

APPENDIX A. pK_a and CLogP Values for Some Drugs and pK_a Values for Miscellaneous Organic Acids and Bases

DAVID A. WILLIAMS

TABLE A.1 pK_a Values for Some Drugs and Miscellaneous Organic Acids and Bases

Drugs	pK_a Values		ClogP*	Drugs	pK_a Values		ClogP*
	HA	HB ⁺			HA	HB ⁺	
Acebutolol		9.2	1.77	Amoxapine		7.6	1.89
Acenocoumarol	4.7		3.24	Amoxicillin	2.4	9.6	-1.99
Acetaminophen	9.7		0.8	Amphetamine		10.0	1.76
Acetanilide		0.5	1.14	Amphotericin B	5.5	10.0	2.30
Acetazolamide	7.4, 9.1		-0.26	Ampicillin	2.5	7.2	-1.28
α -Acetylmethadol		8.6	3.03	Amprenavir	1.76, 11.54		2.68
Acetylsalicylic acid	3.5		1.19	Anileridine		3.7, 7.5	2.96
Acyclovir	9.3	2.3	-1.47	Antazoline		2.5, 10.1	3.58
Adriamycin		8.2	0.10	Antipyrine		1.5	0.28
Ajmaline		8.2	1.81	Apomorphine	8.9	7.0	1.70
Albuterol	10.3	9.3	0.69	Apraclonidine		9.22	0.87
Alclofenac	4.3		2.48	Aprobarbital	8.0		1.28
Alfentanil		6.5	2.16	Aripazole		7.6 ^c	3.76
Alfuzosin		8.13	1.26	Ascorbic acid	4.2, 11.6		-1.64
Allobarbitol	7.8		0.94	Atomoxetine		9.23	3.36
Allopurinol	9.4		-0.14	Atenolol		9.6	0.33
Alphaprodine		8.7	2.49	Atropine		9.8	1.83
Alprenolol		9.7	2.89	Azatadine		9.3	2.69
Altretamine		10.3	2.52	Azathioprine	8.0		0.02
Amantadine		9.0	2.44	Azlocillin	2.8		0.83
Amiloride		8.7	0.93	Aztrenam	0.7, 2.9	3.9	0.49
Aminoacrine		10.0	2.74	Bacampicillin		6.8	3.52
p-Aminobenzoic acid	4.9	2.5	0.78	Baclofen	5.4	9.5	-0.96
Aminocaproic acid	4.4	10.8	-2.70	Barbital	7.9		0.70
Aminopterin	5.5		-0.9	Bendroflumethiazide	8.5		1.95
Aminopyrine		5.0	0.8	Benzocaine		2.5	1.86
p-Aminosalicylic acid	3.6	1.8	1.24	Benzphetamine		6.6	3.84
Aminothiazole		3.2	0.38	Benzquinamide		5.9	0.46
Amiodarone		6.6	7.81	Benztropine		10.0	4.03
Amitriptyline		9.4	4.41	Betaprodine		8.7	2.49
Amlodipine		8.7	3.01	Bethanidine		10.6	1.73
Amobarbital	7.8		1.58	Bitolterol			4.16

TABLE A.1 pK_a Values for Some Drugs and Miscellaneous Organic Acids and Bases (Continued)

Drugs	pK_a Values		ClogP ^a	Drugs	pK_a Values		ClogP ^a
	HA	HB ⁺			HA	HB ⁺	
Brimonidine		7.78	1.20	Cephacetrile			-1.60
Bosentan	5.46		4.36	Cephalexin ^b	3.2		0.35
Bromazepam	11.0	2.9	1.69	L-Cephaloglycin	4.6	7.1	-0.38
Bromocriptine ^a	15	6.6	-	Cephaloridine	3.4		-2.10
Bromodiphenhydramine		4.9	4.03	Cephalothin	2.5		-0.41
Brompheniramine		3.6, 9.8	3.24	Cephapirin			-0.41
Brucine		8.2, 2.5	1.41	Cephadrine			0.48
Bufuralol		8.9	3.54	Cetirizine	2.9	8.3	1.62
Bumetanide	5.2, 10.0		2.88	Cevimeline		8.5	2.44
Bunolol		9.3	1.96	Chloral hydrate	10.0		0.99
Bupivacaine		8.1	3.31	Chlorambucil	5.8		2.61
Buprenorphine		8.42	2.83	Chlorcyclizine		2.1, 8.2	3.24
Bupropion		7.0	2.32	Chlordiazepoxide		4.8	2.49
Butabarbital	7.9		1.67	Chlorhexidine		10.8	4.57
Butacaine		9.0	4.62	Chloroquin		8.1, 9.9	4.41
Butaclamol		7.2	3.81	Chlorothiazide	6.8, 9.5		-0.24
Butamben		5.4	2.85	Chlorpheniramine		9.0	2.97
Butorphanol		8.6	3.54	Chlorphentermine		9.6	2.78
Butylated hydroxytoluene	7.5		5.17	Chlorpromazine		9.3	5.35
Butylparaben	8.5		3.57	Chlorpropamide	4.9		2.30
Caffeine	>14.0	0.6	-0.63	Chlorprothixene		8.8, 7.6	5.31
Camptothecin		10.8	0.95	Chlortetracycline ^c	3.3, 7.4	9.3	1.32
Captopril	3.7, 9.8		1.99	Chlorthalidone	9.4	1	0.70
Carbenicillin	2.7		1.13	Chlorzoxazone	8.3		2.25/1.82 lactam
Carbenoxolone	6.7, 7.1		6.63	Cimetidine		6.8	0.56
Carbidopa	7.8		-1.75	Cinchonine		4.3, 8.4	3.69
Carbinoxamine		8.1	2.69	Ciprofloxacin	6.0	8.8	1.63
Carisoprodol		4.2	2.10	Citalopram		9.59	3.47
Carpindolol		8.8	2.93	Clindamycin		7.5	1.75
Carvedilol		7.8	4.11	Clofibrate	3.5		3.88
Carteolol		9.74	1.34	Clonazepam	10.5	1.5	2.41
Cefaclor	1.5	7.2	0.14	Clonidine		8.3	1.52
Cefamandole	2.7		0.25	Clopendithiol		6.7, 7.6	3.91
Cefazolin	2.1		-0.70	Clopidogrel		4.55	2.50
Cefoperazone	2.6		-1.11	Clotrimazole		4.7	4.92
Cefotaxime	3.4		-0.51	Cloxacillin	2.8		2.83
Cefoxitin	2.2		-0.02	Clozapine		3.7, 7.4	3.94
Ceftazidime	1.8, 2.7	4.1	-2.50	Cocaine		8.7	2.28
Ceftizoxime	2.7	2.1	-0.65	Codeine		8.2	1.39
Ceftriaxone	3.2, 4.1	3.2	-0.54	Colchicine		1.9	1.07
Cefuroxime			0.26	Cromolyn	1.1, 1.9		2.00
Celecoxib	11.2		2.59	Cyclacillin	2.7	7.5	1.21

TABLE A.1 pK_a Values for Some Drugs and Miscellaneous Organic Acids and Bases (Continued)

Drugs	pK_a Values		ClogP ^a	Drugs	pK_a Values		ClogP ^a
	HA	HB ⁺			HA	HB ⁺	
Cyclamate	1.9		1.03	Diethazine		9.1	5.55
Cyclazocine		9.4	3.52	Diethylcarbamazepine		7.7	1.66
Cyclizine		8.0, 2.5	2.47	Diflunisal	3.0		3.65
Cyclobarbital	8.6		1.50	Dihydroergocriptine		6.9	6.37
Cyclobenzaprine		8.5	6.19	Dihydroergocristine		6.9	6.55
Cyclopentamine		11.5	2.46	Dihydroergotamine		6.9	5.69
Cyclopentolate		7.9	0.99	Dihydrostreptomycin		7.8	-1.49
Cycloserine		4.5, 7.4	-2.99	Dilevalol		9.5	3.09
Cyclothiazide ^c	9.1, 10.5		1.73	Diltiazem		7.7	4.73
Cyproheptadine		8.9	4.92	Dimethadione	6.1		0.77
Cytarabine		4.3	-2.17	Dimethisoquin		6.3	4.04
Dacarbazine		4.4	-0.24	Dinoprost ^e	4.9		2.59
Dantrolene	7.5		1.07	Dinoprostone	4.6		2.97
Dapsone		1.3, 2.5	0.99	Diperodon		8.4	4.65
Darifenicin		9.20	3.78	Diphenhydramine		9.1	3.27
Daunorubicin		8.4	0.54	Diphenoxin			3.97
Debrisoquin		11.9	0.75	Diphenoxylate		7.1	4.51
Dehydrocholic acid	5.12		1.89	Diphenylpyraline		8.9	3.43
Demeclocycline	3.3, 7.2	9.4	0.94	Dipipanone		8.5	5.10
Demoxepam		4.5, 10.6	0.73	Dipyridamole		6.4	3.35
Deprenyl		7.4	2.68	Disopyramide	10.2	8.4	2.33
Deserpidine ^d		6.7	4.95	Donepezil		9.1	3.91
Desipramine		10.4	3.97	Dobutamine		9.5	2.53
Desloratadine		4.2, 9.7	3.50	Dopamine	10.6	8.9	0.05
Desvenlafaxine				Dozazosin		6.93	2.85
Dextroamphetamine		9.9	1.76	Doxepin		9.0	3.85
Dextrobrompheniramine		9.3	3.24	Doxorubicin		8.2, 10.2	0.24
Dextrochlorpheniramine		9.2	2.97	Doxycycline	3.4, 7.7	9.5	1.78
Dextrofenfluramine		9.1	3.55	Doxylamine		4.4, 9.2	2.34
Dextroindoprofen	4.6		2.82	Droperidol		7.6	3.10
Dextromethorphan		8.3	3.89	Duloxetine		9.34	4.81
Dextromoramide		7.0	2.53	Emetine		8.2, 7.4	3.82
Diacetylmorphine (heroin)		7.8	1.58	Enalapril	3.0	5.5	3.25
Diatrizoic acid	3.4		0.49	Enalaprilat	2.3, 3.4	8.0	3.63
Diazepam		3.4	2.82	Entacapone	4.5, 10.72		3.02
Diazoxide	8.5		1.09	Ephedrine		9.6	1.43
Dibenzepin		8.3	3.26	Epinephrine	8.9	10.0	-0.54
Dibucaine		8.9	4.40	Ergometrine		7.3	2.48
Dichlorphenamide	7.4, 8.6		0.34	Ergonovine		6.8	2.48
Diclofenac	4.5		4.55	Ergotamine		6.4	7.37
Dicloxacillin	2.8		3.10	Erythromycin		8.8	2.48
Dicoumarol	4.4, 8.0		2.05	Esmolol		9.5	1.92
Dicyclomine		9.0	4.64	Estrone ^f	10.8		3.62

TABLE A.1 pK_a Values for Some Drugs and Miscellaneous Organic Acids and Bases (Continued)

Drugs	pK_a Values		ClogP ^a	Drugs	pK_a Values		ClogP ^a
	HA	HB ⁺			HA	HB ⁺	
Ethacrynic acid	3.50		2.84	Guanethidine		8.3, 11.9	1.10
Ethambutol		6.3, 9.5	-0.29	Guanabenz		8.1	2.66
Ethoheptazine		8.5	2.41	Guanoxan		12.3	0.83
Ethopropazine		9.6	4.77	Haloperidol		8.3	3.76
Ethosuximide	9.5		0.25	Hexobarbital	8.2		1.46
Ethyl biscoumacetate	7.5		1.61	Hexylcaine		9.1	3.65
Ethylmorphine		8.2	1.90	Hexylresorcinol	9.5		3.77
Ethylnorepinephrine		8.4	-0.40	Homatropine		9.7	1.30
Etidocaine		7.9	3.57	Hycanthone		3.4	3.81
Etomidate		4.2	3.05	Hydralazine		0.5, 7.1	1.00
Eugenol	9.8		2.40	Hydrochlorothiazide	7.0, 9.2		-0.02
Fenclofenac	4.5		4.59	Hydrocodone		8.9	2.57
Fenfluramine		9.1	3.55	Hydrocortisone	-		1.76
Fenoterol	10.0	8.6	1.33	Hydroflumethiazide	8.9, 10.7		-0.07
Fenpropfen	4.5		3.72	Hydromorphone		8.2	2.13
Fentanyl		8.4	3.68	Hydroxyamphetamine		9.3	1.14
fesoterodine		9.28	5.08	Hydroxyzine		2.0, 7.1	2.32
Fexofenadine	4.25	9.53	3.73	Hyoscyamine		9.7	1.79
Finasteride		12.4	3.83	Ibuprofen	5.2		3.50
Flurbiprofen	4.3		3.66	Imipramine		9.5	4.35
Flucloxacillin	2.7		2.89	Indacaterol			3.88
Flufenamic acid	3.9		5.22	Indapamide	8.8		1.96
Flumizole	10.7		4.26	Indomethacin	4.5		4.25
Flunitrazepam		1.8	2.13	Indoprofen	5.8		2.82
Fluoxetine		8.7	3.93	Indoramin		7.7	2.87
Flupenthixol		7.8	3.67	Iocetamic acid ^g	4.1 or 4.3		4.57
Fluphenazine enanthate		3.5, 8.2	7.29	Iodipamide	3.5		5.10
Fluphenazine		3.9, 8.1	3.92	Iodoquinol	8.0		4.10
Flurazepam	8.2	1.9	4.84	Iopanoic acid	4.8		4.65
Flutamide	13.12		3.52	Iprindole	8.2		5.02
Formoterol	7.9	9.2	2.03	Iproniazid		8.1	0.41
Furosemide	3.9		2.30	Ipronidazole		2.7	0.96
Fusidic acid	5.4		5.76	Irbesartan	4.9		5.25
Fluvoxamine		9.39	3.71	Isocarboxazid		10.4	1.63
Gabapentin	3.7	10.7	1.08	Isoniazid		2.0, 3.5, 10.8	-0.77
Galantamine		8.2	-0.05	Isoproterenol	10.1, 12.1	8.6	0.32
Gentamicin ^b		8.2	-3.55	Isoxsuprine	9.8	8.0	2.80
Glibenclamide	5.3		3.08	Kanamycin		7.2	-
Glipizide	5.9		1.88	Ketamine		7.5	3.01
Glutethimide	9.2		1.75	Ketobemidone		8.7	0.80
Glyburide	5.3		3.08	Ketoconazole		2.9, 6.5	4.04
Glycylamine		5.5	2.81	Ketoprofen ^h	4.8		2.91
Guanfacine		7.1	1.33	Labetalol	8.7	7.4	2.72

TABLE A.1 pK_a Values for Some Drugs and Miscellaneous Organic Acids and Bases (Continued)

Drugs	pK_a Values		ClogP ^a	Drugs	pK_a Values		ClogP ^a
	HA	HB ⁺			HA	HB ⁺	
Lansoprazole		3.9	2.58	Methenamine		4.8	-0.17
Leucovorin	3.1, 8.1, 10.4		-1.43	Methicillin	3.0		1.02
Levallorphan	4.5	6.9	3.85	Methohexital	8.3		2.01
Levobunolol		9.2	1.96	Methotrexate	3.8, 4.8	5.6	-0.45
Levodopa	2.3, 9.7, 13.4	8.7	-1.15	Methotrimeprazine		9.2	4.94
Levonordefrin	9.8	8.6	-0.91	Methoxamine		9.2	0.61
Levorphanol		9.2	3.26, 3.26	Methoxyphenamine		10.1	2.12
Lidocaine		7.8	2.20	Methyclothiazide	9.4		1.42
Lincomycin		7.5	0.72	Methyl nicotinate		3.1	0.79
Liothyronine	8.4		3.91	Methyl paraben	8.4		1.88
Lisinopril	1.7, 3.3, 11.1	7.0	3.47	Methyl salicylate	9.9		2.52
Loperamide		8.6	4.15	Methyldopa	2.3, 10.4, 12.6	9.2	-0.74
Loratadine		5.0, 9.8	3.90	Methylergonovine		6.6	2.99
Lorazepam	11.5	1.3	2.35	Methylphenidate		8.8	2.31
Losartan	4.9, 4.7		3.46	Methylthiouracil	8.2		0.14
Loxapine		6.6	2.41	Methypylon	12.0		0.65
Lysergide		7.5	2.71	Methysergide		6.62	1.81
Maprotiline		10.2	4.36	Metoclopramide		0.6, 9.3	2.16
Mazindol		8.6	2.36	Metolazone	9.7		3.16
Mecamylamine		11.2	2.98	Metopon		8.1	2.41
Meclizine		3.1, 6.2	5.28	Metoprolol		9.88	1.63
Meclofenamic acid	4.0		5.44	Metronidazole		2.6	-0.14
Medazepam		6.2	3.89	Metyrosine	2.7, 10.1		00.01
Mefenamic acid	4.2		4.83	Mexiletine		9.1	2.12
Memantine		10.8	3.0	Mezlocillin	2.7		0.33
Mepazine		9.3	5.04	Miconazole		6.7	4.97
Meperidine		8.7	2.19	Midazolam		6.2	3.80
Mephentermine		10.4	2.61	Minocycline	2.8, 5.0, 7.8	9.5	2.12
Mephobarbital	7.7		1.23	Minoxidil		4.6	1.62
Mepindolol		8.9	2.30	Mitomycin		10.9	-0.30
Mepivacaine		7.7	1.78	Molindone		6.9	-1.32
Mercaptopurine	7.8	11.0	-0.04	Montelukast	5.7		5.81
Mesalamine	2.7	5.8	0.74	Morphine	9.9	8.0	0.87
Metaproterenol	11.8	8.8	0.28	Morpholine		8.33	-0.79
Metaraminol		8.6	0.25	Moxalactam	2.5, 7.7, 10.2		-2.56
Methacycline	3.5, 7.6	9.5	1.35	Nabilone ^b	13.5		7.25
Methadone		8.3	3.93	Nadolol		9.67	0.56
Methamphetamine		10.0	2.20	Nafcillin	2.7		2.60
Methapyrilene		3.7, 8.9	2.78	Nalbuphine	10.0	8.7	1.21
Methaqualone		2.5	2.50	Nalidixic acid	6.0		0.03
Metharbital	8.2		1.50	Nalorphine		7.8	1.59
Methazolamide	7.3		0.13	Naloxone		7.9	1.78
Methdilazine		7.5	4.64	Naltrexone		8.13	2.05

TABLE A.1 pK_a Values for Some Drugs and Miscellaneous Organic Acids and Bases (Continued)

Drugs	pK_a Values		ClogP ^a	Drugs	pK_a Values		ClogP ^a
	HA	HB ^a			HA	HB ^a	
Naphazoline		10.9	2.99	Pentazocine	10.0	8.5	4.15
Naproxen	4.2		2.88	Pentobarbital	8.1		2.18
Nebivolol		7.1	4.08	Pentoxiphylline		0.3	0.29, 0.29
Nelfinavir	7.53	9.58	7.28	Pergolide		7.8 ^b	3.90
Niacin/nicotinic acid	2.0	4.8	0.22	Perphenazine		3.7, 7.8	3.94
Nicotinamide		0.5, 3.4	-0.37	Perhexilene			6.46
Nicotine		3.1, 8.0	0.57	Phenacetin		2.2	1.66
Nikethamide		3.5	0.92	Phencyclidine		8.5	4.25
Nitrazepam	10.8	3.2	2.35	Phendimetrazine		7.6	1.64
Nitrofurantoin	7.1		-0.47	Phenethicillin	2.8		2.29
Norcodeine		5.7	0.52	Phenindamine		8.3	3.81
Nordefrin	9.8	8.5	-0.91	Phenindione	4.1		3.13
Norepinephrine	9.8, 12.0	8.6	-1.26	Pheniramine		4.2, 9.3	2.20
Norfenephine		8.7	-0.60	Phenmetrazine		8.5	1.74
Normorphine		9.8	0.00	Phenobarbital	7.4		0.53
Nortriptyline		9.7	3.97	Phenolphthalein	9.7		1.91
Noscapine		6.2	2.38	Phenothiazine		2.5	4.15
Novobiocin	4.3, 9.1		3.74	Phenoxybenzamine		4.4	3.69
Nystatin ⁱ	8.9	5.1	2.46	Phentermine		10.1	2.20
Octopamine	9.5	8.9	-0.59	Phentolamine		7.7	4.08
Olanzapine		5.0, 7.4	3.08	Phenylbutazone	4.5		3.38
Omeprazole		4.0	2.36	Phenylephrine	10.1	8.8	0.12
Ondansetron		7.7	1.55	Phenylpropanolamine		9.4	0.36
Orphenadrine		8.4	3.33	Phenylsalicylate	2.98, 8.80 ^c		2.75
Oxacillin	2.7		2.55	Phenyltoloxamine		9.1	3.46
Oxazepam	11.6	1.8	2.22	Phenylramidol		5.9	2.32
Oxprenolol		9.5	2.15	Phenytol	8.3		2.47
Oxybutynin		7.0	5.05	Physostigmine		2.0, 8.2	1.27
Oxycodone		8.9	1.59	Pilocarpine		1.6, 7.1	-0.24
Oxymorphone	9.3	8.5	1.15	Pimozide		7.3, 8.6	5.76
Oxyphenbutazone	4.7		3.28	Pindolol		8.8	1.68
Oxypurinol	7.7		0.18	Piperazine		5.6, 9.8	-1.50
Oxytetracycline ^c	3.3, 7.3	9.1	0.48	Pipradrol		9.7	3.61
Pamaquine		1.3, 3.5, 10.0	4.38	Pirbuterol		3.0, 7.0, 10.3	0.04
Papaverine		6.4	2.95	Piroxicam	4.6		0.59
Pantoprazole	8.19	3.8	1.48	Pivampicillin		7.0	3.88
Pargyline		6.9	1.68	Polythiazide	9.8		2.05
Pemoline		10.5	0.42	Practolol		9.5	0.59
Penbutolol ^c		9.3	4.02	Pramipexole		10.8	2.35
Penicillamine	1.8, 10.5	7.9	0.85	Pramoxine		6.2	2.59
Penicillin G	2.8		1.92	Prasugrel		5.4	4.31
Penicillin V	2.7		1.94	Prazepam		2.9	3.70
Pentamidine		11.4	2.85	Prazosin		6.5	2.14

TABLE A.1 pK_a Values for Some Drugs and Miscellaneous Organic Acids and Bases (Continued)

Drugs	pK_a Values		ClogP*	Drugs	pK_a Values		ClogP*
	HA	HB ⁺			HA	HB ⁺	
Pregabalin	4.2	10.6	1.09	Serotonin	9.8	4.9, 9.1	0.54
Prenalatorol	10.0	9.5	1.27	Sertraline		9.5	5.08
Prilocaine		7.9	2.03	Silodosin			2.52
Probenecid	3.4		2.51	Solifenacin		6.44	3.70
Procainamide		9.2	1.32	Sotalol	8.5	9.8	0.24
Procaine		8.8	2.26	Spiperone		8.3, 9.1	3.25
Procarbazine		6.8	0.06	Streptozocin		1.3	-1.23
Prochlorperazine		3.7, 8.1	4.65	Strychnine		2.3, 8.0	1.93
Promazine		9.4	4.69	Sufentanil		8.0	3.95
Promethazine		9.1	4.89	Sulfacetamide	5.4	1.8	-0.96
Proparacaine		3.2	3.46	Sulfadiazine	6.5	2.0	0.12
Propoxycaine		8.6	2.70	Sulfaguanidine	12.1	2.8	-1.22
Propoxyphene		6.3	4.10	Sulfamerazine	7.1	2.3	0.11
Propranolol		9.5	2.90	Sulfamethazine	7.4	2.4	0.30
Propylhexedrine		10.4	2.98	Sulfamethoxazole	5.6		0.66
Propylthiouracil	7.8		1.15	Sulfasalazine	2.4, 9.7, 11.8		3.05
Pseudoephedrine		9.5	1.43	Sulfathiazole	7.1	2.4	0.05
Pyrazinazine		8.9	4.15	Sulfinpyrazone	2.8		1.89
Pyrazinamide		0.5	-0.17	Sulfisoxazole	5.0		1.01
Pyridoxine	8.96	5.0	-0.83	Sulindac	4.5		2.55
Pyrilamine		4.0, 8.9	2.67	Sulpiride		9.1	0.78
Pyrimethamine		7.3	2.75	Sulthiame	10.0		0.56
Pyrrobutamine		8.8	4.57	p-Synephrine	10.2	9.3	0.13
Quinacrine		8.2, 10.2	5.59	Talbutal	7.8		1.79
Quinidine		4.2, 7.9	2.82	Tamsulosin	10.23	8.37	2.14
Quinine		4.2, 8.5	2.82	Tamoxifen		8.9	5.13
Ranitidine		2.3, 8.2	-0.07	Tapentadol		9.34	3.02
Resperidone	3.11	8.24	3.04	Terazosin		7.1	0.80
Reserpine		6.6	3.65	Temazepam		1.6	2.19
Rifampin	1.7	7.9	2.05	Terbutaline	10.1, 11.2	8.8	0.70
Rimoterol	10.3	8.7	0.74	Tetracaine		8.4	3.75
Ritodrine		9.0	2.04	Tetracycline	3.3, 7.7	9.7	0.62
Rivastigmine		8.85	2.05	Tetrahydrocannabinol (THC)		10.6	6.84
Rolitetracycline	7.4		1.66	Tetrahydrozoline		10.5	2.85
Ropinirole		9.5	2.49	Theobromine	10.1	0.1	-1.06
Rotoxamine		8.1	2.69	Theophylline	8.6	3.5	-0.02
Saccharin	1.6		0.91	Thiazbendazole		4.7	2.47
Salicylamide	8.2		1.35	Thiamylal	7.5		2.81
Salicylic acid	3.0, 13.4		2.01	Thioguanine	8.2		-0.28
Salmeterol	9.26	9.99	3.71	Thiopental	7.5		2.63
Salsalate	3.5, 9.8		3.29	Thiopropazate		3.2, 7.2	4.76
Scopolamine		7.6	0.69	Thioridazine		9.5	5.90
Secobarbital	7.9, 12.6		2.30	Thiothixene		7.7, 7.9	3.72

TABLE A.1 pK_a Values for Some Drugs and Miscellaneous Organic Acids and Bases (Continued)

Drugs	pK_a Values		ClogP [*]	Drugs	pK_a Values		ClogP [*]
	HA	HB ⁺			HA	HB ⁺	
Thiouracil	7.5		0.85	Vidarabine		3.5, 12.5	-1.23
Thonzylamine		2.2, 9.0	1.86	Vigabatrin	4.02	9.72	-0.30
l-Thyroxine	2.2, 6.7	10.1	4.72	Viloxazine		8.1	1.24
tiagabine	3.3	9.4	4.03	Vinblastine		5.4, 7.4	5.92
Ticarcillin	2.6, 3.4		1.24	Vincristinej		5.0, 7.4	5.75
Ticrynafen	2.7		3.05	Vindesine		6.0, 7.7	4.94
Timolol		8.8	1.28	Voriconazole	2.72, 11.54		1.21
Timoprazole		3.1, 8.8	1.22	Warfarin	5.1		3.13
Tiotidine		6.8	0.35	Xylometazoline		10.2	4.59
Tobramycin		6.7, 8.3, 9.9	-4.22	Zimeldine		3.8, 8.74	3.07
Tocainide		7.5	0.81	Zonisamide		10.2	0.72
Tolamolol		7.9	2.03	Miscellaneous organic acids and bases			
Tolazamide	3.1	5.7	1.54	Acetic acid	4.8		
Tolazoline		10.3	1.80	Allylamine			
Tolbutamide	5.4		2.36	6-Aminopenicillanic acid	2.3		
tolcapone	10.63		2.12	Ammonia		9.3	
Tolmetin	3.5		2.68	Aniline		4.63	
Toloteridine		9.87	5.23	Benzoic acid	4.2		
Topiramate	8.67		2.16	Benzyl alcohol	18.0		
Tramadol		9.41	2.32	Benzylamine		9.33	
Tramazoline		10.7	2.78	Butyric acid	4.8		
Tranlycypromine		8.2	1.47	Carbonic acid	6.4, 10.4		
Trazodone		6.7	2.76	Citric acid	3.1, 4.8, 5.4		
Triamterene		6.2	1.16	Diethanolamine		8.9	
Trichlormethiazide	8.6		0.13	Diethylamine		11.09	
Trifluoperazine		3.9, 8.1	4.62	Dimethylamine		10.73	
Triflupromazine		9.2	5.16	Ethanol	15.6		
Trimeprazine		9.0	5.04	Ethanolamine		9.5	
Trimethobenzamide		8.3	1.26	Ethylamine		10.7	
Trimethoprim		6.6	0.91	Ethylenediamine		7.56, 10.71	
Trimipramine		8.0	4.71	Fumaric acid	3.0, 4.4		
Tripeleennamine		4.2, 8.7	2.78	Gluconic acid	3.6		
Triprolidine		6.5	3.25	Glucuronic acid	3.2		
Troleandomycin		6.6	3.46	Guanidine		13.6	
Tropicamide		5.3	0.64	Imidazole		7.0, 14.9	
Tuaminoheptane		10.5	2.43	Isopropylamine		10.63	
Tubocurarine		8.1, 9.1	0.77	Lactic acid	3.9		
Tyramine	10.9	9.3	0.78	Maleic acid	1.9		
Valdenafil	6.13, 2.02	9.11	3.64	Mandelic acid	3.4		
Valproic acid	4.8		2.58	Methylamine		10.66	
Valsartan	6.0		4.02	Monochloroacetic acid	2.9		
Venlafaxine		9.4	2.47	N-propylamine		10.6	
Verapamil		8.9	4.02	Nitromethane	11.0		

TABLE A.1 pK_a Values for Some Drugs and Miscellaneous Organic Acids and Bases (Continued)

Drugs	pK_a Values		ClogP*	Drugs	pK_a Values		ClogP*
	HA	HB ⁺			HA	HB ⁺	
Phenol	9.9			Trichloroacetic acid	0.9		
Phthalic acid	2.9			Triethanolamine		7.8	
Resorcinol	9.2, 11.3			Triethylamine		10.75	
Sorbic acid	4.8			Trimethylamine		9.8	
Succinimide	9.6			Tropic acid	4.1		
Tartaric acid	3.0, 4.4			Tropine		10.8	
p-Toluidine		5.3		Uric acid	5.4		

*ClogP values calculated on basis of unionized molecules. Calculate $\log D_{pH\ 7.4}$ to determine distribution/partition coefficient at pH 7.4. ClogP calculated with ACD/Log P 12v, Advanced Chemical Development, Toronto, Canada, 2010.

^aDetermined in methyl cellosolve/water (8:2 w/w mixture).

^bDetermined in 66% dimethylformamide.

^cDetermined in 25% to 30% ethanol.

^dDetermined in 40% methanol.

^eProstaglandin F_{2α}.

^fSpectrophotometric determination.

^gThe pK_a values of the four optical isomers are 4.1 for two isomers and 4.25 for two isomers.

^hDetermined in methanol/water (3:1 mixture).

ⁱDetermined in dimethylformamide/water (1:1 mixture).

^jDetermined in 33% dimethylformamide.

General References for pK_a and ClogP Values

Albert A, Serjeant EP. The Determination of Ionization Constants of Acids and Bases: A Laboratory Manual, 3rd ed. New York: Chapman and Hall, 1984.

Florey K, ed. Analytical Profiles of Drugs Substances. New York: Academic Press, 1978.

Hansch C, Leo AJ. Substituent Constants for Correlation Analysis in Chemistry and Biology. New York: Wiley, 1979.

Hansch C, Sammes PG, Taylor JB, eds. Comprehensive Medicinal Chemistry, vol 6. Oxford: Pergamon Press, 1990.

O'Neil A, Heckelman PE, Koch CB, et al. The Merck Index, 14th ed. Rahway, NJ: Merck and Co, 2006.

Perrin DD, Dempsey B, Serjeant EP. pK_a Prediction for Organic Acids and Bases. New York: Chapman and Hall, 1981.

Serjeant EP, Dempsey B. Ionization Constants of Organic Acids in Aqueous Solution. IUPAC Chemical Data Series No. 23. Oxford, UK: Pergamon Press, 1979.

Sinko P. Martin's Physical Pharmacy and Pharmaceutical Sciences, 5th ed. Baltimore: Lippincott Williams & Wilkins, 2005.