

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

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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	Ariprazole		7.6 ^c	3.76
Alfuzosin		8.13	1.26	Ascorbic acid	4.2, 11.6		-1.64
Allobarbital	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
Aminothiazazole		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 ^b			HA	HB ^b	
Brimonidide		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	Clopenthiol		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

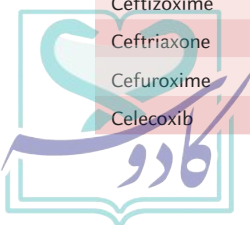


TABLE A.1 pK_a Values for Some Drugs and Miscellaneous Organic Acids and Bases (Continued)

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

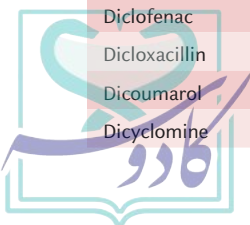


TABLE A.1 pK_a Values for Some Drugs and Miscellaneous Organic Acids and Bases (Continued)

Drugs	pK_a Values		ClogP ^a	Drugs	pK_a Values		ClogP ^a
	HA	HB ^a			HA	HB ^a	
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
Fenopropfen	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	locetamic acid ⁶	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
Glycyclamine		5.5	2.81	Ketoprofen ^h	4.8		2.91
Guanfacine		7.1	1.33	Labetalol	8.7	7.4	2.72

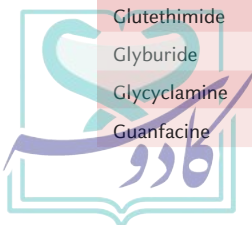


TABLE A.1 pK_a Values for Some Drugs and Miscellaneous Organic Acids and Bases (Continued)

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	Methyprylon	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
Norfenephrine		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	Phenyramidol		5.9	2.32
Oxprenolol		9.5	2.15	Phenytoin	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

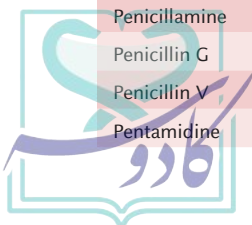


TABLE A.1 pK_a Values for Some Drugs and Miscellaneous Organic Acids and Bases (Continued)

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
Prenalterol	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
Propoxycaïne		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	Sulfapyrazone	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
Pyrrbutamine		8.8	4.57	p-Syneprine	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		
Tripolidine		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 ^a	Drugs	pK_a Values		ClogP ^a
	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		

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

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

^cDetermined in 66% dimethylformamide.

^dDetermined in 25% to 30% ethanol.

^eDetermined in 40% methanol.

^fProstaglandin F_{2α}.

^gSpectrophotometric determination.

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

ⁱDetermined in methanol/water (3:1 mixture).

^jDetermined in dimethylformamide/water (1:1 mixture).

^kDetermined in 33% dimethylformamide.

General References for pK_a and ClogP Values

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