Table 1: Dataset for experimental logBB values.

CID	*Name*	*logBB*	*Canonical SMILES*
11	1,2-dichloroethane	-0.14	C(CCl)Cl
180	acetone	-0.15	CC(=O)C
241	benzene	0.35	C1=CC=CC=C1
263	1-butanol	-0.02	CCCCO
297	methane	0.03	C
338	salicylic acid	-1.11	C1=CC=C(C(=C1)C(=O)O)O
356	octane	0.69	CCCCCCCC
408	cotinine	-0.22	CN1C(CCC1=O)C2=CN=CC=C2
412	nornicotine	0.32	C1CC(NC1)C2=CN=CC=C2
444	bupropion	1.40	CC(C(=O)C1=CC(=CC=C1)Cl)NC(C)(C)C
702	ethanol	-0.16	CCO
887	methanol	0.02	CO
942	nicotine	0.38	CN1CCCC1C2=CN=CC=C2
947	nitrogen	0.03	N#N
948	nitrous oxide	0.03	N#[N+][O-]
962	water	-0.04	O
1031	1-propanol	-0.15	CCCO
1140	toluene	0.36	CC1=CC=CC=C1
1176	urea	-0.14	C(=O)(N)N
1206	pervertin	0.95	CC(CC1=CC=CC=C1)NC
1345	PK 11195	0.48	CCC(C)N(C)C(=O)C1=CC2=CC=CC=C2C(=N1)C3=CC=CC=C3Cl
1775	phenytoin	-0.05	C1=CC=C(C=C1)C2(C(=O)NC(=O)N2)C3=CC=CC=C3
1935	tacrine	-0.12	C1CCC2=NC3=CC=CC=C3C(=C2C1)N
1978	acebutolol	-0.15	CCCC(=O)NC1=CC(=C(C=C1)OCC(CNC(C)C)O)C(=O)C
1983	acetaminophen	-0.37	CC(=O)NC1=CC=C(C=C1)O
2022	acyclovir	-0.84	C1=NC2=C(N1COCCO)NC(=NC2=O)N
2083	salbutamol	-1.14	CC(C)(C)NCC(C1=CC(=C(C=C1)O)CO)O
2118	alprazolam	0.02	CC1=NN=C2N1C3=C(C=C(C=C3)Cl)C(=NC2)C4=CC=CC=C4
2119	alprenolol	-0.23	CC(C)NCC(COC1=CC=CC=C1CC=C)O
2153	theophylline	-0.32	CN1C2=C(C(=O)N(C1=O)C)NC=N2
2160	amitriptyline	0.90	CN(C)CCC=C1C2=CC=CC=C2CCC3=CC=CC=C31
2164	amobarbital	0.11	CCC1(C(=O)NC(=O)NC1=O)CCC(C)C
2206	antipyrine	-0.11	CC1=CC(=O)N(N1C)C2=CC=CC=C2
2244	aspirin	-0.61	CC(=O)OC1=CC=CC=C1C(=O)O
2249	atenolol	-1.14	CC(C)NCC(COC1=CC=C(C=C1)CC(=O)N)O
2294	barbital	-0.14	CCC1(C(=O)NC(=O)NC1=O)CC
2337	benzocaine	0.27	CCOC(=O)C1=CC=C(C=C1)N
2366	betahistine	-0.34	CNCCC1=CC=CC=N1
2369	betaxolol	0.39	CC(C)NCC(COC1=CC=C(C=C1)CCOCC2CC2)O
2381	biperiden	0.85	C1CCN(CC1)CCC(C2CC3CC2C=C3)(C4=CC=CC=C4)O
2443	bromocriptine	-1.10	CC(C)CC1C(=O)N2CCCC2C3(N1C(=O)C(O3)(C(C)C)NC(=O)C4CN(C5CC6=C(NC7=CC=CC(=C67)C5=C4)Br)C)O
2448	bromperidol	1.38	C1CN(CCC1(C2=CC=C(C=C2)Br)O)CCCC(=O)C3=CC=C(C=C3)F
2473	bunitrolol	0.38	CC(C)(C)NCC(COC1=CC=CC=C1C#N)O
2477	buspirone	0.49	C1CCC2(C1)CC(=O)N(C(=O)C2)CCCCN3CCN(CC3)C4=NC=CC=N4
2482	butamben	0.42	CCCCOC(=O)C1=CC=C(C=C1)N
2519	caffeine	-0.04	CN1C=NC2=C1C(=O)N(C(=O)N2C)C
2520	verapamil	-0.64	CC(C)C(CCCN(C)CCC1=CC(=C(C=C1)OC)OC)(C#N)C2=CC(=C(C=C2)OC)OC
2554	carbamazepine	-0.04	C1=CC=C2C(=C1)C=CC3=CC=CC=C3N2C(=O)N
2555	carbamazepine epoxide	-0.34	C1=CC=C2C(=C1)C3C(O3)C4=CC=CC=C4N2C(=O)N
2578	carmustine	-0.52	C(CCl)NC(=O)N(CCCl)N=O
2583	carteolol	0.01	CC(C)(C)NCC(COC1=CC=CC2=C1CCC(=O)N2)O
2678	cetirizine	-2.15	C1CN(CCN1CCOCC(=O)O)C(C2=CC=CC=C2)C3=CC=C(C=C3)Cl

2708	chlorambucil	-1.70	C1=CC(=CC=C1CCCC(=O)O)N(CCCl)CCCl
2726	chlorpromazine	1.02	CN(C)CCCN1C2=CC=CC=C2SC3=C1C=C(C=C3)Cl
2756	cimetidine	-1.06	CC1=C(N=CN1)CSCCNC(=NC)NC#N
2789	clobazam	0.36	CN1C(=O)CC(=O)N(C2=C1C=CC(=C2)Cl)C3=CC=CC=C3
2803	clonidine	0.12	C1CN=C(N1)NC2=C(C=CC=C2Cl)Cl
2995	desipramine	1.08	CNCCCN1C2=CC=CC=C2CCC3=CC=CC=C31
2997	nordiazepam	0.52	C1C(=O)NC2=C(C=C(C=C2)Cl)C(=N1)C3=CC=CC=C3
3007	amphetamine	0.93	CC(CC1=CC=CC=C1)N
3016	diazepam	0.47	CN1C(=O)CN=C(C2=C1C=CC(=C2)Cl)C3=CC=CC=C3
3043	didanosine	-1.30	C1CC(OC1CO)N2C=NC3=C2NC=NC3=O
3100	diphenhydramine	1.26	CN(C)CCOC(C1=CC=CC=C1)C2=CC=CC=C2
3121	valproic acid	-0.41	CCCC(CCC)C(=O)O
3151	domperidone	-0.85	C1CN(CCC1N2C3=C(C=C(C=C3)Cl)NC2=O)CCCN4C5=CC=CC=C5NC4=O
3152	donepezil	0.89	COC1=C(C=C2C(=C1)CC(C2=O)CC3CCN(CC3)CC4=CC=CC=C4)OC
3162	doxylamine	0.64	CC(C1=CC=CC=C1)(C2=CC=CC=N2)OCCN(C)C
3226	enflurane	0.22	C(C(OC(F)F)(F)F)(F)Cl
3230	enoxolone	-1.40	CC1(C2CCC3(C(C2(CCC1O)C)C(=O)C=C4C3(CCC5(C4CC(CC5)(C)C(=O)O)C)C)C)C
3282	ethenzamide	-0.05	CCOC1=CC=CC=C1C(=O)N
3283	ether	0.00	CCOCC
3308	etodolac	-1.42	CCC1=CC=CC2=C1NC3=C2CCOC3(CC)CC(=O)O
3310	etoposide	-2.00	CC1OCC2C(O1)C(C(C(O2)OC3C4COC(=O)C4C(C5=CC6=C(C=C35)OCO6)C7=CC(=C(C(=C7)OC)O)OC)O)O
3345	fentanyl	0.59	CCC(=O)N(C1CCN(CC1)CCC2=CC=CC=C2)C3=CC=CC=C3
3348	fexofenadine	-0.98	CC(C)(C1=CC=C(C=C1)C(CCCN2CCC(CC2)C(C3=CC=CC=C3)(C4=CC=CC=C4)O)O)C(=O)O
3372	triflumethazine	1.51	C1CN(CCN1CCCN2C3=CC=CC=C3SC4=C2C=C(C=C4)C(F)(F)F)CCO
3373	flumazenil	-0.29	CCOC(=O)C1=C2CN(C(=O)C3=C(N2C=N1)C=CC(=C3)F)C
3380	flunitrazepam	0.07	CN1C(=O)CN=C(C2=C1C=CC(=C2)[N+](=O)[O-])C3=CC=CC=C3F
3386	fluoxetine	0.72	CNCCC(C1=CC=CC=C1)OC2=CC=C(C=C2)C(F)(F)F
3469	gentisic acid	0.09	C1=CC(=C(C=C1O)C(=O)O)O
3510	granisetron	-0.69	CN1C2CCCC1CC(C2)NC(=O)C3=NN(C4=CC=CC=C43)C
3559	haloperidol	1.33	C1CN(CCC1(C2=CC=C(C=C2)Cl)O)CCCC(=O)C3=CC=C(C=C3)F
3562	halothane	0.32	C(C(F)(F)F)(Cl)Br
3608	hexobarbital	0.03	CC1(C(=O)NC(=O)N(C1=O)C)C2=CCCCC2
3658	hydroxyzine	0.36	C1CN(CCN1CCOCCO)C(C2=CC=CC=C2)C3=CC=C(C=C3)Cl
3672	ibuprofen	-0.18	CC(C)CC1=CC=C(C=C1)C(C)C(=O)O
3676	lidocaine	0.34	CCN(CC)CC(=O)NC1=C(C=CC=C1C)C
3696	imipramine	0.98	CN(C)CCCN1C2=CC=CC=C2CCC3=CC=CC=C31
3715	indomethacin	-1.26	CC1=C(C2=C(N1C(=O)C3=CC=C(C=C3)Cl)C=CC(=C2)OC)CC(=O)O
3763	isoflurane	0.37	C(C(F)(F)F)(OC(F)F)Cl
3776	isopropanol	-0.15	CC(C)O
3878	lamotrigine	0.29	C1=CC(=C(C(=C1Cl)Cl)Cl)C2=C(N=C(N=N2)N)N
3955	loperamide	0.77	CN(C)C(=O)C(CCN1CCC(CC1)(C2=CC=C(C=C2)Cl)O)(C3=CC=CC=C3)C4=CC=CC=C4
3958	lorazepam	0.44	C1=CC=C(C(=C1)C2=NC(C(=O)NC3=C2C=C(C=C3)Cl)O)Cl
4046	mefloquine	0.63	C1CCNC(C1)C(C2=CC(=NC3=C2C=CC=C3C(F)(F)F)C(F)(F)F)O
4078	mesoridazine	-0.28	CN1CCCCC1CCN2C3=CC=CC=C3SC4=C2C=C(C=C4)S(=O)C
4112	methotrexate	-1.51	CN(CC1=CN=C2C(=N1)C(=NC(=N2)N)N)C3=CC=C(C=C3)C(=O)NC(CCC(=O)O)C(=O)O
4116	methoxyflurane	0.23	COC(C(Cl)Cl)(F)F
4171	metoprolol	1.15	CC(C)NCC(COC1=CC=C(C=C1)CCOC)O
4184	mianserin	0.99	CN1CCN2C(C1)C3=CC=CC=C3CC4=CC=CC=C42
4192	midazolam	0.37	CC1=NC=C2N1C3=C(C=C(C=C3)Cl)C(=NC2)C4=CC=CC=C4F
4205	mirtazapine	0.53	CN1CCN2C(C1)C3=CC=CC=C3CC4=C2N=CC=C4
4421	nalidixic acid	-0.66	CCN1C=C(C(=O)C2=C1N=C(C=C2)C)C(=O)O
4463	nevirapine	0.00	CC1=C2C(=NC=C1)N(C3=C(C=CC=N3)C(=O)N2)C4CC4
4585	olanzapine	0.78	CC1=CC2=C(NC3=CC=CC=C3N=C2S1)N4CCN(CC4)C
4594	omeprazole	-0.82	CC1=CN=C(C(=C1OC)C)CS(=O)C2=NC3=C(N2)C=C(C=C3)OC
4616	oxazepam	0.60	C1=CC=C(C=C1)C2=NC(C(=O)NC3=C2C=C(C=C3)Cl)O

4687	paraxanthine	0.07	CN1C=NC2=C1C(=O)N(C(=O)N2)C
4736	pentazocine	0.51	CC1C2CC3=C(C1(CCN2CC=C(C)C)C)C=C(C=C3)O
4737	pentobarbital	0.08	CCCC(C)C1(C(=O)NC(=O)NC1=O)CC
4781	phenylbutazone	-0.52	CCCCC1C(=O)N(N(C1=O)C2=CC=CC=C2)C3=CC=CC=C3
4828	pindolol	-0.14	CC(C)NCC(COC1=CC=CC2=C1C=CN2)O
4909	primidone	-0.07	CCC1(C(=O)NCNC1=O)C2=CC=CC=C2
4914	procaine	0.05	CCN(CC)CCOC(=O)C1=CC=C(C=C1)N
4926	promazine	1.08	CN(C)CCCN1C2=CC=CC=C2SC3=CC=CC=C31
4943	propofol	0.63	CC(C)C1=C(C(=CC=C1)C(C)C)O
4946	propranolol	0.84	CC(C)NCC(COC1=CC=CC2=CC=CC=C21)O
4992	pyrilamine	0.49	CN(C)CCN(CC1=CC=C(C=C1)OC)C2=CC=CC=N2
5039	ranitidine	-1.23	CNC(=C[N+](=O)[O-])NCCSCC1=CC=C(O1)CN(C)C
5064	ribavirin	-0.67	C1=NC(=NN1C2C(C(C(O2)CO)O)O)C(=O)N
5073	risperidone	-0.02	CC1=C(C(=O)N2CCCCC2=N1)CCN3CCC(CC3)C4=NOC5=C4C=CC(=C5)F
5092	rolipram	0.61	COC1=C(C=C(C=C1)C2CC(=O)NC2)OC3CCCC3
5095	ropinirole	0.08	CCCN(CCC)CCC1=C2CC(=O)NC2=CC=C1
5142	S-methyl-isothiourea	-0.60	CSC(=N)N
5155	stavudine	-0.48	CC1=CN(C(=O)NC1=O)C2C=CC(O2)CO
5184	scopolamine	0.23	CN1C2CC(CC1C3C2O3)OC(=O)C(CO)C4=CC=CC=C4
5193	secobarbital	0.20	CCCC(C)C1(C(=O)NC(=O)NC1=O)CC=C
5206	sevoflurane	0.30	C(OC(C(F)(F)F)C(F)(F)F)F
5253	sotalol	-0.28	CC(C)NCC(C1=CC=C(C=C1)NS(=O)(=O)C)O
5265	spiperone	0.26	C1CN(CCC12C(=O)NCN2C3=CC=CC=C3)CCCC(=O)C4=CC=C(C=C4)F
5402	terbinafine	0.08	CC(C)(C)C#CC=CCN(C)CC1=CC=CC2=CC=CC=C21
5405	terfenadine	0.64	CC(C)(C)C1=CC=C(C=C1)C(CCCN2CCC(CC2)C(C3=CC=CC=C3)(C4=CC=CC=C4)O)O
5416	krypton	-0.16	[Kr]
5429	theobromine	-0.29	CN1C=NC2=C1C(=O)NC(=O)N2C
5452	thioridazine	0.26	CN1CCCCC1CCN2C3=CC=CC=C3SC4=C2C=C(C=C4)SC
5538	tretinoin	-0.49	CC1=C(C(CCC1)(C)C)C=CC(=CC=CC(=CC(=O)O)C)C
5556	triazolam	0.67	CC1=NN=C2N1C3=C(C=C(C=C3)Cl)C(=NC2)C4=CC=CC=C4Cl
5566	trifluoperazine	1.43	CN1CCN(CC1)CCCN2C3=CC=CC=C3SC4=C2C=C(C=C4)C(F)(F)F
5568	triflupromazine	1.44	CN(C)CCCN1C2=CC=CC=C2SC3=C1C=C(C=C3)C(F)(F)F
5726	zidovudine	-0.74	CC1=CN(C(=O)NC1=O)C2CC(C(O2)CO)N=[N+]=[N-]
5732	zolpidem	-0.48	CC1=CC=C(C=C1)C2=C(N3C=C(C=CC3=N2)C)CC(=O)N(C)C
5760	cocaine	0.60	CN1C2CCC1C(C(C2)OC(=O)C3=CC=CC=C3)C(=O)OC
5809	scopolamine	0.23	CN1C2CC(CC1C3C2O3)OC(=O)C(CO)C4=CC=CC=C4
5917	pentylenetetrazol	-0.03	C1CCC2=NN=NN2CC1
5953	quinidine	-0.21	COC1=CC2=C(C=CN=C2C=C1)C(C3CC4CCN3CC4C=C)O
5978	vincristine	-1.03	CCC1(CC2CC(C3=C(CCN(C2)C1)C4=CC=CC=C4N3)(C5=C(C=C6C(=C5)C78CCN9C7C(C=CC9)(C(C(C8N6C=O)(C(=O)OC)O)OC(=O)C)CC)OC)C(=O)OC)O
5983	physostigmine	0.08	CC12CCN(C1N(C3=C2C=C(C=C3)OC(=O)NC)C)C
6009	aminophenazone	0.00	CC1=C(C(=O)N(N1C)C2=CC=CC=C2)N(C)C
6047	levodopa	-0.78	C1=CC(=C(C=C1CC(C(=O)O)N)O)O
6085	AR 1D9859	0.31	CCCCN1CC2CC3=CC(=C(C=C3C2C1)OC)OC.Cl
6212	trichloromethane	0.26	C(Cl)(Cl)Cl
6251	D-mannitol	-1.60	C(C(C(C(C(CO)O)O)O)O)O
6276	1-pentanol	0.20	CCCCCO
6278	methylchloroform	0.24	CC(Cl)(Cl)Cl
6344	methylenechloride	-0.17	C(Cl)Cl
6348	carbon bisulfide	0.60	C(=S)=S
6351	trimethylene	0.03	C1CC1
6354	oxirane	0.01	C1CO1
6358	2-bromopropane	0.56	CC(C)Br
6365	ethylidene chloride	-0.28	CC(Cl)Cl
6386	tert-butylalcohol	0.11	CC(C)(C)O
6403	hexane	1.03	CCC(C)(C)C

6405	amylene hydrate	0.07	CCC(C)(C)O
6408	chlorotrifluoroethane	-0.08	C(C(F)(F)F)Cl
6468	phencyclidine	0.58	C1CCC(CC1)(C2=CC=CC=C2)N3CCCCC3
6473	butethal	0.19	CCCCC1(C(=O)NC(=O)NC1=O)CC
6560	isobutanol	-0.17	CC(C)CO
6569	2-butanone	-0.07	CCC(=O)C
6574	vinyltrichloride	-0.10	C(C(Cl)Cl)Cl
6575	trichloroethene	0.30	C(=C(Cl)Cl)Cl
6584	methylacetate	-0.13	CC(=O)OC
6623	bisphenol A	-0.12	CC(C)(C1=CC=C(C=C1)O)C2=CC=C(C=C2)O
7174	risocaine	0.55	CCCOC(=O)C1=CC=C(C=C1)N
7237	o-xylene	0.39	CC1=CC=CC=C1C
7247	pseudocumene	0.16	CC1=CC(=C(C=C1)C)C
7282	3-methylpentane	1.01	CCC(C)CC
7296	methylcyclopentane	0.93	CC1CCCC1
7366	tert-butylbenzene	0.43	CC(C)(C)C1=CC=CC=C1
7394	4-chlorobenzotrifluoride	0.17	C1=CC(=CC=C1C(F)(F)F)Cl
7500	ethylbenzene	0.22	CCC1=CC=CC=C1
7501	vinylbenzene	0.45	C=CC1=CC=CC=C1
7558	propylhexedrine	1.08	CC(CC1CCCCC1)NC
7809	p-xylene	0.33	CC1=CC=C(C=C1)C
7840	N-propylbromide	0.27	CCCBr
7845	divinyl	-0.17	C=CC=C
7855	acrylonitrile	-0.40	C=CC#N
7859	2-propyn-1-ol	-0.23	C#CCO
7892	isohexane	0.98	CCCC(C)C
7895	2-pentanone	-0.01	CCCC(=O)C
7915	isopropyl acetate	0.40	CC(C)OC(=O)C
7929	m-xylene	0.28	CC1=CC(=CC=C1)C
7962	cyclohexylmethane	0.96	CC1CCCCC1
7997	propyl acetate	0.12	CCCOC(=O)C
8003	n-pentane	0.75	CCCCC
8038	isobutyl acetate	0.45	CC(C)COC(=O)C
8058	n-hexane	0.78	CCCCCC
8078	cyclohexane	0.96	C1CCCCC1
8125	1-octene	0.74	CCCCCCC=C
8141	n-nonane	0.52	CCCCCCCCC
8252	propene	-0.06	CC=C
8522	iodophenazone	-0.10	CC1=C(C(=O)N(N1C)C2=CC=CC=C2)I
8723	sec-butylcarbinol	0.04	CCC(C)CO
8857	ethyl acetate	0.00	CCOC(=O)C
8900	heptane	0.76	CCCCCCC
8942	ortal	0.36	CCCCCCC1(C(=O)NC(=O)NC1=O)CC
9034	methohexitone	-0.07	CCC#CC(C)C1(C(=O)NC(=O)N(C1=O)C)CC=C
9651	galanthamine	0.32	CN1CCC23C=CC(CC2OC4=C(C=CC(=C34)C1)OC)O
9664	1,1-difluorochloroethylene	-0.02	C(=C(F)F)Cl
9844	fluoromar	0.13	C=COCC(F)(F)F
10253	salicylurate	-0.44	C1=CC=C(C(=C1)C(=O)NCC(=O)O)O
10836	metamphetamine	0.93	CC(CC1=CC=CC=C1)NC
11416	hexahydro-o-xylene	1.07	CC1CCCCC1C
11507	2-ethylpentane	0.90	CCCC(C)CC
11594	2-methylheptane	0.86	CCCCCC(C)C
12348	pentyl acetate	0.40	CCCCCOC(=O)C
12418	1,1,1,2-tetrachloroethane	0.33	C(C(Cl)(Cl)Cl)Cl
12512	tert-butylethylether	0.22	CCOC(C)(C)C
12598	butaperazine	0.83	CCCC(=O)C1=CC2=C(C=C1)SC3=CC=CC=C3N2CCCN4CCN(CC4)C

13342	vinblastine	-0.07	CCC1(CC2CC(C3=C(CCN(C2)C1)C4=CC=CC=C4N3)(C5=C(C=C6C(=C5)C78CCN9C7C(C=CC9)(C(C(C8N6C)(C(=O)OC)O)OC(=O)C)CC)OC)C(=O)OC)O
13379	2-methylnonane	1.05	CCCCCCCC(C)C
13381	1-decene	0.96	CCCCCCCCC=C
15413	tert-butylmethylether	0.36	CC(C)(C)OC
15600	decane	0.67	CCCCCCCCCC
17358	elegas	0.37	FS(F)(F)(F)(F)F
18047	toliprolol	0.34	CC1=CC(=CC=C1)OCC(CNC(C)C)O
18508	t-butylcyclohexane	0.61	CC(C)(C)C1CCCCC1
18591	isononane	0.98	CCCCCCC(C)C
22407	cytisine	-1.09	C1C2CNCC1C3=CC=CC(=O)N3C2
23935	neon	0.20	[Ne]
23968	argon	0.03	[Ar]
23991	xenon	0.07	[Xe]
24066	zalcitabine	-1.18	C1CC(OC1CO)N2C=CC(=NC2=O)N
28315	desmonomethylpromazine	0.59	CNCCCN1C2=CC=CC=C2SC3=CC=CC=C31
30322	digoxin	-1.23	CC1C(C(CC(O1)OC2C(OC(CC2O)OC3C(OC(CC3O)OC4CCC5(C(C4)CCC6C5CC(C7(C6(CCC7C8=CC(=O)OC8)O)C)O)C)C)O)O
31272	butyl acetate	0.28	CCCCOC(=O)C
31276	isopentyl acetate	0.55	CC(C)CCOC(=O)C
31285	1-nonene	0.86	CCCCCCCC=C
31300	tefluranum	0.27	C(C(F)(F)F)(F)Br
31373	perchloroethylene	0.37	C(=C(Cl)Cl)(Cl)Cl
31423	pyrene	0.23	C1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2
31703	doxorubicin	-0.83	CC1C(C(CC(O1)OC2CC(CC3=C(C4=C(C(=C23)O)C(=O)C5=C(C4=O)C=CC=C5OC)O)(C(=O)CO)O)N)O
31765	sulforidazine	0.18	CN1CCCCC1CCN2C3=CC=CC=C3SC4=C2C=C(C=C4)S(=O)(=O)C
33039	alovudine	-0.59	CC1=CN(C(=O)NC1=O)C2CC(C(O2)CO)F
37614	miloxacin	-0.92	CON1C=C(C(=O)C2=CC3=C(C=C21)OCO3)C(=O)O
42113	suprane	0.11	C(C(F)(F)F)(OC(F)F)F
43473	5-ethyl-5-heptyl-1,3-diazinane-2,4,6-trione	0.02	CCCCCCCC1(C(=O)NC(=O)NC1=O)CC
46516	5-ethyl-5-propyl-1,3-diazinane-2,4,6-trione	0.09	CCCC1(C(=O)NC(=O)NC1=O)CC
47811	pergolide	0.30	CCCN1CC(CC2C1CC3=CNC4=CC=CC2=C34)CSC
50287	tiotidine	-0.82	CN=C(NCCSCC1=CSC(=N1)N=C(N)N)NC#N
51670	lupitidine	-1.06	CC1=NC=C(C=C1)CC2=CN=C(NC2=O)NCCSCC3=CC=C(O3)C(C)(C)N.Cl.Cl.Cl
51671	lupitidinum	-1.06	CC1=NC=C(C=C1)CC2=CN=C(NC2=O)NCCSCC3=CC=C(O3)C(C)(C)N
53024	yamatetan	-1.89	CN1C(=NN=N1)SCC2=C(N3C(C(C3=O)(NC(=O)C4SC(=C(C(=O)N)C(=O)[O-])S4)OC)SC2)C(=O)[O-].[Na+].[Na+]
53025	cefotetan	-1.89	CN1C(=NN=N1)SCC2=C(N3C(C(C3=O)(NC(=O)C4SC(=C(C(=O)N)C(=O)O)S4)OC)SC2)C(=O)O
55482	temelastine	-1.88	CC1=NC=C(C=C1)CC2=CN=C(NC2=O)NCCCCC3=NC=C(C=C3C)Br
57347	flesinoxan	-0.45	C1CN(CCN1CCNC(=O)C2=CC=C(C=C2)F)C3=C4C(=CC=C3)OC(CO4)CO
60944	indinavir	-0.74	CC(C)(C)NC(=O)C1CN(CCN1CC(CC(CC2=CC=CC=C2)C(=O)NC3C(CC4=CC=CC=C34)O)O)CC5=CN=CC=C5
60949	apaxifylline	-1.40	CCCN1C2=C(C(=O)N(C1=O)CCC)NC(=N2)C3CCC(=O)C3
61247	tert-amylmethylether	0.17	CCC(C)(C)OC
62761	thoron	-0.12	[Rn]
62875	norchlorpromazine	1.38	CNCCCN1C2=CC=CC=C2SC3=C1C=C(C=C3)Cl
64142	nelfinavir mesylate	-0.93	CC1=C(C=CC=C1O)C(=O)NC(CSC2=CC=CC=C2)C(CN3CC4CCCCC4CC3C(=O)NC(C)(C)C)O.CS(=O)(=O)O
64143	nelfinavir	-0.93	CC1=C(C=CC=C1O)C(=O)NC(CSC2=CC=CC=C2)C(CN3CC4CCCCC4CC3C(=O)NC(C)(C)C)O
64814	3-hydroxy-3-phenylpentamide	0.04	CCC(CC(=O)N)(C1=CC=CC=C1)O
65016	amprenavir	-0.56	CC(C)CN(CC(C(CC1=CC=CC=C1)NC(=O)OC2CCOC2)O)S(=O)(=O)C3=CC=C(C=C3)N
66724	4-carboxybiphenyl	-1.26	C1=CC=C(C=C1)C2=CC=C(C=C2)C(=O)O
67101	16a-fluoroestradiol	-0.30	CC12CCC3C(C1CC(C2O)F)CCC4=C3C=CC(=C4)O
68617	sertraline	1.60	CNC1CCC(C2=CC=CC=C12)C3=CC(=C(C=C3)Cl)Cl
69460	kusol	0.67	C1CC2=CC=CC=C2NC1
72108	icotidine	-2.00	CC1=NC=C(C=C1)CC2=CN=C(NC2=O)NCCCCC3=C(C=CC=N3)OC
74981	didemethylchlorpromazine	0.97	C1=CC=C2C(=C1)N(C3=C(S2)C=CC(=C3)Cl)CCCN
77501	1,4-divinyloxybutane	0.12	C=COCCCCOC=C
77991	rivastigmine	0.88	CCN(C)C(=O)OC1=CC=CC(=C1)C(C)N(C)C

80554	N,N-dimethylpyridine-2-ethylamine	-0.27	CN(C)CCC1=CC=CC=N1
83909	chlorambucil-t-butylester	1.00	CC(C)(C)OC(=O)CCCC1=CC=C(C=C1)N(CCCl)CCCl
87653	thiazole-22-aminoethyl	-0.42	C1=CSC(=N1)CCN
89657	norclobazam	0.35	C1C(=O)NC2=C(C=C(C=C2)Cl)N(C1=O)C3=CC=CC=C3
90274	ST 363	0.16	C1CN=C(N1)NC2=C(C=C(C=C2)Cl)Cl
91517	tripropylphosphine	1.02	CC1CCC(C(C1)C)C
91769	zolantidine	0.14	C1CCN(CC1)CC2=CC(=CC=C2)OCCCNC3=NC4=CC=CC=C4S3
92242	fluoromisonidazole	-0.01	C1=CN(C(=N1)[N+](=O)[O-])CC(CF)O
92375	alpha-(4-pyridyl-1-oxide)-N-tert-butylnitrone	-0.38	CC(C)(C)[N+](=O)C=C1C=CN(C=C1)[O-]
94957	4-fluoroantipyrine	-0.05	CC1=CC(=O)N(N1C)C2=CC=C(C=C2)F
95705	NSC 30403	-0.22	CCC1(C(=O)NC(=O)NC1=O)C
104972	norverapamil	-0.64	CC(C)C(CCCNCCC1=CC(=C(C=C1)OC)OC)(C#N)C2=CC(=C(C=C2)OC)OC
107917	1-hydroxymidazolam	-0.08	C1C2=CN=C(N2C3=C(C=C(C=C3)Cl)C(=N1)C4=CC=CC=C4F)CO
107926	bretazenil	-0.09	CC(C)(C)OC(=O)C1=C2C3CCCN3C(=O)C4=C(N2C=N1)C=CC=C4Br
114376	northioridazine	0.76	CSC1=CC2=C(C=C1)SC3=CC=CC=C3N2CCC4CCCNC4
115237	paliperidone	-0.67	CC1=C(C(=O)N2CCCC(C2=N1)O)CCN3CCC(CC3)C4=NOC5=C4C=CC(=C5)F
119146	N-methylspiroperidol	0.46	CN1CN(C2(C1=O)CCN(CC2)CCCC(=O)C3=CC=C(C=C3)F)C4=CC=CC=C4
119329	alaptide	-0.26	CC1C(=O)NC2(CCCC2)C(=O)N1
121249	2-hydroxydesipramine	0.53	CNCCCN1C2=C(CCC3=CC=CC=C31)C=C(C=C2)O
124449	4-hydroxymidazolam	-0.22	CC1=NC=C2N1C3=C(C=C(C=C3)Cl)C(=NC2O)C4=CC=CC=C4F
126761	fluoroethylflumazenil	-0.14	CCOC(=O)C1=C2CN(C(=O)C3=C(N2C=N1)C=CC(=C3)F)CCF
127382	RO 19-4603	-0.25	CC(C)(C)OC(=O)C1=C2CN(C(=O)C3=C(N2C=N1)C=CS3)C
129710	CHEBI 218555	-0.30	CC(C)C1=NC(=NO1)C2=C3CN(C(=O)C4=C(N3C=N2)C=CC=C4Cl)C
133741	7-hydroxy ropinirole	-0.43	CCCN(CCC)CCC1=C2CC(=O)NC2=C(C=C1)O
156386	p-bromospiperone	0.07	C1CN(CCC12C(=O)NCN2C3=CC=C(C=C3)Br)CCCC(=O)C4=CC=C(C=C4)F
159642	didesipramine	1.05	C1CC2=CC=CC=C2N(C3=CC=CC=C31)CCCN
162244	alpha-hydroxyalprazolam	-1.28	C1C2=NN=C(N2C3=C(C=C(C=C3)Cl)C(=N1)C4=CC=CC=C4)CO
166560	beloxepin	0.82	CC1=CC=CC2=C1OC3=CC=CC=C3C4(C2CN(CC4)C)O
174174	atropine	-0.06	CN1C2CCC1CC(C2)OC(=O)C(CO)C3=CC=CC=C3
182017	4-hydroxyalprazolam	-1.48	CC1=NN=C2N1C3=C(C=C(C=C3)Cl)C(=NC2O)C4=CC=CC=C4
192706	phenserine	1.00	CC12CCN(C1N(C3=C2C=C(C=C3)OC(=O)NC4=CC=CC=C4)C)C
198752	zanapezil	1.14	C1CCNC2=C(C1)C=CC(=C2)C(=O)CCC3CCN(CC3)CC4=CC=CC=C4
204104	MP 005-942-485	0.68	CC1C2=CC=CC=C2CCN1C3=NC(=NC(=C3C)C)NC4=CC=C(C=C4)F
441243	saquinavir	-0.95	CC(C)(C)NC(=O)C1CC2CCCCC2CN1CC(C(CC3=CC=CC=C3)NC(=O)C(CC(=O)N)NC(=O)C4=NC5=CC=CC=C5C=C4)O
444008	tibolone	0.40	CC1CC2=C(CCC(=O)C2)C3C1C4CCC(C4(CC3)C)(C#C)O
444031	darifenacin	-0.62	C1CN(CC1C(C2=CC=CC=C2)(C3=CC=CC=C3)C(=O)N)CCC4=CC5=C(C=C4)OCC5
475100	9-hydroxyrisperidone	-0.67	CC1=C(C(=O)N2CC(CCC2=N1)O)CCN3CCC(CC3)C4=NOC5=C4C=CC(=C5)F
547559	phenothiazine	-0.48	CN(C)CCCN1C2=CC=CC=C2S(=O)C3=CC=CC=C31
638186	dioform	0.04	C(=CCl)Cl
643833	cis-dichloroethylene	-0.13	C(=CCl)Cl
2733526	tamoxifen	0.92	CCC(=C(C1=CC=CC=C1)C2=CC=C(C=C2)OCCN(C)C)C3=CC=CC=C3
2776666	CDS1 000170	-0.04	CC1=CSC(=N1)N=C(N)N
3000715	thiopental	-0.19	CCCC(C)C1(C(=O)NC(=S)NC1=O)CC
3035905	thioperamide	-0.17	C1CCC(CC1)NC(=S)N2CCC(CC2)C3=CN=CN3
3763607	N-(4-phenylthiazol-2-yl)-guanidine	-0.18	C1=CC=C(C=C1)C2=CSC(=N2)N=C(N)N
3946663	3-methyl-2-phenyl-N-(1-phenylpropyl)-quinoline-4-carboxamide	0.30	CCC(C1=CC=CC=C1)NC(=O)C2=C(C(=NC3=CC=CC=C32)C4=CC=CC=C4)C
5281708	daidzein	-0.15	C1=CC(=CC=C1C2=COC3=C(C2=O)C=CC(=C3)O)O
5284371	codeine	0.45	CN1CCC23C4C1CC5=C2C(=C(C=C5)OC)OC3C(C=C4)O
5288826	morphine	-0.26	CN1CCC23C4C1CC5=C2C(=C(C=C5)O)OC3C(C=C4)O
5324346	fluvoxamine	0.79	COCCCCC(=NOCCN)C1=CC=C(C=C1)C(F)(F)F
5359272	levorphanol	0.00	CN1CCC23CCCCC2C1CC4=C3C=C(C=C4)O
6433234	tyrylen	0.83	CCCC(=O)C1=CC2=C(C=C1)SC3=CC=CC=C3N2CCCN4CCN(CC4)C.C(=CC(=O)O)C(=O)O.C(=CC(=O)O)C(=O)O
6434601	cyclosporin A	-0.78	CCC1C(=O)N(CC(=O)N(C(C(=O)NC(C(=O)N(C(C(=O)NC(C(=O)NC(C(=O)N(C(C(=O)N(C(C(=O)N(C(C(=O)N1)C(C(C)C=CC)O)C)CC(C)C)C)CC(C)C)C)C)C)C)C)CC

			(C)C)C)C
7138787	ZINC 04226975	-0.87	C1=CC=C(C=C1)C2=CSC(=N2)CC[NH3+]
9796408	CHEBI: 568657	1.64	C1CN(CCN1)C2=NC(=C(C=C2)C(F)(F)F)Cl
9861160	CID 9861160	0.00	C=CCC(C1=CC=CC=C1C2=NOC3=CC=CC=C32)N
9864749	CHEBI: 167165	1.13	C1CN(CCC1COC2=CC=C(C=C2)C#N)CC=CI
9903970	org 5222	1.03	CN1CC2C(C1)C3=C(C=CC(=C3)Cl)OC4=CC=CC=C24
9907401	CHEBI: 568728	0.16	C1CC(=O)N(C1)CCCCN2CCN(CC2)C3=NC=CC(=C3)C(F)(F)F
9971484	CHEBI: 338581	-0.46	CC(=O)NCCCOC1=CC=CC(=C1)CN2CCCCC2
10011896	2-(2-fluoro-ethyl)-isothiourea	-0.27	C(CSC(=N)N)F
10019237	CHEBI: 338033	0.69	C1CCN(CC1)CC2=CC(=CC=C2)OCCCNC3=CC=CC=N3
10091748	CHEBI: 338584	-1.82	CC(CO)(C1=NC(=NO1)C2=C3CN(C(=O)C4=C(N3C=N2)C=CC=C4Cl)C)O
10313352	CID 10313352	0.05	CC(C)(C)[N+](=CC1=CC=CC=C1)[O-]
10352163	MOLI001288	-0.24	C1=CN(C(=N1)[N+](=O)[O-])CCCF
10377120	MOLI001285	-0.17	C1=CN(C(=N1)[N+](=O)[O-])CCCCCCCCF
10384745	CHEBI: 338585	-1.34	CC(C)(C1=NC(=NO1)C2=C3CN(C(=O)C4=C(N3C=N2)C=CC=C4Cl)C)O
10444765	CHEBI: 338140	-0.02	C1CCN(CC1)CC2=CC(=CC=C2)OCCCO
10451635	CID 10451635	0.18	C1=CC(=C(C=C1C2=NC3=C(S2)C=C(C=C3)O)I)N
11115931	3-methylhexane	0.90	CC[CH][C]([CH2])CC
12780299	CHEBI: 385616	0.98	C1CCN(CC1)CC2=CC(=C(C=C2)I)CN3CCCCC3
12889418	CHEBI: 163710	-1.17	CN(C)C1=NC=CC(=C1)C2=NC(=NN2)N
13720676	CHEBI: 287982	1.01	CCCCCCN1CCN(CC1)C2=CC=C(C=C2)I
13755681	5-octyl-5-ethyl barbituric acid	0.24	CCCCCCCCC1(C(=O)NC(=O)NC1=O)CC
14022480	CHEBI: 339093	-0.67	C1=CC(=C(N=C1)CSCCNC2=C(C=CN2)[N+](=O)[O-])Br
14022481	CHEBI: 339092	-0.66	C1=CC=NC(=C1)CSCCNC2=C(C=CN2)[N+](=O)[O-]
14022483	CHEBI: 337303	-0.12	C1=CC=C(C=C1)CC2=CNC(=C2[N+](=O)[O-])NCCSCC3=CC=CC=N3
14022484	CHEBI: 338035	-0.73	CN(C)CC1=CC=C(O1)CSCCNC2=C(C(=CN2)CC3=CC=CC=C3)[N+](=O)[O-]
14022497	CHEBI: 338961	0.44	C1CCN(CC1)CC2=CC(=CC=C2)OCCCNC3=NC=CS3
14022499	CHEBI: 339055	0.22	C1CCN(CC1)CC2=CC(=CC=C2)OCCCNC3=NC4=CC=CC=C4O3
14022509	CHEBI: 338063	-1.15	C1=CC(=CC(=C1)N)C2=CSC(=N2)N=C(N)N
14022517	CHEBI: 338620	-2.15	CCNC(=NCCSCC1=C(C=CC=N1)Br)NC#N
14022519	CHEBI: 145922	-1.54	CN=C(NC#N)NC1=CC=CC(=C1)C2=CSC(=N2)N=C(N)N
14211618	16a-fluoroestradiol	-0.30	CC12CCC3C(C1CC(C2O)F)CCC4=C3C=CC(=C4)O
18356503	MP 001-772-915	0.35	C(C(Cl)Br)C(F)(F)F
22154175	CID 22154175	0.52	CC1=CC=CC2=C1OC3=CC=CC=C3C4(C2CNCC4)O
23235109	CID 23235109	0.27	C(C(F)Br)C(F)(F)F
40508074	ZINC 05140934	0.53	C[NH2+]CCCN1C2=C(CCC3=CC=CC=C31)C=C(C=C2)O
42251614	ZINC 11886332	-0.58	C1=CSC(=N1)CC[NH3+]
45268400	3-bromocytisine	-0.05	C1C2CNC(C1C3=CC=CC(=O)N3C2)Br