Compound	CAS	Sufficient PBPK Data				
		Human	Rat	Mouse	Monkey	Dog
Acetochlor	34256-82-1	Y	Y			
Ametryn	834-12-8	Y	Y			
Bisphenol-A	80-05-7	Y	Y			
boscalid	188425-85-6	Y	Y			
Carbaryl	63-25-2	Y	Y			
Cyproconazole	94361-06-5	Y	Y			
Fenarimol	60168-88-9		Y			
Flusilazole	85509-19-9	Y	Y			
Formetanate hydrochloride	23422-53-9	Y	Y			
Imazalil	35554-44-0		Y			
Isazofos	42509-80-8	Y	Y			
Propyzamide	23950-58-5		Y			
Pyrimethanil	53112-28-0	Y	Y			
Pyrithiobac-sodium	123343-16-8		Y			
Thidiazuron	51707-55-2		Y			
Triflumizole	68694-11-1	Y	Y			
2-Phenylphenol	90-43-7	Y				
Abamectin	71751-41-2	Y				
Aldicarb	116-06-3					
Atrazine	1912-24-9					
Azinphosmethyl	86-50-0	Y				
Azoxystrobin	131860-33-8	Y				
Bendiocarb	22781-23-3	Y				
Bifenazate	149877-41-8	Y				
Bromoxynil	1689-84-5	Y				
Cacodylic acid	75-60-5					

Carboxin	5234-68-4	Y
Chloridazon	1698-60-8	Y
Clomazone	81777-89-1	Y
Clothianidin	210880-92-5	Y

Human Problem										
Clint	Fub	PhysChem	MW	Reference	logP	Reference	pKa	Reference	Human Clint
			269.77	EPI Suite	3.03	EPI Suite	4	ChemNet	8.47E+01
			227.33	EPI Suite	2.98	EPI Suite	4.401	EpiK	3.15E+01
			228.29	EPI Suite	3.32	EPI Suite	7.889	EpiK	1.93E+01
			343.21	EPI Suite	4	EPI Suite	0.296	EpiK	1.73E+01
			201.23	EPI Suite	2.36	EPI Suite	11.902	EpiK	2.73E+01
			291.78	EPI Suite	2.9	EPI Suite	-2.152	EpiK	1.54E+00
Y			331.20	EPI Suite	3.6	EPI Suite	1.5	EpiK	
			315.40	EPI Suite	3.7	EPI Suite	2.5	LookChem	1.99E+01
			257.72	ChemSpid	0.856	ChemSpid	8.169	EpiK	1.37E+01
Y			297.19	EPI Suite	3.82	EPI Suite	7.203	EpiK	
			313.74	EPI Suite	3.82	EPI Suite	-2.457	EpiK	1.95E+01
Y			256.13	EPI Suite	3.43	EPI Suite	11.698	EpiK	
			199.26	EPI Suite	2.84	EPI Suite	4.856	EpiK	4.39E+01
Y			348.74	EPI Suite	0.6	EPI Suite	-0.878	EpiK	
Y			220.25	EPI Suite	1.77	EPI Suite	2.388	EpiK	
			345.75	EPI Suite	1.4	EPI Suite	2.666	EpiK	1.42E+01
			170.21	EPI Suite	3.09	EPI Suite	9.82	EpiK	2.08E+00
			873.10	EPI Suite	4.39	EPI Suite	11.144	EpiK	5.24E+00
Y			190.26	EPI Suite	1.13	EPI Suite	-2.95	EpiK	
Y			215.69	EPI Suite	2.61	EPI Suite	0.789	EpiK	
			317.32	EPI Suite	2.75	EPI Suite	-0.424	EpiK	3.26E+01
			403.40	EPI Suite	2.5	EPI Suite	0.612	EpiK	3.24E+01
			223.23	EPI Suite	1.7	EPI Suite	11.902	EpiK	2.17E+01
			300.36	EPI Suite	4.14	EPI Suite	0.641	EpiK	4.12E+01
			276.92	EPI Suite	3.39	EPI Suite	5.26	EpiK	7.87E+00
Y			138.00	EPI Suite	0.36	EPI Suite	6.3	Wikipedia	

	235.30	EPI Suite	2.14	EPI Suite	9.276	EpiK	2.44E+01
	221.65	EPI Suite	0.76	EPI Suite	-0.004	EpiK	1.87E+00
	239.70	EPI Suite	2.5	EPI Suite	0.51	EpiK	3.04E+00
	249.68	EPI Suite	0.64	EPI Suite	-2.203	EpiK	1.07E+01

Reference	Human Fut	Reference	Human Fab	Reference	Human Rbp	Reference	Rat Clint	Reference	Rat Fub	al. Human Values Metabolism 1 uM
Wetmore ∈	0.13497	Wetmore et al. 2012					59.28	Wetmore ∈	0.19229	84.7136
Wetmore ∈	0.00395	Wetmore et al. 2012					42.06	Wetmore ∈	0.18232	31.5146
Wetmore ∈	0.25708	Wetmore et al. 2012					2.326	Wetmore ∈	0.71812	19.2933
Wetmore ∈	0.03201	Wetmore et al. 2012					12.038	Wetmore ∈	0.04664	17.2820
Wetmore ∈	0.69225	Wetmore et al. 2012					14.966	Wetmore ∈	0.37532	27.2736
Wetmore ∈	0.10856	Wetmore et al. 2012					2.312	Wetmore ∈	0.11946	1.5380
Wetmore ∈	0.03671	Wetmore et al. 2012					1.5696	Wetmore ∈	0.02760	3.7881
Wetmore ∈	0.23177	Wetmore et al. 2012					5.002	Wetmore ∈	0.07926	19.9210
Wetmore ∈	0.88531	Wetmore et al. 2012					11.178	Wetmore ∈	0.74850	13.7157
Wetmore ∈	0.02956	Wetmore et al. 2012					46.44	Wetmore ∈	0.04829	1.0246
Wetmore ∈	0.06539	Wetmore et al. 2012					81.88	Wetmore ∈	0.10721	19.5295
Wetmore ∈	0.06756	Wetmore et al. 2012					1.7096	Wetmore ∈	0.09361	5.3997
Wetmore ∈	0.01673	Wetmore et al. 2012					11.412	Wetmore ∈	0.07924	43.8884
Wetmore ∈	0.02909	Wetmore et al. 2012					1.9488	Wetmore ∈	0.00927	3.9849
Wetmore ∈	0.02837	Wetmore et al. 2012					2.142	Wetmore ∈	0.16446	4.9203
Wetmore ∈	0.00417	Wetmore et al. 2012					20.62	Wetmore ∈	0.00946	14.2471
Wetmore ∈	0.04105	Wetmore et al. 2012								2.0771
Wetmore ∈	0.06687	Wetmore et al. 2012								5.2404
Wetmore ∈	0.48092	Wetmore et al. 2012								0.7456
Wetmore ∈	0.10035	Wetmore et al. 2012								6.2094
Wetmore ∈	0.21368	Wetmore et al. 2012								32.6341
Wetmore ∈	0.04763	Wetmore et al. 2012								32.3940
Wetmore ∈	0.19710	Wetmore et al. 2012								21.6613
Wetmore ∈	0.83603	Wetmore et al. 2012								41.1507
Wetmore ∈	0.50008	Wetmore et al. 2012								7.8663
Wetmore ∈	0.90583	Wetmore et al. 2012								0.1976

Wetmore ϵ	0.17504	Wetmore et al. 2012		24.4088
Wetmore ϵ	0.42733	Wetmore et al. 2012	0.48892	1.8714
Wetmore ϵ	0.17336	Wetmore et al. 2012		3.0380
Wetmore ϵ	0.52851	Wetmore et al. 2012		10.7271

Wetmore et al. and Rotroff et al.
Human Values

Metabolism

10 uM
47.2104
2.6939
25.0375
5.8173
9.6124
1.5875
0.0288
14.3384
11.6074
-3.2673
9.2460
1.4207
8.9220
-0.6018
-8.6644
8.6690
9.4356
3.6216
0.3636
0.4766
12.2981
14.2876
10.0244
5.6355
4.2829
0.5997

8.7904
3.8752
2.6120
10.2263

Compound	CAS	Clint (hepatocyte)	Clint (Microsomes)	CLh	fub	Reference
Alprazolam	28981-97-7	33	180	19	0.35	Unpublished
Alprenolol	#N/A	36	80	24	1	6
Aminopyrine	#N/A	4.1	6.6	2	1	6
Antipyrine	60-80-0	0.8	3.6	1.4	1	6
Bosentan	#N/A	ND	40	14	0.02	7
Butylbarbitone	#N/A	1.9	ND	1.2	0.6	6
Caffeine	58-08-2	1.4	4.3	3	1	3
Carbamazepine	298-46-4	ND	2.2	0.78	1	6
Chlordiazepoxide	#N/A	8	4.6	2.5	0.15	Unpublished
Clobazam	#N/A	27	110	7.9	0.21	Unpublished
Clonazepam	#N/A	15	18	4.9	0.21	Unpublished
Codeine	#N/A	290	ND	23	1	6
Dextromethorphan	#N/A	110	450	20	0.45	15
Diazepam	53320-84-6	82	81	17	0.15	3
Diclofenac	15307-86-5	110	110	3.6	0.017	16
Diltiazem	33286-22-5	ND	250	12	0.198	8
Dofetilide	#N/A	ND	18	7.8	0.47	3
Ethoxybenzamide	#N/A	1.3	4.5	2.2	0.5	6
Ethoxycoumarin	#N/A	(ECOD)	26	50	14	0.22
Felodipine	#N/A	ND	500	5.9	0.07	6
FK1052	129299-72	ND	550	13	0.025	8
FK480	150408-73	ND	130	8.6	0.016	8
Flunitrazepam	#N/A	46	89	12	0.25	Unpublished
Heptabarbitone	#N/A	29	ND	16	0.62	6
Heptylbarbitone	#N/A	33	ND	5.2	0.066	6
Hexobarbitone	#N/A	ND	330	16	0.62	6
Hexylbarbitone	#N/A	21	ND	4.9	0.18	6
Ibuprofen	15687-27-1	ND	29	0.6	0.01	6
Imipramine	50-49-7	990	4500	22	0.107	6
Indinavir	#N/A	ND	70	16	0.3	9,10
Ketoconazole	#N/A	55	42	6.4	0.062	17
L-738,372	#N/A	ND	4.3	3.8	1	11
Lignocaine	#N/A	ND	200	24	1	6
Loxtidine	#N/A	11	ND	5.5	0.96	6
Metoprolol	#N/A	ND	44	22	1	6
Midazolam	59467-70-8	74	81	11	0.07	Unpublished
Mofarotene	#N/A	ND	130	4	0	7
Nicardipine	#N/A	ND	6700	13	0.084	8
Nilvadipine	#N/A	ND	36000	14	0.013	8
Omeprazole	#N/A	ND	330	13	0.16	8
Ondansetron	#N/A	110	320	15	0.25	3
Oxodipine	#N/A	ND	5.3	4.5	1	6
Phenacetin	#N/A	78	33	21	1	6
Phenytoin	#N/A	37	35	7	0.2	3
Propranolol	#N/A	1800	4300	25	0.72	12,13
R-acenocoumarol	66556-77-2	ND	11	0.33	0.012	3
R-warfarin	#N/A	ND	7	0.13	0.023	3
S-acenocoumarol	66556-78-3	ND	30	1.2	0.009	3
S-warfarin	#N/A	ND	2.1	0.046	0.011	3
Tacrine	#N/A	1000	ND	21	1	3
Tolbutamide	64-77-7	1.6	6.2	0.12	0.08	3
Triazolam	28911-01-5	140	130	21	0.28	Unpublished
YM796	#N/A	ND	870	24	0.694	14
Zolpidem	82626-48-0	ND	83	9.1	0.146	8

Compounc	CAS	Chemical (	Fub	Clint Predicted	Clint Observed	CLh Predic	CLh observ
Acetamino	103-90-2	N	0.79	2.53	6.71	1.81	4
Antipyrine	60-80-0	N	0.94	0.82	0.69	0.74	0.6
Antipyrine	60-80-0	N	0.94	0.23	0.6	0.212	0.55
Bosentan	#N/A	A	0.02	0.67	42.1	0.0134	3.65
Buspirone	#N/A	B	0.05	613.8	1582	12.11	19.2f
Caffeine	58-08-2	N	0.685	2.89	2.25	2.07	1.4
Caffeine	58-08-2	N	0.83	0.37	1.4	0.303	1.05
Carvedilol	#N/A	B	0.03	281.58	521.97	5.87	8.7
Chlorprom	50-53-3	B	0.03	230.33	502.92	5.14	8.6
Cimetidine	51481-61-9	B	0.9	3.35	4.23	2.62	3.2
Cyclospori	#N/A	Ab	N	0.04	13.46	155.27	0.52
Desipramir	50-47-5	B	0.17	127.16	124.92	10.39	10.3
Diazepam	53320-84-0	N	0.012	6.41	31.29	0.08	0.43
Diazepam	53320-84-0	N	0.012	3.44	42.78	0.04	0.5
Diclofenac	15307-86-5	A	0.0055	618.36	2083.46	2.92	7.33
Diflunisal	#N/A	A	0.0053	9.86	34.8	0.05	0.18
Diltiazem	33286-22-5	B	0.22	77.81	143.61	10.7	12.8
Diltiazem	33286-22-5	B	0.22	8.45	205.44	1.7	13.35
Etodolac	#N/A	A	0.02	81.2	82.84	1.28	1.31
Felodipine	#N/A	N	0.004	72.08	6111.11	0.28	11
Fenoprofei	#N/A	A	0.01	56.52	216.15	0.47	1.69
FK079	#N/A	N	0.0288	56.38	636	0.91	4.4
FK1052	129299-72	N	0.021	32.38	1570	0.64	12.2
FK480	150408-73	N	0.008	49.41	336	0.4	2.4
Furosemid	#N/A	A	0.029	5.95	22.85	0.14	0.59
Gemfibrozi	#N/A	A	0.005	325.82	773.37	1.43	3.09
Glipizide	#N/A	A	0.02	7.13	60.52	0.12	0.96
Granisetro	#N/A	B	0.7	29.72	35.14	10.17	11
Ibuprofen	15687-27-1	A	0.0182	71.34	82.7	0.64	1.4
Imipramine	50-49-7	B	0.1	92.57	125.59	6.33	9.46
Indometha	#N/A	A	0.02	27.13	145.77	0.46	2.24
Irbesartan	#N/A	A	0.04	58.75	131.31	1.93	3.85
Ketoprofer	#N/A	A	0.02	22.44	103.95	0.52	2.22
Lidocaine	#N/A	B	0.3	24.61	100.68	5.34	15
Lorazepan	#N/A	N	0.094	1.16	12.38	0.11	1.1
Lorazepan	#N/A	N	0.094	1.24	16.71	0.12	1.45
Methylprec	#N/A	N	0.23	37.08	52.17	5.98	7.5
Metoprolol	#N/A	B	0.747	13.87	40.62	5.95	12.15
Mibefradil	#N/A	B	0.005	41.3	4888.9	0.2	11
Midazolam	59467-70-8	N	0.04	40.08	246.27	1.48	6.6
Midazolam	59467-70-8	N	0.04	25.74	599.04	0.98	10.9
Montelukas	#N/A	A	0.0009	96.27	1495.15	0.09	1.27
Naloxone	#N/A	B	0.56	150.28	924.35	16.16	19.5f
Nifedipine	#N/A	N	0.05	32.6	253.7	1.46	7.8
Ondansetr	#N/A	N	0.68	5.23	12.4	3	5.9
Oxaprozin	#N/A	A	0.0007	24.4	100.36	0.02	0.07
Oxazepam	#N/A	N	0.03	8.23	38.8	0.24	1.1
Oxazepam	#N/A	N	0.03	1.52	36.94	0.046	1.05
Phenacetir	#N/A	N	0.594	76.01	212.5	13.9	19.2f
Pindolol	#N/A	B	0.9	9.28	5.91	5.89	4.2
Prazosin	#N/A	N	0.07	6.16	42.23	0.45	2.7
Prednisolo	#N/A	N	0.26	35.54	59.22	6.32	8.7
Propranolc	#N/A	B	0.12	59.2	291.87	6.46	16.11

Propranolc	#N/A	B	0.1	21.67	388.75	1.96	13.2
Quinidin	#N/A	B	0.15	12.95	48.63	1.73	5.33
Ranitidine	#N/A	B	0.77	3	4.4	2.07	2.9
Ritonavir	#N/A	N	0.0148	30.51	86.26	0.44	1.2
Sildenafil	#N/A	N	0.04	24.35	214.29	0.93	6
Tenoxicam	59804-37-4	A	0.0164	8.77	4.46	0.14	0.073
Theophyllin	#N/A	N	0.4	1.67	1.68	0.65	0.65
Theophyllin	#N/A	N	0.4	0.35	1.55	0.141	0.6
Timolol	#N/A	B	0.4	6.55	22.75	2.32	9.17
Tiprolidin	#N/A	B	0.1	39.61	133.33	3.31	8
Tolbutamic	64-77-7	A	0.04	6.91	8.99	0.24	0.3
Tolcapone	#N/A	A	0.0018	6.41	1650.32	0.074	2.65
Troglitazor	97322-87-7	A	0.0017	306.36	10000	0.51	9
Verapamil	52-53-9	B	0.115	278.92	388.33	11.65	14.66
Warfarin	81-81-2	A	0.018	3.69	8.22	0.07	0.16
Warfarin	81-81-2	A	0.018	0.34	6.02	0.006	0.12

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Compound	CAS	logP	logD	logMA	pKa	Compound	Fub	Reference
Acebutolol	68107-81-3	1.71	-0.51	1.4	9.7	B	0.79	4
Acebutolol	37517-30-9	1.71	-0.51	1.4	9.7	B	0.73	4
Alprazolam	28981-97-7	2.12	2.12	2.5	2.4	B	0.35	5
Barbital	#N/A	0.65	0.5	0.36	7.8	A	0.93	1
Betaxolol-F	#N/A	2.591	0.63	2.2	9.4	B	0.53	4
Betaxolol-S	#N/A	2.591	0.63	2.2	9.4	B	0.54	4
Cefazolin	#N/A	-0.58	-3.58	0.9	2.2	A	0.14	1
Ceftazidim	#N/A	-1.36	-4.35	1	4.7	A	0.9	1
Chlorprom	50-53-3	5.41	3.19	3.63	9.7	B	0.1	1
Clomipram	#N/A	4.82	2.34	3.23	10	B	0.07	1
Clozapine	5786-21-0	3.23	2.88	2.95	7.5	B	0.5	1
Cotinine	486-56-6	-0.253	-0.25	0.3	8.1	B	0.97	1
Diazepam	53320-84-6	2.82	2.82	2.76	3.3	B	0.15	5
Dicloxacilli	#N/A	2.91	-0.06	1.85	3.3	A	0.03	5
Digoxin	#N/A	1.26	1.26	1.48		N	0.87	1
Fleroxacin	#N/A	0.24	0.24	1.3		Z	0.75	1
Flunitrazep	#N/A	2.6	2.6	2.5	1.8	B	0.25	5
Glycyrrhizi	#N/A	2.8	-0.19	0.6	5.3	A	0.05	1
Haloperido	#N/A	4.3	2.99	3.72	8.7	B	0.23	1
Hexobarbit	56-29-1	0.873	0.87	0.95	8.1	A	0.7	1
Imipramine	50-49-7	4.8	2.75	3	9.5	B	0.24	3
Lidocaine	#N/A	2.44	1.74	1.8	8	B	0.38	3
Methotrexa	#N/A	-1.85	-4.77	1.18	1.3	M	0.5	1
Metoprolol	#N/A	1.88	-0.34	1.5	9.7	B	0.8	4
Metoprolol	#N/A	1.88	-0.34	1.5	9.7	B	0.81	4
Midazolam	59467-70-8	2.74	2.69	2.9	5.8	B	0.07	5
Nicotine	54-11-5	1.17	0.63	0.7	7.8	B	0.84	3
Norfloxacir	#N/A	-1.03	-1.03	0.95		Z	0.58	1
Oxprenolol	#N/A	2.181	-0.2	2.3	9.9	B	0.24	4
Oxprenolol	#N/A	2.181	-0.2	2.3	9.9	B	0.36	4
Pefloxacin	#N/A	0.27	0.27	1.08		Z	0.8	1
Penicillin	#N/A	-4.623	-4.62	1.04	2.8	A	0.15	1
Pentazocir	#N/A	3.315	2.18	2.6	8.5	B	0.46	3
Pentobarbi	#N/A	2.1	2.02	1	8.1	A	0.66	2
Phenobarb	50-06-6	1.47	1.14	0.8	7.35	A	0.78	2
Phenytoin	#N/A	2.47	2.38	2	8.06	A	0.06	2
Pindolol-R	#N/A	1.75	-0.12	2.2	9.3	B	0.51	4
Pindolol-S	#N/A	1.75	-0.12	2.2	9.3	B	0.76	4
Pipemidic a	#N/A	-2.15	-2.15	1.43		Z	0.85	1
p-Phenylbe	#N/A	2.813	2.81	0.3	4.2	A	0.03	1
Prednisolo	#N/A	1.62	1.62	1.9		N	0.23	1
Procainam	#N/A	0.88	-0.81	0.95	9.1	B	0.92	3
Promazine	#N/A	4.55	2.86	3.82	9.1	B	0.05	1
Promethaz	#N/A	4.81	3.12	3.2	9.1	B	0.22	1
Propranolc	#N/A	3.48	1.52	2.95	9.4	B	0.08	6
Propranolc	#N/A	3.48	1.43	3	9.5	B	0.017	4
Propranolc	#N/A	3.48	1.43	3	9.5	B	0.127	4
Pyridostigr	#N/A	-3.733	-3.73	1.04	10	B	0.5	1
Quinidine	56-54-2	3.44	2.22	2.3	8.6	B	0.33	3
Salicylic ac	#N/A	2.26	-0.72	0.6	3	A	0.4	1
Tetracyclin	#N/A	-1.3	-3.08	1.7	3.6	M	0.5	1
Thiopental	#N/A	2.85	2.6	1.58	7.5	A	0.25	2
Thioridazin	#N/A	5.9	3.85	3.81	9.5	B	0.01	1

Timolol-S	#N/A	1.83	0.05	1.5	9.2	B	0.63	4
Tolbutamic	64-77-7	2.34	0.47	1.41	5.5	A	0.24	1
trans-Retir	#N/A	2.853	2.85	1.73	6.4	A	0.1	1
Trihexylph	#N/A	6.3	3.84	2.41	10	B	0.37	1
Valproic ac	#N/A	2.75	0.29	1.04	4.8	A	0.22	1
Verapamil	52-53-9	3.79	2.66	3.2	8.5	B	0.05	3

Compounc	CAS	Fu,hep fraction	Cluint,iv ml/min/kg	Well Stirre	Dispersion	Rat Clint,iv ml/min/kg	Clint,iv SD ml/min/kg	Cluint,iv ch	Clint ml/min/10^
FK1052	129299-72	0.244	2600	10.7	3.1	635	24	2602.5	0.1322916
FK480	150408-73	0.202	1120	5.1	3.4	226	13	1118.8	0.0470833
Diazepam	53320-84-6	0.705	489	1.6	1	345	39	489.4	0.071875
Diltiazem	33286-22-5	0.529	6240	0.3	0.1	3300	1330	6238.2	0.6875
Quinotolas	101193-40	0.937	58.3	9.8	8.4	54.6	3.4	58.3	0.011375
Troglitazor	97322-87-7	0.217	4280	15.8	10.2	928	9	4276.5	0.1933333
FK079		0.713	6.66	4.3	4.2	4.75	0.14	6.7	0.0009895
Zidovudine	30516-87-1	1	14.3	1.4	1.3	14.3	1	14.3	0.0029791
Acetamino	103-90-2	0.933	76.4	0.7	0.5	71.3	10.9	76.4	0.0148541

	Rat	Human
Number of	120000000	120000000
Liver weigh	40	25.7
Liver blooc	55.2	20.7
Concentra	uM	1

120000000

Clint SD ml/min/10^6 cell	Fabsorbed	Fub,p	RatioB:P	Human Clint,iv ml/min/kg	Clint,iv SD ml/min/kg	Fabsorbed	Fub,p	RatioB:P	Clint ml/min/10^
0.005	0.95	0.03	1.21	7.89	8.44	0.016	0.78		0.00256
0.0027083	0.7	0.01	0.626	9.98	11.6	0.005	0.6		0.00324
0.008125	1	0.137	1.04	4.14	3.24	0.032	1.04		0.00134
0.2770833	1	0.184	0.93	72.4	67.9	0.22	1		0.02348
0.0007083	1	0.033	0.65			0.59	0.59		
0.001875	0.718	0.00092	0.594	67.4	39.1	0.548	0.548		0.02185
0.0000291	1	0.06	0.63	40.2	18.6	0.059	0.59		0.01304
0.0002083	1	0.786	1	9.87	5.52	0.098	0.98		0.00320
0.0022708	1	0.82	1	2.39	2.29	0.79	1		0.00077

Clint SD ml/min/10^6 cell
0.00274
0.00376
0.00105
0.02202
0.01268
0.00603
0.00179
0.00074

Compouund	CAS	pKa	Koc	LogKow	Kd l/kg	Dow
Paracetamol	103-90-2	9.4	61.7	0.46	0.4139	2.8721
Metformin hydroch	1115-70-4	12.4	105.8	-2.64	0.0003	0.0023
Ibuprofen	15687-27-	4.9	394	3.5	453.79	2.0404
Amoxycillin	26787-78-0		865	0.87	1.06	
Sodium valproate	1069-66-5		24.1	-0.85	0.02	
Sulphasalazine	599-79-1		1.84E+03	3.81	926.51	
Mesalazine	89-57-6		10	0.98	1.37	
Carbamazepine	298-46-4	13.9	3.87E+03	2.25	25.52	177.8279
Ferrous sulphate	7782-63-0		14.6	-0.37	0.06	
Ranitidine hydroch	66357-59-	3.5				
Cimetidine	51481-61-	6.8	690	0.4	0.36	0.9718
Naproxen	22204-53-	4.2	349	3.18	217.2	2.1349
Atenolol	29122-68-	9.2	148	0.16	0.21	1.4355
Oxytetracycline	79-57-2	3.3	97.2	-0.9	0.02	2.34E-05
Erythromycin	114-07-8	8.9	10	3.06	164.76	1133.2149
Diclofenac sodium	15307-79-	4.2	833	0.7	0.72	0.0076
Flucloxacillin sodi	1847-24-1					
Phenoxymethylpe	87-08-1		177	2.09	17.65	
Allopurinol	315-30-0	9.3	19.4	-0.55	0.04	0.2805
Diltiazem hydroch	33286-22-	7.7	9.50E+03	2.7	71.92	417.821
Gliclazide	21187-98-4		1.27E+04	2.12	18.92	
Aspirin	50-78-2	3.5	10	1.19	2.22	0.0048
Quinine sulphate	804-63-7		1.85E+08	5.4	36045.57	
Mebeverine hydro	2753-45-9		6.66E+05	3.82	948.1	
Mefenamic acid	61-68-7		461	5.12	18916.98	

Compound	CAS	Fraction U	Blood-to-P	Normal Clearance (ml/min/kg) Plasma	Blood	References
Chlorprom	50-53-3	0.05	0.78	8.6	11	Dahl and Strandjard, 1974; Maxwell et al., 1972; L
Propafenon	54063-53-5	0.04	0.7	13	19	Bryson et al., 1993
Verapamil	52-53-9	0.1	0.77	15	19	Eichelbaum et al., 1984
Diphenhyd	58-73-1	0.22	0.65	6.2	9.5	Blyden et al., 1986
Lorcainide	59729-31-6	0.15	0.77	14	18	Somani et al., 1987; Klotz et al., 1978
Diltiazem	33286-22-5	0.22	1	12	12	Echizen and Eichelbaum, 1986; Smith et al., 1983
Amitriptylin	50-48-6	0.05	0.86	10	12	Schulz et al., 1983
Desipramin	50-47-5	0.18	0.96	12	12	Brosen and Gram, 1988
Imipramine	50-49-7	0.1	1.1	13	12	Sallee and Pollack, 1990; Abernathy et al., 1985
Ketamine	6740-88-1	0.88	0.82	16	20	White et al., 1985
Quinidine	56-54-2	0.13	0.92	2.5	2.7	Greenblatt et al., 1977; Rakhit et al., 1984; Hughes
Clozapine	5786-21-0	0.05	0.87	2.5	2.9	Cheng et al., 1988
Dexameth	50-02-2	0.32	0.93	3.5	3.8	Tseui et al., 1979; Peterson et al., 1983
Prednison	53-03-2	0.25	0.83	4.1	4.9	Schalm et al., 1977
Diazepam	53320-84-6	0.013	0.71	0.4	0.6	Greenblatt et al., 1980; Maguire et al., 1980
Midazolam	59467-70-8	0.05	0.53	4.6	8.7	Heizmann et al., 1983
Methoxsal	298-81-7	0.09	0.67	12	18	Billard et al., 1995; Pibouin et al., 1987
Alprazolam	28981-97-7	0.32	0.78	0.59	0.76	Smith et al., 1984
Triazolam	28911-01-5	0.1	0.62	2.9	4.7	Smith et al., 1987
Zolpidem	82626-48-0	0.08	0.76	4.3	5.7	Durand et al., 1992
Diclofenac	15307-86-5	0.005	0.55	4.2	7.6	Willis et al., 1979; Chan et al., 1987
Ibuprofen	15687-27-1	0.01	0.55	0.8	1.5	Martin et al., 1990
Tolbutamic	64-77-7	0.04	0.55	0.2	0.36	Balant, 1981; Scott and Poffenbarger, 1979
Warfarin	81-81-2	0.01	0.55	0.045	0.081	O'Reilly, 1972
Tenidap	120210-48	0.0007	0.56	0.058	0.1	Gardner et al., 1995
Tenoxicam	59804-37-4	0.009	0.67	0.02	0.03	Heintz et al., 1984
Amobarbit	57-43-2	0.39	1.5	0.53	0.35	Bachmann, 1987; Sawada et al., 1985
Hexobarbit	56-29-1	0.53	1	3.6	3.6	Breimer et al., 1975; Sawada et al., 1985
Methohexit	151-83-7	0.27	0.7	11	16	Breimer, 1976; Gillis et al., 1976

All clearance values from the literature were from i.v. dosing. In the case of dependence of clearance on genetic poly
excluded. Nonrenal clearance values were calculated by: Clnon-renal 5 Cltotal z (1 2 fraction of the dose excreted un
b Chlorpromazine clearance values from i.m. dose; assumes complete absorption from i.m. route.
c Denotes blood-to-plasma ratios that were unavailable in the scientific literature. Values were determined in duplica
for 45 min.

und, 1980

et al., 1975

morphism of drug-metabolizing enzymes, data from poor metabolizers was changed in urine).

te after incubation of drug at 1.0 mg/mL in whole blood at ambient temperature

Compound	CAS
Picloram	1918-02-1
Cloprop	101-10-0
Quinotolast	101193-40-2
Flumioxazin	103361-09-7
Acetaminophen	103-90-2
Paracetamol	103-90-2
Imazapic	104098-48-8
Resmethrin	10453-86-8
Carbendazim	10605-21-7
Trimethyltin	1066-45-1
Sodium valproate	1069-66-5
Toluene	108-88-3
Diethylene glycol	111-46-6
Metformin hydrocl	1115-70-4
Cycloate	1134-23-2
MGK	113-48-4
Erythromycin	114-07-8
Endosulfan	115-29-7
Dicofol	115-32-2
Novaluron	116714-46-6
Diethyhexyl phtha	117-81-7
Hexachlorobenze ne	118-74-1
Tebufenpyrad	119168-77-3
Dichlobenil	1194-65-6
Fipronil	120068-37-3
Tenidap	120210-48-2
Clorophene	120-32-1
Paraben	120-47-8
Cyprodinil	121552-61-2
Malathion	121-75-5
Fenitrothion	122-14-5
Rimsulfuron	122931-48-0
Quinoxyfen	124495-18-7
Trimethadione	127-48-0
Pyrene	129-00-0
FK1052	129299-72-5
dimethyl phthalate	131-11-3
Ethoprop	13194-48-4
Rifampicin	13292-46-1
Flutamide	13311-84-7
Isoxaflutole	141112-29-0
Flufenacet	142459-58-3

Domoic acid	14277-97-5
FK480	150408-73-4
FK480	150408-73-4
Potassium cyanide	151-50-8
Methohexital	151-83-7
Napropamide	15299-99-7
Diclofenac sodium	15307-79-6
Diclofenac	15307-86-5
Ibuprofen	15687-27-1
Trifluralin	1582-09-8
Prometon	1610-18-0
Foramsulfuron	173159-57-4
Indoxacarb	173584-44-6
Pyraclostrobin	175013-18-0
Flucloxacillin sodi	1847-24-1
Nitrapyrin	1929-82-4
Oxadiazon	19666-30-9
Trifloxysulfuron-s	199119-58-9
Mesosulfuron-me	208465-21-8
Gliclazide	21187-98-4
Molinate	2212-67-1
Naproxen	22204-53-1
Tri-allate	2303-17-5
Phosalone	2310-17-0
Oxamyl	23135-22-0
Etridiazole	2593-15-9
Ethofumesate	26225-79-6
Chloroneb	2675-77-6
Amoxycillin	26787-78-0
Mebeverine hydr	2753-45-9
Diquat	2764-72-9
Thiobencarb	28249-77-6
S-Bioallethrin	28434-00-6
Triazolam	28911-01-5
Alprazolam	28981-97-7
Prodiamine	29091-21-2
Atenolol	29122-68-7
Chlorpyrifos	2921-88-2
Pirimiphos-methyl	29232-93-7
Methyl Parathion	298-00-0
Disulfoton	298-04-4
Carbamazepine	298-46-4
Methoxsalen	298-81-7

Gossypol	303-45-7
Ochratoxin A	303-47-9
Zidovudine	30516-87-1
Paraoxon	311-45-5
Allopurinol	315-30-0
Diltiazem	33286-22-5
Diltiazem hydroch	33286-22-5
Diazinon	333-41-5
Triclosan	3380-34-5
Iprodione	36734-19-7
Acebutolol-S	37517-30-9
Pendimethalin	40487-42-1
Oxyfluorfen	42874-03-3
Triadimefon	43121-43-3
Difenzoquat meth	43222-48-6
Genistein	446-72-0
Cotinine	486-56-6
Cotinine	486-56-6
Fenofibrate	49562-28-9
Dexamethasone	50-02-2
Phenobarbital	50-06-6
Vinclozolin	50471-44-8
Desipramine	50-47-5
Amitriptyline	50-48-6
Imipramine	50-49-7
Chlorpromazine	50-53-3
Aspirin	50-78-2
Wyeth-14643	50892-23-4
Piperonyl butoxid	51-03-6
Metolachlor	51218-45-2
Diclofop-methyl	51338-27-3
Cimetidine	51481-61-9
Verapamil	52-53-9
Permethrin	52645-53-1
Deltamethrin	52918-63-5
Prednisone	53-03-2
Diazepam	53320-84-6
Propafenone	54063-53-5
Nicotine	54-11-5
Chlorethoxyfos	54593-83-8
Triadimenol	55219-65-3
Ethalfluralin	55283-68-6
Fenthion	55-38-9
Chlorpyrifos-meth	5598-13-0

Hexobarbital	56-29-1
Parathion	56-38-2
Quinidine	56-54-2
Coumaphos	56-72-4
Glycidamide	5694-00-8
Amobarbital	57-43-2
Metalaxyl	57837-19-1
Clozapine	5786-21-0
Caffeine	58-08-2
d-cis,trans- Alleth	584-79-2
Diphenhydramine	58-73-1
Lindane	58-89-9
Midazolam	59467-70-8
Lorcainide	59729-31-6
Tenoxicam	59804-37-4
Sulphasalazine	599-79-1
Antipyrine	60-80-0
Lead acetate	6080-56-4
Oxytetracycline di	6153-64-6
Mefenamic acid	61-68-7
Flumetralin	62924-70-3
Clofibrate	637-07-0
Tolbutamide	64-77-7
Esfenvalerate	66230-04-4
Ranitidine hydroc	66357-59-3
Fenoxaprop-ethyl	66441-23-4
R-acenocoumarol	66556-77-2
S-acenocoumarol	66556-78-3
Ketamine	6740-88-1
Acebutolol-R	68107-81-3
Hexachlorophene	70-30-4
Propanil	709-98-8
Methoxychlor	72-43-5
Prometryn	7287-19-6
Clofentezine	74115-24-5
EPTC	759-94-4
Fentin hydroxide	76-87-9
Tetramethrin	7696-12-0
Lactofen	77501-63-4
Ferrous sulphate	7782-63-0
Tribufos	78-48-8
Hexythiazox	78587-05-0
Fluazifop-P-butyl	79241-46-6

Tefluthrin	79538-32-2
Oxytetracycline	79-57-2
Quinine sulphate	804-63-7
Fluroxypyr-mepty	81406-37-3
Warfarin	81-81-2
Zolpidem	82626-48-0
Quintozene	82-68-8
Diniconazole	83657-18-5
Rotenone	83-79-4
Quinclorac	84087-01-4
Dibutyl phthalate	84-74-2
Phenanthrene	85-01-8
Phenoxymethylpe	87-08-1
Dimethenamid	87674-68-8
Cinmethylin	87818-31-3
Pentachlorophenol	87-86-5
Mesalazine	89-57-6
Prosulfuron	94125-34-5
MCPA	94-74-6
Tebupirimfos	96182-53-5
pyridaben	96489-71-3
Troglitazone	97322-87-7
Dithiopyr	97886-45-8
Fosthiazate	98886-44-3
Dichloran	99-30-9
Alprenolol	#N/A
Aminopyrine	#N/A
Barbital	#N/A
Betaxolol-R	#N/A
Betaxolol-S	#N/A
Bosentan	#N/A
Buspirone	#N/A
Butylbarbitone	#N/A
Carbamazepine	#N/A
Carvedilol	#N/A
Cefazolin	#N/A
Ceftazidime	#N/A
Chlordiazepoxide	#N/A
Chlorpromazine	#N/A
Clobazam	#N/A
Clomipramine	#N/A
Clonazepam	#N/A
Codeine	#N/A

Cyclosporin	#N/A
Desipramine	#N/A
Dextromethorphan	#N/A
Dicloxacillin	#N/A
Diflunisal	#N/A
Digoxin	#N/A
Dofetilide	#N/A
Ethoxybenzamide	#N/A
Ethoxycoumarin	#N/A
Etodolac	#N/A
Felodipine	#N/A
Fenoprofen	#N/A
FK079	#N/A
Fleroxacin	#N/A
Flunitrazepam	#N/A
Furosemide	#N/A
Gemfibrozil	#N/A
Glipizide	#N/A
Glycyrrhizin	#N/A
Granisetron	#N/A
Haloperidol	#N/A
Heptabarbitone	#N/A
Heptylbarbitone	#N/A
Hexobarbitone	#N/A
Hexylbarbitone	#N/A
Indinavir	#N/A
Indomethacin	#N/A
Irbesartan	#N/A
Ketoconazole	#N/A
Ketoprofen	#N/A
L-738,372	#N/A
Lidocaine	#N/A
Lignocaine	#N/A
Lorazepam	#N/A
Loxtidine	#N/A
Methotrexate	#N/A
Methylprednisolon	#N/A
Metoprolol	#N/A
Metoprolol-R	#N/A
Metoprolol-S	#N/A
Mibefradil	#N/A
Mofarotene	#N/A
Montelukast	#N/A
Naloxone	#N/A

Nicardipine	#N/A
Nifedipine	#N/A
Nilvadipine	#N/A
Norfloxacin	#N/A
Omeprazole	#N/A
Ondansetron	#N/A
Ondansetron	#N/A
Oxaprozin	#N/A
Oxazepam	#N/A
Oxodipine	#N/A
Oxprenolol-R	#N/A
Oxprenolol-S	#N/A
Pefloxacin	#N/A
Penicillin	#N/A
Pentazocine	#N/A
Pentobarbital	#N/A
Phenacetin	#N/A
Phenytoin	#N/A
Phenytoin	#N/A
Pindolol	#N/A
Pindolol-R	#N/A
Pindolol-S	#N/A
Pipemidic acid	#N/A
p-Phenylbenzoic a	#N/A
Prazosin	#N/A
Prednisolone	#N/A
Procainamide	#N/A
Promazine	#N/A
Promethazine	#N/A
Propranolol	#N/A
Propranolol-R	#N/A
Propranolol-S	#N/A
Pyridostigmine	#N/A
Ranitidine	#N/A
Ritonavir	#N/A
R-warfarin	#N/A
Salicylic acid	#N/A
Sildenafil	#N/A
S-warfarin	#N/A
Tacrine	#N/A
Tenoxicam	#N/A
Tetracycline	#N/A
Theophylline	#N/A
Thiopental	#N/A

Thioridazine	#N/A
Timolol	#N/A
Timolol-S	#N/A
Tiprolidin	#N/A
Tolcapone	#N/A
trans-Retinoic aci	#N/A
Trihexylphenidil	#N/A
Valproic acid	#N/A
YM796	#N/A

Source	Compound name	CAS #	vLiver Table?	logP	ion	pKa1	pKa2	fup	Rbp
									Uchimura (2010) Biopharm Drug Dispos 31(5-6):286-297
EPA/Hamner	2,4-D	94-75-7		630.96	mpa	2.73	NA	0.040	2.11
EPA/Hamner	Acetochlor	34256-82-1		13803.84	neu	NA	NA	0.160	0.87
EPA/Hamner	Acifluorfen	50594-66-6		35481.34	mpa	2.03	NA	0.005	0.64
EPA/Hamner	Alachlor	15972-60-8		3890.45	neu	NA	NA	0.133	0.85
EPA/Hamner	Ametryn	834-12-8		398.11	mpb	5.74	NA	0.005	0.64
EPA/Hamner	Bensulide	741-58-2		2818.38	mpb	10.18	NA	0.006	0.65
EPA/Hamner	Bentazone	25057-89-0		5.75	mpb	8.02	NA	0.020	0.71
EPA/Hamner	Bisphenol-A	80-05-7		10964.78	dpa	9.78	10.39	0.068	0.79
EPA/Hamner	Boscalid	188425-85-6		83176.38	mpa	10.70	NA	0.032	0.74
EPA/Hamner	Carbaryl	63-25-2		288.40	mpa	14.77	NA	0.692	0.85
EPA/Hamner	Chloridazon	1698-60-8		12.88	neu	NA	NA	0.427	0.92
EPA/Hamner	Chlorpropham	101-21-3		7943.28	mpa	5.22	NA	0.005	0.64
EPA/Hamner	Cyclanilide	113136-77-9		263.03	dpa	3.56	12.61	0.984	0.61
EPA/Hamner	Cyproconazole	94361-06-5		707.95	zwi	2.26 (base)	13.34 (acid)	0.109	0.84
EPA/Hamner	Cyprodinil	121552-61-2		1621.81	zwi	3.63 (base)	13.63 (acid)	0.005	0.64
EPA/Hamner	Diazoxon	962-58-3		2398.83	mpb	3.80	NA	0.327	0.92
EPA/Hamner	Dichlobenil	1194-65-6		1096.48	neu	NA	NA	0.062	0.79
EPA/Hamner	Diethylhexyl phthalate (DEHP)	117-81-7		107151930.52	neu	NA	NA		
EPA/Hamner	Dimethanimid	87674-68-8		831.76	neu	NA	NA	0.232	0.90
EPA/Hamner	Diphenylamine	122-39-4		2570.40	mpb	0.78	NA	0.005	0.64
EPA/Hamner	Dithiopyr	97886-45-8		588843.66	neu	NA	NA	0.005	0.64
EPA/Hamner	Diuron	330-54-1		338.84	mpa	13.18	NA	0.161	0.87
EPA/Hamner	Ethofumesate	26225-79-6		218.78	neu	NA	NA	0.131	0.85
EPA/Hamner	Ethoprop	13194-48-4		1659.59	neu	NA	NA	0.093	0.82
EPA/Hamner	Etoxazole	153233-91-1		416869.38	mpb	0.74	NA	0.005	0.64

EPA/Hamner	Fenarimol	60168-88-9	8317.64	zwi	1.04 (base)	12.13 (acid)	0.037	0.75
EPA/Hamner	Fenbuconazole	114369-43-6	22387.21	mpb	2.27	NA	0.005	0.64
EPA/Hamner	Fludioxonil	131341-86-1	3715.35	mpa	14.66	NA	0.005	0.64
EPA/Hamner	Flufenacet	142459-58-3	1659.59	mpa	12.58	NA	0.137	0.86
EPA/Hamner	Flusilazole	85509-19-9	47863.01	mpb	2.32	NA	0.029	0.73
EPA/Hamner	Formetanate hydrochloride	23422-53-9	12.02	zwi	8.89 (base)	14.77 (acid)	0.885	0.73
EPA/Hamner	Halosulfuron-methyl	100784-20-1	28.18	zwi	1.69 (base)	5.03 (acid)	0.009	0.67
EPA/Hamner	Hexaconazole	79983-71-4	5128.61	zwi	2.26 (base)	13.35 (acid)	0.041	0.76
EPA/Hamner	Imazalil	35554-44-0	5754.40	mpb	6.77	NA	0.030	0.73
EPA/Hamner	Imidacloprid	138261-41-3	12.59	zwi	5.28 (base)	9.39 (acid)	0.656	0.87
EPA/Hamner	Isazofos	42509-80-8	3019.95	neu	NA	NA	0.065	0.79
EPA/Hamner	Isoxaflutole	141112-29-0	138.04	neu	NA	NA	0.017	0.70
EPA/Hamner	Lindane	58-89-9	22387.21	neu	NA	NA	0.005	0.64
EPA/Hamner	MCPA	94-74-6	562.34	mpa	3.07	NA	0.590	1.30
EPA/Hamner	Novaluron	116714-46-6	1737800.83	dpa	6.30	13.89	0.005	0.64
EPA/Hamner	Oxadiazon	19666-30-9	204173.79	neu	NA	NA	0.005	0.64
EPA/Hamner	Perfluorooctane sulfonic acid	1763-23-1	269153.48	mpa	-3.32	NA	0.005	0.64
EPA/Hamner	Perfluorooctanoic acid	335-67-1	128824.96	mpa	-4.20	NA	0.005	0.64
EPA/Hamner	Permethrin	52645-53-1	501187.23	neu	NA	NA	0.005	0.64
EPA/Hamner	Propamocarb hydrochloride	25606-41-1	5.89	mpa	9.30	NA	0.843	0.76
EPA/Hamner	Propyzamide	23950-58-5	1513.56	mpa	14.21	NA	0.068	0.79
EPA/Hamner	Pryrithiobac-sodium	123343-16-8	7762.47	zwi	0.53 (base)	2.21 (acid)	0.027	0.73
EPA/Hamner	Pyrimethanil	53112-28-0	269.15	zwi	3.96 (base)	13.67 (acid)	0.017	0.70
EPA/Hamner	Resmethrin	10453-86-8	117489.76	neu	NA	NA	0.005	0.64
EPA/Hamner	Rimsulfuron	122931-48-0	6.76	zwi	1.69 (base)	4.95 (acid)	0.628	0.88
EPA/Hamner	S-Bioallethrin	28434-00-6	11481.54	neu	NA	NA	0.237	0.90
EPA/Hamner	Simazine	122-34-9	60.26	mpb	3.23	NA	0.284	0.91
EPA/Hamner	Tetraconazole	112281-77-3	7244.36	mpb	2.28	NA	0.025	0.72
EPA/Hamner	Thidiazuron	51707-55-2	74.13	mpa	8.93	NA	0.028	0.73
EPA/Hamner	Triadimefon	43121-43-3	9332.54	mpb	1.93	NA	0.114	0.84
EPA/Hamner	Triclosan	3380-34-5	95499.26	mpa	7.68	NA	0.005	0.64

EPA/Hamner	Triflumizole	68694-11-1	3801.89	dpb	3.52	6.31	0.005	0.64
EPA/Hamner	Triticonazole	131983-72-7	2238.72	zwi	2.26 (base)	13.33 (acid)	0.137	0.86
EPA/Hamner	Zoxamide	156052-68-5	43651.58	neu	NA	NA	0.010	0.67
TNO	Acrylamide	79-06-1	0.21	neu	NA	NA		
TNO	Chlorpyrifos	2921-88-2	50118.72336	neu	NA	NA	0.03	0.73
TNO	Warfarin	81-81-2	3235.94	mpa	5.00	NA	0.007	0.55
TNO	Phenytoin	57-41-0	141.25	dpa	6.46	14.71	0.200	0.89
TNO	Valproic acid	99-66-1	524.81	mpa	4.56	NA	0.366	0.74
TNO	Diazepam	53320-84-6	630.96	mpb	2.92	NA	0.012	0.70
TNO	Cyclosporin A	59865-13-3	831.76	neu	NA	NA	0.062	1.28
TNO	Methoxyacetic acid	625-45-6	0.32	mpa	3.57	NA		
Ito/Riley	Alprazolam	28981-97-7	234.42	dpa	1.42	8.19	0.35	0.78
Ito/Riley	Bosentan	147536-97-8	87096.36	mpb	5.80	NA	0.02	0.71
Ito/Riley	Caffeine	58-08-2	0.28	neu	NA	NA	1	0.80
Ito/Riley	Diclofenac	64118-84-9	9120.11	dpa	3.76	8.61	0.017	0.70
Ito/Riley	Diltiazem	42399-41-7	537.03	zwi	8.18 (base)	12.86 (acid)	0.198	0.89
Ito/Riley	Hexobarbitone	56-29-1	17.78	mpa	8.41	NA	0.62	0.88
Ito/Riley	Ibuprofen	15687-27-1	6918.31	mpa	4.85	NA	0.01	0.55
Ito/Riley	Imipramine	50-49-7	19054.61	mpb	9.20	NA	0.107	1.10
Ito/Riley	Metoprolol	37350-58-6	57.54	zwi	9.67 (base)	14.09 (acid)	1	1.00
Ito/Riley	Midazolam	59467-70-8	2137.96	dpb	5.67	7.42	0.07	0.80
Ito/Riley	Nicardipine	55985-32-5	3630.78	dpb	5.42	8.18	0.084	0.71
Ito/Riley	Nilvadipine	75530-68-6	173.78	neu	NA	NA	0.013	0.68
Ito/Riley	Ondansetron	99614-02-5	223.87	mpb	7.34	NA	0.25	0.83
Ito/Riley	Phenacetin	62-44-2	25.70	neu	NA	NA	1	1.01
Ito/Riley	Tolbutamide	64-77-7	199.53	mpa	4.33	NA	0.08	0.55
ECVAM	Antipyrine	60-80-0	2.40	mpb	0.37	NA	1	0.56
ECVAM	2,5-Hexanedione	110-13-4	0.54	neu	NA	NA	0.93	0.69
ECVAM	Acetylsalicylic acid	50-78-2	15.49	mpa	3.41	NA	0.085	0.81
ECVAM	Acrylamide	79-06-1	0.21	zwi	0.83	16.70	0.75 (BSA)	0.82
ECVAM	Benz(a)anthracene	56-55-3	575439.94	neu	NA	NA	0.01	0.67
ECVAM	Benzene	71-43-2	134.90	neu	NA	NA	0.40	0.91
ECVAM	Bisphenol A	80-05-7	2089.30	dpa	9.78	10.39	0.05	0.77
ECVAM	Carbendazim	10605-21-7	33.11	zwi	4.28 (acid)	9.70 (base)	0.26 - 0.4 (rat)	0.92
ECVAM	Chlorpyrifos	2921-88-2	91201.08	neu	NA	NA	0.01	0.67
ECVAM	Deltamethrin	52918-63-5	1584893.19	mpa	10.62	NA	0.01	0.67
ECVAM	Diethylene glycol	111-46-6	0.07	dpa	14.82	15.42	0.07	0.63
ECVAM	Diquat	2764-72-9	46.77	neu	NA	NA	0.99	0.89
ECVAM	Domoic acid	14277-97-5	0.85	ppa & zwi	1.68 (acid)	4.22 (acid) & 4.86 (acid) & 11.59 (base)	0.92	0.70
ECVAM	Endosulfan	115-29-7	6760.83	neu	NA	NA	0.33	0.84

ECVAM	Flutamide	13311-84-7	N	2238.72	mpa	13.17	NA	0.17	0.67
ECVAM	Genistein	446-72-0	N	208.93	ppa	6.61	8.79 & 9.46	0.01 (rat)	0.67
ECVAM	Glycidamide	5694-00-8	N	0.06	mpa	15.25	NA	0.98	0.61
ECVAM	Gossypol	303-45-7	N	446683.59	ppa	7.80	8.29 & 8.74 & 9.32 & 11.77 & 12.37	0.81	0.67
ECVAM	Hexachlorobenzene	118-74-1	N	537031.80	neu	NA	NA	0.01	0.67
ECVAM	Hexachlorophene	70-30-4	N	34673685.05	dpa	5.15	8.79	0.08	0.81
ECVAM	Ketoconazole	65277-42-1		22387.21	dpb	3.69	6.75	0.037 (rat)	0.75
ECVAM	Lead acetate	6080-56-4	N	1.86	NA	NA	NA	0.85	0.74
ECVAM	Lindane	58-89-9		5248.07	neu	NA	NA	0.02	0.71
ECVAM	Nicotine	54-11-5	N	14.79	dpb	2.70	8.86	0.75	0.82
ECVAM	Ochratoxin A	303-47-9	N	54954.09	dpa	3.17	7.95	0.0002	0.58
ECVAM	Paraben	120-47-8	N	91.20	mpa	8.50	NA	0.51	0.91
ECVAM	Parathion	56-38-2		6760.83	neu	NA	NA	0.04	0.75
ECVAM	Pentachlorophenol (=2,4-D)	87-86-5	N	131825.67	mpa	4.98	NA	0.014 (mouse)	0.69
ECVAM	Phenanthrene	85-01-8	N	28840.32	neu	NA	NA	0.04	0.78
ECVAM	Potassium cyanide	151-50-8	N	1.02	mpb	9.50	NA	0.91	0.71
ECVAM	Pyrene	129-00-0	N	75857.76	neu	NA	NA	0.03	0.75
ECVAM	Toluene	108-88-3	N	537.03	neu	NA	NA	0.34	0.91
ECVAM	Trimethadione	127-48-0		1.58	neu	NA	NA	0.89	0.73
ECVAM	Trimethyltin	1066-45-1		43.65	neu	NA	NA	0.60	0.89

MW	VP	fvol	CLint,h		Papp
	http://www.ncbi.nlm.nih.gov/pccompound				\\tsn.tno.nl\Data\Projects\031\2\20496\ToxCast\Relevant information from ToxCast database\ToxCast_QikProp_20091214.xlsx
g/mol	133.3224 mmHg / Pa		*L/h/xx*	*hep /1E6 cells; mic /mg prot*	*cm/s*
221.04	1.10E-05	0	#N/A		2.32E-05
269.77	4.53E-06	0	#N/A		6.36E-04
361.66	2.00E-06	1	1.25E+00	hep	5.36E-06
269.77	3.05E-03	1	8.47E+01	hep	5.54E-04
227.33	3.65E-04	1	1.77E+00	hep	2.97E-04
397.51	1.07E-04	1	6.29E+01	hep	2.14E-04
240.28	9.20E-06	0	3.15E+01	hep	7.71E-05
228.29	5.20E-05	1	2.50E+02	hep	9.08E-05
343.21	7.20E-07	0	0.00E+00	hep	2.85E-04
201.23	1.81E-04	1	1.93E+01	hep	2.94E-04
221.65	6.00E-05	1	1.73E+01	hep	9.19E-05
213.67	2.40E-02	1	2.73E+01	hep	2.12E-04
274.11	1.21E-06	0	1.87E+00	hep	1.79E-05
291.78	4.48E-07	1	4.38E+01	hep	2.49E-04
225.30	4.91E-04	1	3.36E-01	hep	5.19E-04
288.29	NA	0	1.54E+00	hep	3.93E-04
172.01	8.80E-02	1	3.78E+01	hep	2.48E-04
390.57	1.89E-05	1	3.46E+01	hep	9.99E-05
275.80	NA	0	7.04E+00	hep	6.20E-04
169.23	8.93E-02	1	2.65E+00	hep	7.83E-04
401.41	NA	0	1.99E+01	hep	3.40E-04
233.10	9.20E-06	0	6.46E+01	hep	2.52E-04
286.35	6.53E-04	1	1.32E+01	hep	1.68E-04
242.33	5.07E-02	1	1.22E+01	hep	4.36E-04
359.42	2.19E-06	0	1.76E+01	hep	7.95E-04

331.20	NA	0	2.09E+01	hep	1.70E-04
336.83	NA	0	1.85E+01	hep	1.33E-04
248.19	NA	0	3.79E+00	hep	1.24E-04
363.33	9.00E-05	1	1.12E+01	hep	1.40E-04
315.40	NA	0	3.70E+01	hep	3.79E-04
257.70	0.00E+00	0	2.90E+01	hep	1.53E-04
434.81	NA	0	6.96E+00	hep	9.44E-06
314.22	NA	0	1.37E+01	hep	2.63E-04
297.19	1.60E-04	1	0.00E+00	hep	4.73E-04
255.67	4.00E-10	0	1.62E+01	hep	3.45E-05
313.74	1.16E-02	1	1.02E+00	hep	5.59E-04
359.32	1.00E-08	0	2.81E+00	hep	5.02E-05
290.83	5.60E-03	1	1.95E+01	hep	9.91E-04
200.62	7.87E-04	1	2.04E+01	hep	2.74E-05
492.71	NA	0	1.32E+01	hep	8.56E-05
345.23	1.53E-05	1	0.00E+00	hep	2.88E-04
500.13	2.67E-01	1	2.87E+00	hep	1.51E-05
414.07	2.00E+01	1	1.40E+01	hep	2.94E-05
391.30	2.91E-06	1	0.00E+00	hep	4.76E-04
224.77	NA	0	1.64E+00	hep	3.43E-05
256.13	NA	0	4.62E+01	hep	4.96E-04
348.74	NA	0	5.82E+00	hep	3.20E-05
199.26	2.20E-03	1	5.40E+00	hep	4.82E-04
338.45	1.51E-06	0	3.98E+00	hep	5.63E-04
431.44	NA	0	4.39E+01	hep	8.36E-06
302.42	1.60E-02	1	9.90E+01	hep	1.29E-04
201.66	2.93E-06	1	0.00E+00	hep	2.27E-04
372.15	1.80E-04	1	0.00E+00	hep	3.30E-04
220.25	3.07E-09	0	6.33E+00	hep	3.46E-05
293.76	2.00E-06	0	0.00E+00	hep	1.84E-04
289.55	1.37E-08	0	4.92E+00	hep	4.74E-04

345.75	NA	0	1.46E+01	hep	4.05E-04
317.82	NA	0	1.19E+02	hep	3.90E-04
336.65	8.80E-07	1	1.42E+01	hep	3.00E-04
71.08	9.33E-01	1			2.70E-05
350.59	2.69E-03	0			NA
308.33	1.55E-05	1	3.30E-02	hep	2.45E-05
252.27	1.60E-08	0	2.22E-03	mic	2.67E-05
166.20	6.13E+00	1			4.80E-05
284.74	NA	0	1.88E+00	(L/h/kg) in vivo human	4.38E-05
1202.61	NA	0			8.60E-07
90.08	4.04E+01	1			NA
308.77	NA	0	1.98E-03	hep	2.55E-05
551.61	NA	0	2.40E+00	mic	1.05E-06
194.19	9.73E-07	0	8.40E-05	hep	4.46E-05
312.15	8.13E-06	1	6.60E-03	hep	
414.52	NA	0	1.50E+01	mic	4.17E-05
236.27	NA	0	1.98E+01	mic	NA
206.28	6.27E-03	1	1.74E+00	mic	5.25E-05
280.41	NA	0	5.94E-02	hep	1.41E-05
267.36	3.73E-05	1	2.64E+00	mic	2.30E-05
325.77	NA	0	4.44E-03	hep	3.24E-05
479.53	NA	0	4.02E+02	mic	1.98E-05
385.37	NA	0	2.16E+03	mic	NA
293.36	NA	0	6.60E-03	hep	2.23E-05
179.22	9.23E-05	1	4.68E-03	hep	5.06E-05
270.35	NA	0	9.60E-05	hep	5.25E-05
188.23	NA	0	4.80E-05	hep	4.15E-05
114.14	5.73E+01	1			
180.16	3.33E-03	1			1.22E-05
71.08	9.33E-01	0			2.70E-05
228.29	2.53E-04	1			
78.12	1.26E+04	1			
228.29	5.20E-05	1			9.08E-05
191.19	1.00E-09	0			
350.59	2.69E-03	1			
505.20	2.00E-06	0			
106.12	7.60E-01	1			
344.05	<<1.33E-05	0			
311.33	NA	0			
406.93	2.31E-05	1			

276.21			
270.24	6.93E-10	0	
87.08	7.81E+01	1	
518.55	NA	0	
284.78	6.53E-03	1	
406.90	1.37E-08	0	
531.43	NA	0	
325.30	NA	0	
290.83	5.60E-03	1	
162.23	5.07E-01	1	1.94E-05
403.81	1.01E-12	0	
152.15	NA	0	
291.26	8.91E-04	1	
266.34	1.10E-05	0	2.32E-05
178.23	1.61E-02	1	
65.12	NA	0	
202.25	6.00E-04	1	
92.14	3.79E+03	1	
143.14	NA	0	
164.82	NA	0	