

Experimentally determined Caco-2 P_{app} values and standard deviations

Compound	P_{app} / cm/s (pH6.5)	SD	P_{app} / cm/s (pH7.4)	SD	Compound	P_{app} / cm/s (pH6.5)	SD	P_{app} / cm/s (pH7.4)	SD
acarbose	1.51E-07	5.34E-08	1.12E-07	2.13E-08	gabapentin	4.83E-07	7.48E-10	6.46E-07	8.80E-08
acebutolol	3.84E-07	2.33E-08	1.31E-07	8.92E-09	guanabenz	1.97E-05	1.76E-07	2.95E-05	4.03E-06
acetaminophen	2.89E-05	2.83E-06	2.35E-05	1.52E-06	hydrocortisone	1.46E-05	1.45E-06	1.87E-05	1.16E-07
acyclovir	9.11E-07	1.52E-07			imipramine	1.31E-05	5.41E-07	2.25E-05	2.31E-06
adefovir	2.18E-07	2.90E-08			indomethacin	5.32E-05	1.62E-06	2.50E-05	1.75E-07
alprazolam	3.81E-05	3.69E-06			isradipine	2.99E-05	1.15E-06		
alprenolol	1.52E-05	8.76E-07	3.18E-05	1.40E-06	ketoprofen	6.40E-05	1.93E-06	2.76E-05	1.63E-06
amiloride	2.91E-06	4.27E-08	1.94E-06	6.01E-08	lansoprazole	3.00E-05	1.08E-06	2.66E-05	1.92E-06
aminopyrine	4.44E-05	2.94E-06			lisinopril	2.01E-07	3.36E-08		
amoxicillin	6.93E-07	1.14E-07			metaproterenol	3.78E-07	6.84E-08	3.62E-07	9.86E-08
ampicillin	2.33E-07	5.17E-08	3.85E-07	1.95E-07	methotrexate	1.29E-06	4.24E-08		
amrinone	5.47E-06	3.96E-07	1.00E-05	6.97E-07	metolazone	3.82E-06	6.80E-08	2.63E-06	2.57E-07
antipyrine	4.21E-05	4.32E-06	4.85E-05	2.41E-06	mexiletine	1.95E-05	1.02E-07	4.57E-05	2.17E-06
atenolol	3.90E-07	1.33E-09	2.79E-07		minoxidil	7.60E-06	3.71E-07	5.74E-06	7.70E-07
atropine	4.28E-06	1.91E-08			nadolol	4.52E-07	2.05E-08	2.81E-07	6.00E-08
azithromycin	2.15E-07				naloxone	2.00E-05	6.01E-07	3.90E-05	7.51E-07
benazepril	7.29E-07	3.87E-08			naproxen	7.51E-05	1.87E-06	4.94E-05	2.05E-06
betaxolol	1.26E-05	5.62E-07			nitrendipine	2.14E-05	1.87E-06	1.80E-05	5.77E-07
caffeine	4.79E-05	5.51E-07	4.45E-05	2.14E-07	ofloxacin	6.57E-06	4.86E-07	5.13E-06	2.12E-07
captopril	4.50E-07	7.72E-08	3.41E-07	3.01E-08	omeprazole	3.35E-05	8.20E-07	2.30E-05	2.34E-06
cefazolin	2.44E-07	8.45E-08			oxazepam	4.25E-05	3.38E-06		
cefmetazole	3.34E-07	4.15E-08			phenytoin	4.21E-05	1.96E-06		
cimetidine	1.060E-06	4.15E-08			pindolol	7.07E-06	5.76E-07	1.81E-05	2.68E-08
ciprofloxacin	2.56E-06	9.45E-08			piroxicam	6.66E-05	4.37E-06	3.81E-05	2.99E-07
clonidine	1.91E-05	1.93E-06			prednisolone	8.84E-06	6.07E-07	6.99E-06	9.23E-07
cymarin	2.97E-06	2.16E-07	2.34E-06	1.20E-07	progesterone	3.06E-05	2.48E-06	2.54E-05	1.35E-06
desipramine	1.09E-05	1.43E-06	2.22E-05	2.41E-06	propranolol	1.29E-05	3.49E-07	3.09E-05	1.77E-06
dexamethasone	1.49E-05	3.17E-07	1.46E-05	2.59E-06	quinidine	3.40E-06	5.39E-07	1.17E-05	9.16E-07
diazepam	4.39E-05	2.02E-06			ranitidine	7.33E-07	1.16E-07	6.59E-07	4.41E-08

diclofenac	4.57E-05	4.05E-06	2.77E-05	1.57E-06	sulfasalazin	1.66E-07	6.49E-08		
digoxin	1.39E-06	3.04E-09			sulindac	1.67E-05	2.40E-07	4.91E-06	3.47E-08
doxorubicin	1.40E-07	8.00E-09			sulpiride	4.61E-07	5.62E-08	3.07E-07	5.94E-08
enalapril	2.42E-07	3.23E-08	1.11E-07	1.67E-08	talinalolol	3.94E-07	3.89E-08	3.29E-07	2.82E-08
enalaprilat	1.79E-07	1.16E-08	1.76E-07	3.26E-08	terazosin	4.79E-06	5.19E-07	4.69E-06	2.71E-07
erythromycin	1.49E-07	2.08E-08	4.42E-08	1.53E-09	terbutaline	2.51E-07	6.44E-08		
etoposide	1.98E-07	5.86E-08	2.30E-07	9.15E-09	tetracycline	1.59E-06	2.72E-07		
famciclovir	5.51E-06	3.76E-07	3.20E-06	1.13E-06	theophylline	2.99E-05	2.90E-07	2.55E-05	1.24E-06
famotidine	5.78E-07	3.69E-08	5.06E-07	1.01E-07	trimethoprim	1.73E-05	3.80E-07	2.07E-05	1.53E-06
felodipine	4.71E-06	9.93E-08			urapidil	7.03E-06	1.30E-06		
fenoterol	2.86E-07	5.23E-08			verapamil	1.28E-05	8.79E-07	2.14E-05	6.55E-07
flecainide	6.68E-06	1.16E-06	1.23E-05	1.15E-07	warfarin	5.85E-05	3.54E-06	3.19E-05	5.48E-06
fluconazole	2.45E-05	1.19E-06			xamoterol	4.93E-07	1.15E-07		
fosinopril	2.59E-06	7.54E-07							

Parameter	Range
Molecular weight	151-749
H-bond acceptors	2-14
H-bond donors	0-8
TPSA	6.48-210
