N_2$	1-Methylimidazol		25	6.95
$C_4H_6N_4O_3$	Allantoin		25	8.96
$C_4H_6N_4O_3S_2$	Acetazolamide			7.2
$C_4H_6O_2$	*trans*-Crotonic acid		25	4.69
$C_4H_6O_2$	3-Butenoic acid		25	4.34
$C_4H_6O_2$	Cyclopropanecarboxylic acid		25	4.83
$C_4H_6O_3$	2-Oxobutanoic acid		25	2.50
$C_4H_6O_3$	Acetoacetic acid		25	3.6
$C_4H_6O_4$	Succinic acid	1	25	4.21
		2	25	5.64
$C_4H_6O_4$	Methylmalonic acid	1	25	3.07
		2	25	5.76
$C_4H_6O_5$	Malic acid	1	25	3.40
		2	25	5.11
$C_4H_6O_6$	*DL*-Tartaric acid	1	25	3.03
		2	25	4.37
$C_4H_6O_6$	*meso*-Tartaric acid	1	25	3.17
		2	25	4.91
$C_4H_6O_6$	*L*-Tartaric acid	1	25	2.98
		2	25	4.34
$C_4H_6O_8$	Dihydroxytartaric acid		25	1.92
$C_4H_7ClO_2$	2-Chlorobutanoic acid			2.86
$C_4H_7ClO_2$	3-Chlorobutanoic acid			4.05
$C_4H_7ClO_2$	4-Chlorobutanoic acid			4.52
$C_4H_7NO_2$	4-Cyanobutanoic acid		25	2.42
$C_4H_7NO_3$	*N*-Acetylglycine		25	3.67
$C_4H_7NO_4$	Iminodiacetic acid	1		2.98
		2		9.89
$C_4H_7NO_4$	*L*-Aspartic acid	1	25	1.99
		2	25	3.90
		3	25	9.90
$C_4H_7N_3O$	Creatinine	1	25	4.8
		2		9.2
$C_4H_7N_5$	2,4,6-Pyrimidinetriamine		20	6.84
$C_4H_8N_2O_3$	*L*-Asparagine	1	20	2.1
		2	20	8.80
$C_4H_8N_2O_3$	*N*-Glycylglycine	1	25	3.14
		2		8.17
$C_4H_8O_2$	Butanoic acid		25	4.83
$C_4H_8O_2$	2-Methylpropanoic acid		20	4.84
$C_4H_8O_3$	3-Hydroxybutanoic acid, (±)		25	4.70
$C_4H_8O_3$	4-Hydroxybutanoic acid		25	4.72
$C_4H_8O_3$	Ethoxyacetic acid		18	3.65
C_4H_9N	Pyrrolidine		25	11.31

Mol. form.	Name	Step	*t*/°C	pK_a
C_4H_9NO	Morpholine		25	8.50
$C_4H_9NO_2$	2-Methylalanine	1	25	2.36
		2	25	10.21
$C_4H_9NO_2$	*N,N*-Dimethylglycine		25	9.89
$C_4H_9NO_2$	*DL*-2-Aminobutanoic acid	1	25	2.29
		2	25	9.83
$C_4H_9NO_2$	4-Aminobutanoic acid	1	25	4.031
		2	25	10.556
$C_4H_9NO_2S$	*DL*-Homocysteine	1	25	2.22
		2	25	8.87
		3	25	10.86
$C_4H_9NO_3$	*L*-Threonine	1	25	2.09
		2	25	9.10
$C_4H_9NO_3$	*L*-Homoserine	1	25	2.71
		2	25	9.62
$C_4H_9N_3O_2$	Creatine	1	25	2.63
		2	25	14.3
$C_4H_{10}N_2$	Piperazine	1	25	9.73
		2	25	5.33
$C_4H_{10}N_2O_2$	2,4-Diaminobutanoic acid	1	25	1.85
		2	25	8.24
		3	25	10.44
$C_4H_{10}O_4$	1,2,3,4-Butanetetrol			13.9
$C_4H_{11}N$	Butylamine		25	10.60
$C_4H_{11}N$	*sec*-Butylamine		25	10.56
$C_4H_{11}N$	*tert*-Butylamine		25	10.68
$C_4H_{11}N$	Diethylamine		25	10.84
$C_4H_{11}NO_3$	Tris(hydroxymethyl) methylamine		20	8.3
$C_4H_{12}N_2$	1,4-Butanediamine	1	25	10.80
		2	25	9.63
C_5H_4BrN	3-Bromopyridine		25	2.84
C_5H_4ClN	2-Chloropyridine		25	0.49
C_5H_4ClN	3-Chloropyridine		25	2.81
C_5H_4ClN	4-Chloropyridine		25	3.83
C_5H_4FN	2-Fluoropyridine		25	-0.44
$C_5H_4N_2O_2$	4-Nitropyridine		25	1.61
$C_5H_4N_4$	1*H*-Purine	1	20	2.30
		2	20	8.96
$C_5H_4N_4O$	Hypoxanthine		25	8.7
$C_5H_4N_4O$	Allopurinol			10.2
$C_5H_4N_4O_3$	Uric acid		12	3.89
$C_5H_4N_4S$	1,7-Dihydro-6H-purine-6-thione	1		7.77
		2		11.17
$C_5H_4O_2S$	2-Thiophenecarboxylic acid		25	3.49
$C_5H_4O_2S$	3-Thiophenecarboxylic acid		25	4.1
$C_5H_4O_3$	2-Furancarboxylic acid		25	3.16
$C_5H_4O_3$	3-Furancarboxylic acid		25	3.9
C_5H_5N	Pyridine		25	5.23
C_5H_5NO	2-Pyridinol	1	20	0.75
		2	20	11.65
C_5H_5NO	3-Pyridinol	1	20	4.79
		2	20	8.75
C_5H_5NO	4-Pyridinol	1	20	3.20
		2	20	11.12
C_5H_5NO	2(1H)-Pyridinone	1	20	0.75
		2	20	11.65
C_5H_5NO	Pyridine-1-oxide		24	0.79
$C_5H_5NO_2$	1*H*-Pyrrole-2-carboxylic acid		20	4.45
$C_5H_5NO_2$	1*H*-Pyrrole-3-carboxylic acid		20	5.00
$C_5H_5N_3O$	Pyrazinecarboxamide			0.5
$C_5H_5N_5$	Adenine	1		4.3
		2		9.83
$C_5H_5N_5O$	Guanine		40	9.92
$C_5H_6N_2$	2-Pyridinamine		20	6.82
$C_5H_6N_2$	3-Pyridinamine		25	6.04
$C_5H_6N_2$	4-Pyridinamine		25	9.11
$C_5H_6N_2$	2-Methylpyrazine		27	1.45
$C_5H_6N_2O_2$	Thymine		25	9.94
$C_5H_6O_4$	1,1-Cyclopropanedi-carboxylic acid	1	25	1.82
		2	25	7.43
$C_5H_6O_4$	*trans*-1-Propene-1,2-dicarboxylic acid	1	25	3.09
		2	25	4.75
$C_5H_6O_4$	1-Propene-2,3-dicarboxylic acid	1	25	3.85
		2	25	5.45
$C_5H_6O_5$	2-Oxoglutaric acid	1	25	2.47
		2	25	4.68
$C_5H_7NO_3$	5,5-Dimethyl-2,4-oxazolidinedione		37	6.13
$C_5H_7NO_3$	*L*-Pyroglutamic acid		25	3.32
$C_5H_7N_3$	2,5-Pyridinediamine		20	6.48
$C_5H_7N_3$	Methylaminopyrazine		25	3.39
$C_5H_7N_3O_4$	Azaserine			8.55
$C_5H_8N_2$	2,4-Dimethylimidazole		25	8.36
$C_5H_8N_4O_3S_2$	Methazolamide			7.30
$C_5H_8O_2$	*trans*-3-Pentenoic acid		25	4.51
$C_5H_8O_4$	Dimethylmalonic acid		25	3.15
$C_5H_8O_4$	Glutaric acid	1	18	4.32
		2	25	5.42
$C_5H_8O_4$	Methylsuccinic acid	1	25	4.13
		2	25	5.64
$C_5H_9NO_2$	*L*-Proline	1	25	1.95
		2	25	10.64
$C_5H_9NO_3$	5-Amino-4-oxopentanoic acid	1	25	4.05
		2	25	8.90
$C_5H_9NO_3$	*trans*-4-Hydroxyproline	1	25	1.82
		2	25	9.66
$C_5H_9NO_4$	*L*-Glutamic acid	1	25	2.13
		2	25	4.31
		3		9.67
$C_5H_9N_3$	Histamine	1	25	6.04
		2	25	9.75
$C_5H_{10}N_2O_3$	Glycylalanine		25	3.15
$C_5H_{10}N_2O_3$	*L*-Glutamine	1	25	2.17
		2	25	9.13
$C_5H_{10}N_2O_4$	Glycylserine	1	25	2.98
		2	25	8.38
$C_5H_{10}O_2$	Pentanoic acid		20	4.83
$C_5H_{10}O_2$	2-Methylbutanoic acid		25	4.80
$C_5H_{10}O_2$	3-Methylbutanoic acid		25	4.77
$C_5H_{10}O_2$	2,2-Dimethylpropanoic acid		20	5.03
$C_5H_{10}O_4$	*D*-2-Deoxyribose		25	12.61
$C_5H_{10}O_5$	*L*-Ribose		25	12.22
$C_5H_{10}O_5$	*D*-Xylose		18	12.14
$C_5H_{11}N$	Piperidine		25	11.123
$C_5H_{11}N$	*N*-Methylpyrrolidine		25	10.46
$C_5H_{11}NO$	4-Methylmorpholine		25	7.38
$C_5H_{11}NO_2$	*L*-Valine	1	25	2.29
		2	25	9.74

Mol. form.	Name	Step	t/°C	pK_a
$C_5H_{11}NO_2$	*DL*-Norvaline	1		2.36
		2		9.72
$C_5H_{11}NO_2$	*L*-Norvaline	1	25	2.32
		2	25	9.81
$C_5H_{11}NO_2$	*N*-Propylglycine	1	25	2.35
		2	25	10.19
$C_5H_{11}NO_2$	5-Aminopentanoic acid	1	25	4.27
		2	25	10.77
$C_5H_{11}NO_2$	Betaine		0	1.83
$C_5H_{11}NO_2S$	*L*-Methionine	1	25	2.13
		2	25	9.27
$C_5H_{12}N_2O$	Tetramethylurea			2
$C_5H_{12}N_2O_2$	*L*-Ornithine	1	25	1.71
		2	25	8.69
		3	25	10.76
$C_5H_{13}N$	Pentylamine		25	10.63
$C_5H_{13}N$	3-Pentanamine		17	10.59
$C_5H_{13}N$	3-Methyl-1-butanamine		25	10.60
$C_5H_{13}N$	2-Methyl-2-butanamine		19	10.85
$C_5H_{13}N$	2,2-Dimethylpropylamine		25	10.15
$C_5H_{13}N$	Diethylmethylamine		25	10.35
$C_5H_{14}NO$	Choline		25	13.9
$C_5H_{14}N_2$	1,5-Pentanediamine	1	25	10.05
		2	25	10.93
$C_6H_3Cl_3N_2O_2$	4-Amino-3,5,6-trichloro-2-pyridinecarboxlic acid			3.6
$C_6H_3N_3O_7$	2,4,6-Trinitrophenol		24	0.42
$C_6H_4Cl_2O$	2,3-Dichlorophenol		25	7.44
$C_6H_4N_2O_5$	2,4-Dinitrophenol		25	4.07
$C_6H_4N_2O_5$	2,5-Dinitrophenol		15	5.15
$C_6H_4N_4$	Pteridine		20	4.05
C_6H_5BrO	2-Bromophenol		25	8.45
C_6H_5BrO	3-Bromophenol		25	9.03
C_6H_5BrO	4-Bromophenol		25	9.37
$C_6H_5Br_2N$	3,5-Dibromoaniline		25	2.34
C_6H_5ClO	2-Chlorophenol		25	8.56
C_6H_5ClO	3-Chlorophenol		25	9.12
C_6H_5ClO	4-Chlorophenol		25	9.41
$C_6H_5Cl_2N$	2,4-Dichloroaniline		22	2.05
C_6H_5FO	2-Fluorophenol		25	8.73
C_6H_5FO	3-Fluorophenol		25	9.29
C_6H_5FO	4-Fluorophenol		25	9.89
C_6H_5IO	2-Iodophenol		25	8.51
C_6H_5IO	3-Iodophenol		25	9.03
C_6H_5IO	4-Iodophenol		25	9.33
C_6H_5NO	2-Pyridinecarboxaldehyde		25	12.68
C_6H_5NO	4-Pyridinecarboxaldehyde		30	12.05
$C_6H_5NO_2$	Nitrobenzene		0	3.98
$C_6H_5NO_2$	2-Pyridinecarboxylic acid	1	20	0.99
		2	20	5.39
$C_6H_5NO_2$	3-Pyridinecarboxylic acid	1	25	2.00
		2	25	4.82
$C_6H_5NO_2$	4-Pyridinecarboxylic acid	1	25	1.77
		2	25	4.84
$C_6H_5NO_3$	2-Nitrophenol		25	7.23
$C_6H_5NO_3$	3-Nitrophenol		25	8.36
$C_6H_5NO_3$	4-Nitrophenol		25	7.15
$C_6H_5N_3$	1*H*-Benzotriazole		20	1.6
$C_6H_5N_5O$	2-Amino-4-hydroxypteridine	1	20	2.27
		2	20	7.96
$C_6H_5N_5O_2$	Xanthopterin	2	20	6.59
		3	20	9.31
C_6H_6BrN	2-Bromoaniline		25	2.53
C_6H_6BrN	3-Bromoaniline		25	3.53
C_6H_6BrN	4-Bromoaniline		25	3.89
C_6H_6ClN	2-Chloroaniline		25	2.66
C_6H_6ClN	3-Chloroaniline		25	3.52
C_6H_6ClN	4-Chloroaniline		25	3.98
C_6H_6FN	2-Fluoroaniline		25	3.20
C_6H_6FN	3-Fluoroaniline		25	3.59
C_6H_6FN	4-Fluoroaniline		25	4.65
C_6H_6IN	2-Iodoaniline		25	2.54
C_6H_6IN	3-Iodoaniline		25	3.58
C_6H_6IN	4-Iodoaniline		25	3.81
$C_6H_6N_2O$	3-Pyridinecarboxamide		20	3.3
$C_6H_6N_2O$	2-Pyridinecarboxaldehyde oxime	1	20	3.59
		2	20	10.18
$C_6H_6N_2O_2$	2-Nitroaniline		25	-0.25
$C_6H_6N_2O_2$	3-Nitroaniline		25	2.46
$C_6H_6N_2O_2$	4-Nitroaniline		25	1.02
C_6H_6O	Phenol		25	9.99
$C_6H_6O_2$	*p*-Hydroquinone	1	25	9.85
		2	25	11.4
$C_6H_6O_2$	Pyrocatechol	1	25	9.34
		2	25	12.6
$C_6H_6O_2$	Resorcinol	1	25	9.32
		2	25	11.1
$C_6H_6O_2S$	Benzenesulfinic acid		20	1.3
$C_6H_6O_3S$	Benzenesulfonic acid		25	0.70
$C_6H_6O_4$	5-Hydroxy-2-(hydroxymethyl)-4H-pyran-4-one			7.9
$C_6H_6O_4S$	3-Hydroxybenzenesulfonic acid		25	9.07
$C_6H_6O_4S$	4-Hydroxybenzenesulfonic acid		25	9.11
$C_6H_6O_6$	*cis*-1-Propene-1,2,3-tricarboxylic acid		25	1.95
$C_6H_6O_6$	*trans*-1-Propene-1,2,3-tricarboxylic acid	1	25	2.80
		2	25	4.46
C_6H_6S	Benzenethiol		25	6.62
$C_6H_7BO_2$	Benzeneboronic acid			8.83
C_6H_7N	Aniline		25	4.87
C_6H_7N	2-Methylpyridine		25	6.00
C_6H_7N	3-Methylpyridine		25	5.70
C_6H_7N	4-Methylpyridine		25	5.99
C_6H_7NO	2-Aminophenol	1	20	4.78
		2	20	9.97
C_6H_7NO	3-Aminophenol	1	20	4.37
		2	20	9.82
C_6H_7NO	4-Aminophenol	1	25	5.48
		2	25	10.30
C_6H_7NO	2-Methoxypyridine		20	3.28
C_6H_7NO	3-Methoxypyridine		25	4.78
C_6H_7NO	4-Methoxypyridine		25	6.58
$C_6H_7NO_3S$	2-Aminobenzenesulfonic acid		25	2.46
$C_6H_7NO_3S$	3-Aminobenzenesulfonic acid		25	3.74
$C_6H_7NO_3S$	4-Aminobenzenesulfonic acid		25	3.23
$C_6H_8N_2$	*N*-Methylpyridinamine		20	9.65
$C_6H_8N_2$	*o*-Phenylenediamine	1	20	4.57

Mol. form.	Name	Step	t/°C	pK_a
		2	20	0.80
$C_6H_8N_2$	*m*-Phenylenediamine	1	20	5.11
		2	20	2.50
$C_6H_8N_2$	*p*-Phenylenediamine	1	20	6.31
		2	20	2.97
$C_6H_8N_2$	Phenylhydrazine		15	8.79
$C_6H_8O_2$	2,4-Hexadienoic acid		25	4.76
$C_6H_8O_2$	1,3-Cyclohexanedione		25	5.26
$C_6H_8O_4$	2,2-Dimethyl-1,3-dioxane-4,6-dione			5.1
$C_6H_8O_6$	*L*-Ascorbic acid	1	25	4.04
		2	16	11.7
$C_6H_8O_7$	Citric acid	1	25	3.13
		2	25	4.76
		3	25	6.40
$C_6H_8O_7$	Isocitric acid	1	25	3.29
		2	25	4.71
		3	25	6.40
$C_6H_9NO_6$	Nitrilotriacetic acid	1	20	3.03
		2	20	3.07
		3	20	10.70
$C_6H_9NO_6$	*L*-γ-Carboxyglutamic acid	1	25	1.7
		2	25	3.2
		3	25	4.75
		4	25	9.9
$C_6H_9N_3$	4,6-Dimethylpyrimidinamine		20	4.82
$C_6H_9N_3O_2$	*L*-Histidine	1	25	1.80
		2	25	6.04
		3	25	9.33
$C_6H_{10}O_2$	Cyclopentanecarboxylic acid		25	4.99
$C_6H_{10}O_3$	Ethyl acetoacetate		25	10.68
$C_6H_{10}O_4$	3-Methylglutaric acid		25	4.24
$C_6H_{10}O_4$	Adipic acid	1	18	4.41
		2	18	5.41
$C_6H_{11}NO_2$	2-Piperidinecarboxylic acid	1	25	2.28
		2	25	10.72
$C_6H_{11}NO_3$	Adipamic acid		25	4.63
$C_6H_{11}NO_4$	2-Aminoadipic acid	1	25	2.14
		2	25	4.21
		3	25	9.77
$C_6H_{11}N_3O_4$	*N*-(*N*-Glycylglycyl)glycine	1	25	3.225
		2	25	8.09
$C_6H_{11}N_3O_4$	Glycylasparagine	1	25	2.942
		2	18	8.44
$C_6H_{12}N_2$	Triethylenediamine	1		3.0
		2		8.7
$C_6H_{12}N_2O_4S_2$	*L*-Cystine	1		1
		2		2.1
		3		8.02
		4		8.71
$C_6H_{12}O_2$	Hexanoic acid		25	4.85
$C_6H_{12}O_2$	4-Methylpentanoic acid		18	4.84
$C_6H_{12}O_6$	β-*D*-Fructose		25	12.27
$C_6H_{12}O_6$	α-*D*-Glucose		25	12.46
$C_6H_{12}O_6$	*D*-Mannose		25	12.08
$C_6H_{13}N$	Cyclohexylamine		25	10.64
$C_6H_{13}N$	1-Methylpiperidine		25	10.38
$C_6H_{13}N$	1,2-Dimethylpyrrolidine		26	10.20
$C_6H_{13}NO$	*N*-Ethylmorpholine		25	7.67
$C_6H_{13}NO_2$	*L*-Leucine	1	25	2.33
		2	25	9.74
$C_6H_{13}NO_2$	*L*-Isoleucine	1	25	2.32
		2	25	9.76
$C_6H_{13}NO_2$	*L*-Norleucine	1	25	2.34
		2	25	9.83
$C_6H_{13}NO_2$	6-Aminohexanoic acid	1	25	4.37
		2	25	10.80
$C_6H_{13}NO_4$	*N,N*-Bis(2-hydroxyethyl)glycine	2	20	8.35
$C_6H_{13}N_3O_3$	Citrulline	1	25	2.43
		2	25	9.69
$C_6H_{14}N_2$	*cis*-1,2-Cyclohexanediamine	1	20	9.93
		2	20	6.13
$C_6H_{14}N_2$	*trans*-1,2-Cyclohexanediamine	1	20	9.94
		2	20	6.47
$C_6H_{14}N_2$	*cis*-2,5-Dimethylpiperazine	1	25	9.66
		2	25	5.20
$C_6H_{14}N_2O_2$	*L*-Lysine	1	25	2.16
		2	25	9.06
		3	25	10.54
$C_6H_{14}N_4O_2$	*L*-Arginine	1	25	1.82
		2	25	8.99
		3	25	12.5
$C_6H_{14}O_6$	*D*-Mannitol		18	13.5
$C_6H_{15}N$	Hexylamine		25	10.56
$C_6H_{15}N$	Diisopropylamine		25	11.05
$C_6H_{15}N$	Triethylamine		25	10.75
$C_6H_{15}NO_3$	Triethanolamine		25	7.76
$C_6H_{16}N_2$	1,6-Hexanediamine	1	0	11.86
		2	0	10.76
$C_6H_{16}N_2$	*N,N,N',N'*-Tetramethyl-1,2-ethanediamine	1	25	10.40
		2	25	8.26
$C_6H_{19}NSi_2$	Hexamethyldisilazane			7.55
$C_7HF_5O_2$	Pentafluorobenzoic acid		25	1.75
$C_7H_3Br_2NO$	3,5-Dibromo-4-hydroxybenzonitrile			4.06
$C_7H_3N_3O_8$	2,4,6-Trinitrobenzoic acid		25	0.65
$C_7H_4Cl_3NO_3$	Triclopyr			2.68
$C_7H_4N_2O_6$	2,4-Dinitrobenzoic acid		25	1.43
$C_7H_5BrO_2$	2-Bromobenzoic acid		25	2.85
$C_7H_5BrO_2$	3-Bromobenzoic acid		25	3.81
$C_7H_5BrO_2$	4-Bromobenzoic acid		25	3.96
$C_7H_5ClO_2$	2-Chlorobenzoic acid		25	2.90
$C_7H_5ClO_2$	3-Chlorobenzoic acid		25	3.84
$C_7H_5ClO_2$	4-Chlorobenzoic acid		25	4.00
$C_7H_5FO_2$	2-Fluorobenzoic acid		25	3.27
$C_7H_5FO_2$	3-Fluorobenzoic acid		25	3.86
$C_7H_5FO_2$	4-Fluorobenzoic acid		25	4.15
$C_7H_5F_3O$	2-(Trifluoromethyl)phenol		25	8.95
$C_7H_5F_3O$	3-(Trifluoromethyl)phenol		25	8.68
$C_7H_5IO_2$	2-Iodobenzoic acid		25	2.86
$C_7H_5IO_2$	3-Iodobenzoic acid		25	3.87
$C_7H_5IO_2$	4-Iodobenzoic acid		25	4.00
C_7H_5NO	2-Hydroxybenzonitrile		25	6.86
C_7H_5NO	3-Hydroxybenzonitrile		25	8.61
C_7H_5NO	4-Hydroxybenzonitrile		25	7.97
$C_7H_5NO_3S$	Saccharin		18	11.68
$C_7H_5NO_4$	2-Nitrobenzoic acid		25	2.17
$C_7H_5NO_4$	3-Nitrobenzoic acid		25	3.46
$C_7H_5NO_4$	4-Nitrobenzoic acid		25	3.43

Mol. form.	Name	Step	t/°C	pK_a
$C_7H_5NO_4$	2,3-Pyridinedicarboxylic acid	1	25	2.43
		2	25	4.78
$C_7H_5NO_4$	2,4-Pyridinedicarboxylic acid	1	25	2.15
$C_7H_5NO_4$	2,6-Pyridinedicarboxylic acid	1	25	2.16
		2	25	4.76
$C_7H_5NO_4$	3,5-Pyridinedicarboxylic acid	1	25	2.80
	Chlorothiazide	1		6.85
$C_7H_6ClN_3O_4S_2$		2		9.45
$C_7H_6F_3N$	3-(Trifluoromethyl)aniline		25	3.49
$C_7H_6F_3N$	4-(Trifluoromethyl)aniline		25	2.45
$C_7H_6N_2$	1*H*-Benzimidazole		25	5.53
$C_7H_6N_2$	2-Aminobenzonitrile		25	0.77
$C_7H_6N_2$	3-Aminobenzonitrile		25	2.75
$C_7H_6N_2$	4-Aminobenzonitrile		25	1.74
C_7H_6O	Benzaldehyde		25	14.90
$C_7H_6O_2$	Benzoic acid		25	4.204
$C_7H_6O_2$	Salicylaldehyde		25	8.37
$C_7H_6O_2$	3-Hydroxybenzaldehyde		25	8.98
$C_7H_6O_2$	4-Hydroxybenzaldehyde		25	7.61
$C_7H_6O_3$	2-Hydroxybenzoic acid	1	20	2.98
		2	20	13.6
$C_7H_6O_3$	3-Hydroxybenzoic acid	1	25	4.08
		2	19	9.92
$C_7H_6O_3$	4-Hydroxybenzoic acid	1	25	4.57
		2	25	9.46
$C_7H_6O_4$	2,4-Dihydroxybenzoic acid	1	25	3.11
		2	25	8.55
		3	25	14.0
$C_7H_6O_4$	2,5-Dihydroxybenzoic acid	1	25	2.97
$C_7H_6O_4$	3,4-Dihydroxybenzoic acid	1	25	4.48
		2	25	8.83
		3	25	12.6
$C_7H_6O_4$	3,5-Dihydroxybenzoic acid	1	25	4.04
$C_7H_6O_5$	2,4,6-Trihydroxybenzoic acid		25	1.68
$C_7H_6O_5$	3,4,5-Trihydroxybenzoic acid		25	4.41
C_7H_7NO	Benzamide		25	~13
$C_7H_7NO_2$	Aniline-2-carboxylic acid	1	25	2.17
		2	25	4.85
$C_7H_7NO_2$	Aniline-3-carboxylic acid	1	25	3.07
		2	25	4.79
$C_7H_7NO_2$	Aniline-4-carboxylic acid	1	25	2.50
		2	25	4.87
$C_7H_7NO_3$	4-Amino-2-hydroxy-benzoic acid			3.25
$C_7H_8ClN_3O_4S_2$	Hydrochlorothiazide	1		7.9
		2		9.2
$C_7H_8N_4O_2$	Theobromine		18	7.89
$C_7H_8N_4O_2$	Theophylline	1	25	8.77
C_7H_8O	*o*-Cresol		25	10.29
C_7H_8O	*m*-Cresol		25	10.09
C_7H_8O	*p*-Cresol		25	10.26
C_7H_8OS	4-(Methylthio)phenol		25	9.53
$C_7H_8O_2$	2-Methoxyphenol		25	9.98
$C_7H_8O_2$	3-Methoxyphenol		25	9.65
$C_7H_8O_2$	4-Methoxyphenol		25	10.21
C_7H_8S	Benzenemethanethiol		25	9.43
C_7H_9N	Benzylamine		25	9.34
C_7H_9N	2-Methylaniline		25	4.45
C_7H_9N	3-Methylaniline		25	4.71
C_7H_9N	4-Methylaniline		25	5.08
C_7H_9N	*N*-Methylaniline		25	4.85
C_7H_9N	2-Ethylpyridine		25	5.89
C_7H_9N	2,3-Dimethylpyridine		25	6.57
C_7H_9N	2,4-Dimethylpyridine		25	6.99
C_7H_9N	2,5-Dimethylpyridine		25	6.40
C_7H_9N	2,6-Dimethylpyridine		25	6.65
C_7H_9N	3,4-Dimethylpyridine		25	6.46
C_7H_9N	3,5-Dimethylpyridine		25	6.15
C_7H_9NO	2-Methoxyaniline		25	4.53
C_7H_9NO	3-Methoxyaniline		25	4.20
C_7H_9NO	4-Methoxyaniline		25	5.36
C_7H_9NS	2-(Methylthio)aniline		25	3.45
C_7H_9NS	4-(Methylthio)aniline		25	4.35
$C_7H_9N_5$	2-Dimethylaminopurine	1	20	4.00
		2	20	10.24
$C_7H_{11}N_3O_2$	*L*-1-Methylhistidine	1	25	1.69
		2	25	6.48
		3	25	8.85
$C_7H_{11}N_3O_2$	*L*-3-Methylhistidine	1	25	1.92
		2	25	6.56
		3	25	8.73
$C_7H_{12}O_2$	Cyclohexanecarboxylic acid		25	4.91
$C_7H_{12}O_4$	Heptanedioic acid	1	25	4.71
		2	25	5.58
$C_7H_{12}O_4$	Butylpropanedioic acid	1	5	2.96
$C_7H_{13}NO_4$	α-Ethylglutamic acid	1	25	3.846
		2	25	7.838
$C_7H_{14}O_2$	Heptanoic acid		25	4.89
$C_7H_{14}O_6$	α-Methylglucoside		25	13.71
$C_7H_{15}N$	1-Ethylpiperidine		23	10.45
$C_7H_{15}N$	1,2-Dimethylpiperidine,(±)		25	10.22
$C_7H_{15}NO_3$	Carnitine		25	3.80
$C_7H_{17}N$	Heptylamine		25	10.67
$C_7H_{17}N$	2-Heptanamine		19	10.7
$C_8H_5NO_2$	3-Cyanobenzoic acid		25	3.60
$C_8H_5NO_2$	4-Cyanobenzoic acid		25	3.55
$C_8H_6N_2$	Cinnoline		20	2.37
$C_8H_6N_2$	Quinazoline		29	3.43
$C_8H_6N_2$	Quinoxaline		20	0.56
$C_8H_6N_2$	Phthalazine		20	3.47
$C_8H_6N_4O_5$	Nitrofurantoin			7.2
$C_8H_6O_3$	3-Formylbenzoic acid		25	3.84
$C_8H_6O_3$	4-Formylbenzoic acid		25	3.77
$C_8H_6O_4$	Phthalic acid	1	25	2.943
		2	25	5.432
$C_8H_6O_4$	Isophthalic acid	1	25	3.70
		2	25	4.60
$C_8H_6O_4$	Terephthalic acid	1	25	3.54
		2	25	4.34
$C_8H_7ClO_2$	2-Chlorobenzeneacetic acid		25	4.07
$C_8H_7ClO_2$	3-Chlorobenzeneacetic acid		25	4.14
$C_8H_7ClO_2$	4-Chlorobenzeneacetic acid		25	4.19
$C_8H_7ClO_3$	2-Chlorophenoxyacetic acid		25	3.05
$C_8H_7ClO_3$	3-Chlorophenoxyacetic acid		25	3.10
$C_8H_7NO_4$	2-Nitrobenzeneacetic acid		25	4.00
$C_8H_7NO_4$	3-Nitrobenzeneacetic acid		25	3.97
$C_8H_7NO_4$	4-Nitrobenzeneacetic acid		25	3.85
$C_8H_8F_3N_3O_4S_2$	Hydroflumethiazide	1		8.9

Mol. form.	Name	Step	*t*/°C	pK_a
		2		9.7
$C_8H_8N_2$	2-Methyl-1*H*-benzimidazole	1	25	6.19
$C_8H_8O_2$	*o*-Toluic acid		25	3.91
$C_8H_8O_2$	*m*-Toluic acid		25	4.25
$C_8H_8O_2$	*p*-Toluic acid		25	4.37
$C_8H_8O_2$	Benzeneacetic acid		25	4.31
$C_8H_8O_2$	1-(2-Hydroxyphenyl)ethanone		25	10.06
$C_8H_8O_2$	1-(3-Hydroxyphenyl)ethanone		25	9.19
$C_8H_8O_2$	1-(4-Hydroxyphenyl)ethanone		25	8.05
$C_8H_8O_3$	2-Methoxybenzoic acid		25	4.08
$C_8H_8O_3$	3-Methoxybenzoic acid		25	4.10
$C_8H_8O_3$	4-Methoxybenzoic acid		25	4.50
$C_8H_8O_3$	Phenoxyacetic acid		25	3.17
$C_8H_8O_3$	Mandelic acid		25	3.37
$C_8H_8O_4$	2,5-Hydroxybenzeneacetic acid		25	4.40
C_8H_9NO	Acetanilide		25	0.5
$C_8H_9NO_2$	2-(Methylamino)benzoic acid		25	5.34
$C_8H_9NO_2$	3-(Methylamino)benzoic acid		25	5.10
$C_8H_9NO_2$	4-(Methylamino)benzoic acid		25	5.04
$C_8H_9NO_2$	*N*-Phenylglycine	1	25	1.83
		2		4.39
$C_8H_{10}BrN$	4-Bromo-*N,N*-dimethylaniline		25	4.23
$C_8H_{10}ClN$	3-Chloro-*N,N*-dimethylaniline		20	3.83
$C_8H_{10}ClN$	4-Chloro-*N,N*-dimethylaniline		20	4.39
$C_8H_{10}N_2O_2$	*N,N*-Dimethyl-3-nitroaniline		25	2.62
$C_8H_{11}N$	*N*-Ethylaniline		25	5.12
$C_8H_{11}N$	*N,N*-Dimethylaniline		25	5.07
$C_8H_{11}N$	2,6-Dimethylaniline		25	3.89
$C_8H_{11}N$	Benzeneethanamine		25	9.83
$C_8H_{11}N$	2,4,6-Trimethylpyridine		25	7.43
$C_8H_{11}NO$	2-Ethoxyaniline		28	4.43
$C_8H_{11}NO$	3-Ethoxyaniline		25	4.18
$C_8H_{11}NO$	4-Ethoxyaniline		28	5.20
$C_8H_{11}NO$	4-(2-Aminoethyl)phenol	1	25	9.74
		2	25	10.52
$C_8H_{11}NO$	2-(2-Methoxyethyl)pyridine			5.5
$C_8H_{11}NO_2$	Dopamine	1	25	8.9
		2	25	10.6
$C_8H_{11}NO_3$	Norepinephrine	1	25	8.64
		2	25	9.70
$C_8H_{11}N_3O_6$	6-Azauridine			6.70
$C_8H_{11}N_5$	Phenylbiguanide	1		10.76
		2		2.13
$C_8H_{12}N_2O_3$	Barbital		25	7.43
$C_8H_{12}O_2$	5,5-Dimethyl-1,3-cyclohexanedione		25	5.15
$C_8H_{13}NO_2$	Arecoline			6.84
$C_8H_{14}O_2S_2$	Thioctic acid			5.4
$C_8H_{14}O_4$	Octanedioic acid	1	25	4.52
$C_8H_{15}NO$	Tropine		15	3.80
$C_8H_{15}NO$	Pseudotropine		15	3.80
$C_8H_{16}N_2O_3$	*N*-Glycylleucine		25	3.18
$C_8H_{16}N_2O_3$	*N*-Leucylglycine	1	25	3.25
		2	25	8.2
$C_8H_{16}N_2O_4S_2$	Homocystine	1	25	1.59
		2	25	2.54
		3	25	8.52
		4	25	9.44
$C_8H_{16}O_2$	Octanoic acid		25	4.89
$C_8H_{16}O_2$	2-Propylpentanoic acid			4.6
$C_8H_{17}N$	2-Propylpiperidine,(*S*)			10.9
$C_8H_{17}N$	2,2,4-Trimethylpiperidine		30	11.04
$C_8H_{17}NO$	*trans*-6-Propyl-3-piperidinol,(3*S*)			10.3
$C_8H_{19}N$	Octylamine		25	10.65
$C_8H_{19}N$	*N*-Methyl-2-heptanamine		17	10.99
$C_8H_{19}N$	Dibutylamine		21	11.25
$C_8H_{20}N_2$	1,8-Octanediamine	1	20	11.00
		2	20	10.1
C_9H_6BrN	3-Bromoquinoline		25	2.69
$C_9H_7ClO_2$	*trans-o*-Chlorocinnamic acid		25	4.23
$C_9H_7ClO_2$	*trans-m*-Chlorocinnamic acid		25	4.29
$C_9H_7ClO_2$	*trans-p*-Chlorocinnamic acid		25	4.41
C_9H_7N	Quinoline		20	4.90
C_9H_7N	Isoquinoline		20	5.40
C_9H_7NO	2-Quinolinol	1	20	-0.31
		2	20	11.76
C_9H_7NO	3-Quinolinol	1	20	4.28
		2	20	8.08
C_9H_7NO	4-Quinolinol	1	20	2.23
		2	20	11.28
C_9H_7NO	6-Quinolinol	1	20	5.15
		2	20	8.90
C_9H_7NO	8-Quinolinol	1	25	4.91
		2	25	9.81
C_9H_7NO	7-Isoquinolinol	1	20	5.68
		2	20	8.90
$C_9H_7NO_3$	2-Cyanophenoxyacetic acid		25	2.98
$C_9H_7NO_3$	3-Cyanophenoxyacetic acid		25	3.03
$C_9H_7NO_3$	4-Cyanophenoxyacetic acid		25	2.93
$C_9H_7N_7O_2S$	Azathioprine			8.2
$C_9H_8N_2$	2-Quinolinamine		20	7.34
$C_9H_8N_2$	3-Quinolinamine		20	4.91
$C_9H_8N_2$	4-Quinolinamine		20	9.17
$C_9H_8N_2$	1-Isoquinolinamine		20	7.62
$C_9H_8N_2$	3-Isoquinolinamine		20	5.05
$C_9H_8O_2$	*cis*-Cinnamic acid		25	3.88
$C_9H_8O_2$	*trans*-Cinnamic acid		25	4.44
$C_9H_8O_2$	α-Methylenebenezene-acetic acid			4.35
$C_9H_8O_4$	2-(Acetyloxy)benzoic acid		25	3.48
$C_9H_9Br_2NO_3$	3,5-Dibromo-*L*-tyrosine	1		2.17
		2		6.45
		3		7.60
$C_9H_9ClO_2$	3-(2-Chlorophenyl)-propanoic acid		25	4.58
$C_9H_9ClO_2$	3-(3-Chlorophenyl)-propanoic acid		25	4.59
$C_9H_9ClO_2$	3-(4-Chlorophenyl)-propanoic acid		25	4.61
$C_9H_9I_2NO_3$	*L*-3,5-Diiodotyrosine	1	25	2.12

Mol. form.	Name	Step	t/°C	pK_a
		2	25	5.32
		3	25	9.48
$C_9H_9NO_3$	*N*-Benzoylglycine		25	3.62
$C_9H_9NO_4$	3-(2-Nitrophenyl)-propanoic acid		25	4.50
$C_9H_9NO_4$	3-(4-Nitrophenyl)-propanoic acid		25	4.47
$C_9H_9N_3O_2$	Carbendazim			4.48
$C_9H_9N_3O_2S_2$	Sulfathiazole			7.2
$C_9H_{10}INO_3$	*L*-3-Iodotyrosine	1	25	2.2
		2	25	8.7
		3	25	9.1
$C_9H_{10}N_2$	2-Ethylbenzimidazole		25	6.18
$C_9H_{10}O_2$	3,5-Dimethylbenzoic acid		25	4.32
$C_9H_{10}O_2$	Benzenepropanoic acid		25	4.66
$C_9H_{10}O_2$	α-Methylbenzeneacetic acid		25	4.64
$C_9H_{10}O_3$	α-Hydroxy-α-methyl-benezeneacetic acid		25	3.47
$C_9H_{11}Cl_2N_3O_4S_2$	Methylclothiazide			9.4
$C_9H_{11}N$	*N*-Allylaniline		25	4.17
$C_9H_{11}N$	1-Indanamine		22	9.21
$C_9H_{11}NO_2$	4-(Dimethylamino)-benzoic acid	1		6.03
		2		11.49
$C_9H_{11}NO_2$	Ethyl 4-aminobenzoate			2.5
$C_9H_{11}NO_2$	*L*-Phenylalanine	1	25	2.20
		2	25	9.31
$C_9H_{11}NO_3$	*L*-Tyrosine	1	25	2.20
		2	25	9.11
		3	25	10.1
$C_9H_{11}NO_4$	Levodopa	1	25	2.32
		2	25	8.72
		3	25	9.96
		4	25	11.79
$C_9H_{12}N_2O_2$	Tyrosineamide		25	7.33
$C_9H_{13}N$	*N*-Isopropylaniline		25	5.77
$C_9H_{13}NO_3$	Epinephrine	1	25	8.66
		2	25	9.95
$C_9H_{13}N_2O_9P$	5'-Uridylic acid	1		6.4
		2		9.5
$C_9H_{13}N_3O_5$	Cytidine	1		4.22
		2		12.5
$C_9H_{14}ClNO$	Phenylpropanolamine hydrochloride			9.44
$C_9H_{14}N_2O_3$	Metharbital			8.45
$C_9H_{14}N_3O_8P$	3'-Cytidylic acid	1		0.8
		2		4.28
		3		6.0
$C_9H_{14}N_4O_3$	Carnosine	1	20	2.73
		2	20	6.87
		3	20	9.73
$C_9H_{15}NO_3S$	Captopril	1		3.7
		2		9.8
$C_9H_{15}N_5O$	Minoxidil			4.61
$C_9H_{16}O_4$	Nonanedioic acid	1	25	4.53
		2	25	5.33
$C_9H_{18}O_2$	Nonanoic acid		25	4.96
$C_9H_{19}N$	*N*-Butylpiperidine		23	10.47
$C_9H_{19}N$	2,2,6,6-Tetramethyl-piperidine		25	11.07
$C_9H_{21}N$	Nonylamine		25	10.64
$C_{10}H_7NO_2$	8-Quinolinecarboxylic acid		25	1.82
$C_{10}H_8O$	1-Naphthol		25	9.39
$C_{10}H_8O$	2-Naphthol		25	9.63
$C_{10}H_9N$	1-Naphthylamine		25	3.92
$C_{10}H_9N$	2-Naphthylamine		25	4.16
$C_{10}H_9N$	2-Methylquinoline		20	5.83
$C_{10}H_9N$	4-Methylquinoline		20	5.67
$C_{10}H_9N$	5-Methylquinoline		20	5.20
$C_{10}H_9NO$	5-Amino-1-naphthol		25	3.97
$C_{10}H_9NO$	6-Methoxyquinoline		20	5.03
$C_{10}H_9NO_2$	1H-Indole-3-acetic acid			4.75
$C_{10}H_{10}O_2$	*o*-Methylcinnamic acid		25	4.50
$C_{10}H_{10}O_2$	*m*-Methylcinnamic acid		25	4.44
$C_{10}H_{10}O_2$	*p*-Methylcinnamic acid		25	4.56
$C_{10}H_{12}N_2$	Tryptamine		25	10.2
$C_{10}H_{12}N_2O$	5-Hydroxytryptamine	1	25	9.8
		2	25	11.1
$C_{10}H_{12}N_2O_5$	Dinoseb			4.62
$C_{10}H_{12}N_4O_3$	Dideoxyinosine			9.12
$C_{10}H_{12}O$	5,6,7,8-Tetrahydro-2-naphthalenol		25	10.48
$C_{10}H_{12}O_2$	Benzenebutanoic acid		25	4.76
$C_{10}H_{12}O_5$	Propyl 3,4,5-trihydroxy-benzoate			8.11
$C_{10}H_{13}N_5O_4$	Adenosine	1	25	3.6
		2	25	12.4
$C_{10}H_{14}N_2$	*L*-Nicotine	1		8.02
		2		3.12
$C_{10}H_{14}N_5O_7P$	5'-Adenylic acid	1		3.8
		2		6.2
$C_{10}H_{14}O$	2-*tert*-Butylphenol		25	10.62
$C_{10}H_{14}O$	3-*tert*-Butylphenol		25	10.12
$C_{10}H_{14}O$	4-*tert*-Butylphenol		25	10.23
$C_{10}H_{15}N$	*N*-*tert*-Butylaniline		25	7.00
$C_{10}H_{15}N$	*N*,*N*-Diethylaniline		25	6.57
$C_{10}H_{15}NO$	*d*-Ephedrine		10	10.139
$C_{10}H_{15}NO$	*l*-Ephedrine		10	9.958
$C_{10}H_{17}N_3O_6S$	*l*-Glutathione	1	25	2.12
		2	25	3.59
		3	25	8.75
		4	25	9.65
$C_{10}H_{18}N_4O_5$	*L*-Argininosuccinic acid	1	25	1.62
		2	25	2.70
		3	25	4.26
		4	25	9.58
$C_{10}H_{18}O_4$	Sebacic acid	1		4.59
		2		5.59
$C_{10}H_{19}N$	Bornylamine		25	10.17
$C_{10}H_{19}N$	Neobornylamine		25	10.01
$C_{10}H_{21}N$	Butylcyclohexylamine		25	11.23
$C_{10}H_{21}N$	1,2,2,6,6-Pentamethyl-piperidine		30	11.25
$C_{10}H_{23}N$	Decylamine		25	10.64
$C_{11}H_8N_2$	1*H*-Perimidine		20	6.35
$C_{11}H_8O_2$	1-Naphthalenecarboxylic acid		25	3.69
$C_{11}H_8O_2$	2-Naphthalenecarboxylic acid		25	4.16
$C_{11}H_{11}N$	Methyl-1-naphthylamine		27	3.67
$C_{11}H_{12}I_3NO_2$	Iopanoic acid			4.8
$C_{11}H_{12}N_2O_2$	*L*-Tryptophan	1	25	2.46
		2	25	9.41

Mol. form.	Name	Step	*t*/°C	pK_a
$C_{11}H_{12}N_4O_3S$	Sulfamethoxypyridazine			6.7
$C_{11}H_{13}F_3N_2O_3S$	Mefluidide			4.6
$C_{11}H_{13}NO_3$	Hydrastinine			11.38
$C_{11}H_{13}N_3O_3S$	Sulfisoxazole			5
$C_{11}H_{14}N_2O$	Cytisine	1		6.11
		2		13.08
$C_{11}H_{14}O_2$	2-*tert*-Butylbenzoic acid		25	3.54
$C_{11}H_{14}O_2$	3-*tert*-Butylbenzoic acid		25	4.20
$C_{11}H_{14}O_2$	4-*tert*-Butylbenzoic acid		25	4.38
$C_{11}H_{16}N_2O_2$	Pilocarpine	1	25	1.6
		2	25	6.9
$C_{11}H_{16}N_4O_4$	Pentostatin			5.2
$C_{11}H_{17}N$	*N,N*-Diethyl-2-methyl-aniline		25	7.24
$C_{11}H_{17}NO_3$	Isoproterenol			8.64
$C_{11}H_{17}N_3O_8$	Tetrodotoxin			8.76
$C_{11}H_{18}ClNO_3$	Methoxamine hydrochloride		25	9.2
$C_{11}H_{18}N_2O_3$	Amobarbital		25	8.0
$C_{11}H_{25}N$	Undecylamine		25	10.63
$C_{11}H_{26}NO_2PS$	Methylphosphonothioic acid *S*[2-[bis(1-isopropyl)amino]-ethyl], *O*-ethylester			7.9
$C_{12}H_6Cl_4O_2S$	Bithionol	1		4.82
		2		10.50
$C_{12}H_8N_2$	1,10-Phenanthroline		25	4.84
$C_{12}H_8N_2$	Phenazine		20	1.20
$C_{12}H_{10}O$	2-Hydroxybiphenyl		25	10.01
$C_{12}H_{10}O$	3-Hydroxybiphenyl		25	9.64
$C_{12}H_{10}O$	4-Hydroxybiphenyl		25	9.55
$C_{12}H_{11}N$	Diphenylamine		25	0.79
$C_{12}H_{11}N$	2-Aminobiphenyl		25	3.83
$C_{12}H_{11}N$	3-Aminobiphenyl		18	4.25
$C_{12}H_{11}N$	4-Aminobiphenyl		18	4.35
$C_{12}H_{11}N$	2-Benzylpyridine		25	5.13
$C_{12}H_{11}N_3$	4-Aminoazobenzene		25	2.82
$C_{12}H_{12}N_2$	*p*-Benzidine	1	20	4.65
		2	20	3.43
$C_{12}H_{12}N_2O_3$	Phenobarbital	1		7.3
		2		11.8
$C_{12}H_{13}I_3N_2O_3$	Iocetamic acid			4
$C_{12}H_{13}N$	*N,N*-Dimethyl-1-naphthylamine		25	4.83
$C_{12}H_{13}N$	*N,N*-Dimethyl-2-naphthylamine		25	4.566
$C_{12}H_{14}N_4O_2S$	Sulfamethazine	1		7.4
		2		2.65
$C_{12}H_{14}N_4O_3S$	Sulfacytine			6.9
$C_{12}H_{17}N_3O_4$	Agaritine	1		3.4
		2		8.86
$C_{12}H_{20}N_2O_2$	Aspergillic acid			5.5
$C_{12}H_{21}N_5O_2S_2$	Nizatidine	1		2.1
		2		6.8
$C_{12}H_{22}O_{11}$	Sucrose		25	12.7
$C_{12}H_{22}O_{11}$	α-Maltose		21	12.05
$C_{12}H_{23}N$	Dicyclohexylamine			10.4
$C_{12}H_{27}N$	Dodecylamine		25	10.63
$C_{13}H_9N$	Acridine		20	5.58
$C_{13}H_9N$	Phenanthridine		20	5.58
$C_{13}H_{10}N_2$	9-Acridinamine		20	9.99
$C_{13}H_{10}N_2$	2-Phenylbenzimidazole	1	25	5.23
		2	25	11.91
$C_{13}H_{10}O_2$	2-Phenylbenzoic acid		25	3.46
$C_{13}H_{10}O_3$	2-Phenoxybenzoic acid		25	3.53
$C_{13}H_{10}O_3$	3-Phenoxybenzoic acid		25	3.95
$C_{13}H_{10}O_3$	4-Phenoxybenzoic acid		25	4.57
$C_{13}H_{11}N_3$	3,6-Acridinediamine		20	9.65
$C_{13}H_{12}Cl_2O_4$	Ethacrynic acid			3.50
$C_{13}H_{12}N_2O$	Harmine			7.70
$C_{13}H_{12}N_2O_3S$	Sulfabenzamide		25	4.57
$C_{13}H_{13}N$	4-Benzylaniline		25	2.17
$C_{13}H_{14}N_2O_{13}$	Harmaline			4.2
$C_{13}H_{15}N_3O_3$	Imazapyr	1		1.9
		2		3.6
$C_{13}H_{16}ClNO$	Ketamine			7.5
$C_{13}H_{19}NO_4S$	4-[(Dipropylamino)-sulfonyl]benzoic acid			5.8
$C_{13}H_{21}N$	2,6-Di-*tert*-butylpyridine			3.58
$C_{13}H_{29}N$	(Tridecyl)amine		25	10.63
$C_{14}H_{12}F_3NO_4S_2$	Perfluidone			2.5
$C_{14}H_{12}O_2$	α-Phenylbenzeneacetic acid		25	3.94
$C_{14}H_{12}O_3$	α-Hydroxy-**α**-phenyl-benezeneacetic acid		25	3.04
$C_{14}H_{18}N_4O_3$	Trimethoprim			6.6
$C_{14}H_{19}NO_2$	Methylphenidate			8.9
$C_{14}H_{21}N_3O_3S$	Tolazamide		25	3.6
$C_{14}H_{22}N_2O_3$	Atenolol			9.6
$C_{14}H_{31}N$	Tetradecylamine		25	10.62
$C_{15}H_{10}ClN_3O_3$	Clonazepam	1		1.5
		2		10.5
$C_{15}H_{11}I_4NO_4$	*L*-Thyroxine	1	25	2.2
		2	25	6.45
		3	25	10.1
$C_{15}H_{14}O_3$	Fenoprofen			7.3
$C_{15}H_{15}NO_2$	Mefenamic acid			4.2
$C_{15}H_{15}N_3O_2$	Methyl Red	1		2.5
		2		9.5
$C_{15}H_{17}ClN_4$	NeutralRed			6.7
$C_{15}H_{19}NO_2$	Tropacocaine		15	4.32
$C_{15}H_{19}N_3O_3$	Imazethapyr	1		2.1
		2		3.9
$C_{15}H_{21}N_3O_2$	Physostigmine	1		6.12
		2		12.24
$C_{15}H_{26}N_2$	Sparteine	1	20	2.24
		2	20	9.46
$C_{15}H_{33}N$	Pentadecylamine		25	10.61
$C_{16}H_{13}ClN_2O$	Valium			3.4
$C_{16}H_{14}ClN_3O$	Chlorodiazepoxide			4.8
$C_{16}H_{16}N_2O_2$	Lysergic acid	1		3.44
		2		7.68
$C_{16}H_{17}N_3O_4S$	Cephalexin	1		5.2
		2		7.3
$C_{16}H_{19}N_3O_4S$	Cephradine	1		2.63
		2		7.27
$C_{16}H_{22}N_2$	Lycodine	1		3.97
		2		8.08
$C_{16}H_{35}N$	Hexadecylamine		25	10.61
$C_{17}H_{17}NO_2$	Apomorphine	1		7.0
		2		8.92
$C_{17}H_{19}NO_3$	Piperine		18	12.22
$C_{17}H_{19}NO_3$	Morphine	1	25	8.21
		2	20	9.85
$C_{17}H_{20}N_4O_6$	Riboflavin	1		1.7

Mol. form.	Name	Step	*t*/°C	pK_a
		2	25	9.69
$C_{17}H_{20}O_6$	Mycophenolic acid			4.5
$C_{17}H_{23}NO_3$	Hyoscyamine		21	9.7
$C_{17}H_{27}NO_4$	Nadolol			9.67
$C_{18}H_{19}ClN_4$	Clozapine	1		3.70
		2		7.60
$C_{18}H_{21}NO_3$	Codeine			8.21
$C_{18}H_{21}N_3O$	Dibenzepin			8.25
$C_{18}H_{32}O_2$	Linoleic acid			7.6
$C_{18}H_{33}ClN_2O_5S$	Clindamycin			7.6
$C_{18}H_{39}N$	Octadecylamine		25	10.60
$C_{19}H_{10}Br_4O_5S$	Bromophenol Blue			4.0
$C_{19}H_{14}O_5S$	Phenol Red			7.9
$C_{19}H_{16}ClNO_4$	Indomethacin			4.5
$C_{19}H_{17}N_3O_4S_2$	Cephaloridine			3.2
$C_{19}H_{20}N_2O_2$	Phenylbutazone			4.5
$C_{19}H_{21}N$	Protriptyline			8.2
$C_{19}H_{21}NO_3$	Thebaine		15	6.05
$C_{19}H_{22}N_2O$	Cinchonine	1		5.85
		2		9.92
$C_{19}H_{22}N_2O$	Cinchonidine	1		5.80
		2		10.03
$C_{19}H_{22}N_2O_2$	Cupreine			6.57
$C_{19}H_{22}O_6$	Gibberellic acid			4.0
$C_{19}H_{23}N_3O_2$	Ergometrinine			7.3
$C_{19}H_{23}N_3O_2$	Ergonovine			6.8
$C_{20}H_{14}O_4$	Phenolphthalein		25	9.7
$C_{20}H_{21}NO_4$	Papaverine			6.4
$C_{20}H_{23}N$	Amitriptyline			9.4
$C_{20}H_{23}N_7O_7$	Folinic acid	1		3.1
		2		4.8
		3		10.4
$C_{20}H_{24}N_2O_2$	Quinine	1	25	8.52
		2	25	4.13
$C_{20}H_{24}N_2O_2$	Quinidine	1	20	5.4
		2	20	10.0
$C_{20}H_{26}N_2O_2$	Hydroquinine			5.33
$C_{21}H_{14}Br_4O_5S$	Bromocresol Green			4.7
$C_{21}H_{16}Br_2O_5S$	Bromocresol Purple			6.3
$C_{21}H_{18}O_5S$	CresolRed			8.3
$C_{21}H_{21}NO_6$	Hydrastine			7.8
$C_{21}H_{22}N_2O_2$	Strychnine		25	8.26
$C_{21}H_{23}ClFNO_2$	Haloperidol			8.3
$C_{21}H_{31}NO_4$	Furethidine			7.48
$C_{21}H_{35}N_3O_7$	Lisinopril	1		2.5
		2		4.0
		3		6.7
		4		10.1
$C_{22}H_{18}O_4$	*o*-Cresolphthalein			9.4
$C_{22}H_{22}FN_3O_2$	Droperidol			7.64
$C_{22}H_{23}NO_7$	Noscapine			7.8
$C_{22}H_{25}NO_6$	Colchicine		20	12.36
$C_{22}H_{25}N_3O$	Benzpiperylon	1		6.73
		2		9.13
$C_{22}H_{33}NO_2$	Atisine			12.2
$C_{23}H_{26}N_2O_4$	Brucine	1		6.04
		2		11.07
$C_{24}H_{40}O_4$	Deoxycholic acid			6.58
$C_{24}H_{40}O_5$	Cholic acid			6.4
$C_{25}H_{29}I_2NO_3$	Amiodarone		25	6.56
$C_{25}H_{41}NO_9$	Aconine			9.52
$C_{26}H_{43}NO_6$	Glycocholic acid			4.4
$C_{26}H_{45}NO_7S$	Taurocholic acid			1.4
$C_{27}H_{28}Br_2O_5S$	Bromothymol Blue			7.0
$C_{27}H_{38}N_2O_4$	Verapamil			8.6
$C_{29}H_{32}O_{13}$	Etoposide			9.8
$C_{29}H_{40}N_2O_4$	Emetine	1		5.77
		2		6.64
$C_{30}H_{23}BrO_4$	Bromadiolone		21	4.04
$C_{30}H_{48}O_3$	Oleanolic acid			2.52
$C_{31}H_{36}N_2O_{11}$	Novobiocin	1		4.3
		2		9.1
$C_{32}H_{32}O_{13}S$	Teniposide			10.13
$C_{33}H_{40}N_2O_9$	Reserpine			6.6
$C_{34}H_{47}NO_{11}$	Aconitine			5.88
$C_{36}H_{51}NO_{11}$	Veratridine			9.54
$C_{37}H_{67}NO_{13}$	Erythromycin			8.8
$C_{43}H_{58}N_4O_{12}$	Rifampin	1		1.7
		2		7.9
$C_{45}H_{73}NO_{15}$	Solanine		15	6.66
$C_{46}H_{56}N_4O_{10}$	Vincristine			5.4
$C_{46}H_{58}N_4O_9$	Vinblastine	1		5.4
		2		7.4