Chemical Name	SMILES Code	Sal +/-	SsCH3	SdCH2	SssCH2	StCH	SdsCH	SaaCH	SsssCH	SddC	StsC	SdssC	SaasC	SaaaC	SssssC	SsNH3p	SsNH2	SssNH2p	SdNH	SssNH	SaaNH	StN	SssssNHp	SdsN
Acenaphtho[1,2-d]pyrz-8-amino	n3c(N)cnc4c1c2c(ccc1)cccc2c34	+						14.8630					0.4663	6.5743			5.7199							
acetal	O(C(C)OCC)CC	+	5.8370		1.4468				-0.3738															
acetic acid [glacial; sodium; calcium]	O=C(O)C	-	1.8333									-0.8333												
Acetyl-2-picolinoylhydrazine, 1- [NSC68626]	O=C(NNC(=O)C)c1ncccc1	-	1.3427					6.4491				-0.7638	0.2642							4.3627				
acetyl-5-nitropyrrole, 2-	O=C(C)C1nC(N(=O)=O)=CC=1	+	1.3116					2.5389				-0.2656	-0.1464											
Acitretin	O(C)c1c(C)c(C)c(C=CC(C)=CC=CC(C)=CC(=O)O)c(C)c1	-	11.7480				1.9360	2.5656				0.8548	5.6576											
adiponitrile	N#CCCCCC#N	-			2.9280						4.3437											16.6540		
aflatoxin B2	C1=C(OC)C4=C(C2=C1OC3C2CCO3)OC(=O)C5=C4CCC5=C	+	1.5573		2.3162			1.8796	-0.2836			0.1958	3.2695											
aflatoxin derivative (AA34-3-82107)	C=C1Cc2c3c(cc(c2C2=C1C(=C)CC2)CC)CC1C3C=CC1	+	2.3165	8.7497	7.1863		4.8758	2.5418	1.4931			5.6136	8.8828											
Alizarin-2-beta-d-glucopyrano	O4C(CO)C(O)C(O)C(O)C4Oc2c(O)c1C(=O)c3c(C(=O)c1cc2)cccc3	+			-0.6487			8.7660	-7.6727			-0.9893	-0.7487											
allyl acrylate	O(C(=O)C=C)CC=C	-		6.5697	0.2548		2.6160					-0.4121												
allyl glycidyl ether	O1C(COCC=C)C1	+		3.5121	2.2392		1.7385		0.3842															
Alosetron [anhydrous;]	C1=CC=C2C(=C1)C4=C(N2C)CCN(CC3=C(C)NC=N3)C4=C	-	3.9693		2.1340			9.6572				0.9764	3.7665	2.1593										
Amino-2,5-dimethylaniline, 4-	Nc1c(C)cc(N)c(C)c1	+	3.8997					3.7874					3.7126				11.2680							
Amino-2-methoxy-3,5-dimethylaniline, 4-	O(C)c1c(N)cc(C)c(N)c1C	-	5.4198					1.8263					3.9738				11.5126							
Amino-3-nitro-6-chloroaniline, 4-	Clc1c(N)cc(N(=O)=O)c(N)c1	+						2.3955					0.1594				1.6449							
amino-4-(5-nitro-2-thienyl)thiazole, 2-	S2=C(N)nC(c1sc(N(=O)=O)cc1)=C2	+						4.9283					2.5360				5.4674							
amino-4,6-dinitrophenol, 2- [Picramic acid]	O=N(=O)c1cc(N(=O)=O)c(O)c(N)c1	+						1.4948					-2.4767				5.1382							
Amino-4-nitro-phenoxyethanol, 3-	O(c1cc(N)c(N(=O)=O)cc1)CCO	-			0.2197			4.5555					0.2999				5.4986							
amino-4-thiazoline HCl, 2-	NC1=NCCS1	+			1.9884							0.7454					5.2477							3.8935
Aminoanthracene, 1- [Anthramine, 1-]	Nc3c1c(cc2c(c1)cccc2)ccc3	+						18.7447					0.8457	4.8365			5.9472							
aminoanthraquinone, 2-	O=C1c3c(C(=O)c2c1cccc2)ccc(N)c3	+						11.6612				-0.2521	2.2419				5.6460							
aminobenzenesulfonic acid, m- [Aminobenzenesulfonic acid, 3-]	S(=O)(=O)(O)c1cc(N)ccc1	-						5.4525					0.1229				5.2797							
aminobenzothiazole, 2-	s1c2c(nc1N)cccc2	-						7.9236					0.6400	2.1435			5.4980							
aminoquinoline, 2-	Nc1ccc2c(n1)cccc2	+						11.6830					0.5729	2.7796			5.5128							
aminoquinoline, 8-	n2c1c(cccc1N)ccc2	+						11.4373					0.7390	1.9745			5.6937							
aminotriazole, 3-	n1nc(N)nc1	-						1.3932					0.2315				4.9936							
Amrinone	O=C2NC=C(c1ccncc1)C=C2N	-					3.2799	7.9722				0.8395	0.9750				5.4987			2.5657				
antipyrine [component A of dichloralphenazone]	O=C1N(c2ccccc2)N(C(=C1)C)C	-	3.7962				1.6319	9.6113				0.9676	0.8964											
Atracurium [Topiramate]	S(=O)(=O)(N)OCC23OCC1OC(C)(C)OC1C2OC(C)(C)O3	-	6.9685		-0.2590				-1.5474						-3.1956		4.8917							
aziridine ethanol, 1-	OCCN1CC1	+			3.5844																			
azoxyanisole, p-	O(C)c2ccc(N=N(=O)c1ccc(OC)cc1)cc2	+	3.1619					13.6599					2.4219											3.9416
Balsalazide	C2(C(=O)O)C=C(N=NC1=CC=C(C(=O)NCCC(=O)O)C=C1)C=CC=2C	-			-0.1440			9.6759				-2.7553	-0.5982							2.4767				7.7741
benomyl	O(C)C(=O)NC1[n+](C(=O)NCCCC)C2=C(N=1)C=CC=C2	-	3.2983		2.4434			7.1628				-1.3273	0.1362	1.2431						5.2525				
benzidine [anhydrous; HCl; Diaminodiphenylenesulfate, 4,4-]	Nc2ccc(-c1ccc(N)cc1)cc2	+						15.5816					3.8674				11.2177							
benzidine-2,2"-disulfonic acid	S(=O)(=O)(O)c2c(-c1c(S(=O)(=O)O)cc(N)cc1)ccc(N)c2	-						7.5870					-1.3289				1.9740							
benzo(a)pyrene-7,8-diol-9,10-epoxide, 7r-anti-	OC1C2C(O2)c2c(cc3c4c2ccc2cccc(c24)cc3)C1O	+						16.8664	-2.6912				1.8617	7.1985										
benzo(a)pyrene-7,8-diol-9,10-epoxide, syn-(+)-	OC1C2C(O2)c2c(cc3c4c2ccc2cccc(c24)cc3)C1O	+						16.8664	-2.6912				1.8617	7.1985										
Benzotrifluoride [Trifouromethylbenzene]	FC(F)(F)c1ccccc1	-						6.3620					-0.6185		-4.2780									
benzyl salicylate	O(C(=O)c1c(O)cccc1)Cc2ccccc2	-			0.2239			15.7230				-0.5213	1.3265											
benzylpiperazinyl)-4-nitrobenzofuroxan, 7-(	o1n(=O)c4c(n1)c(N(=O)=O)ccc4N3CCN(Cc2ccccc2)CC3	+			3.9623			13.2198					1.6399	0.8789										
Bimatoprost [anhydrous;]	C1C(O)C(CC=CCCCC(=O)NCC)C(C=CC(O)CCC)C1C	-	3.9265		5.5275		7.6982		-1.7169			0.8433								2.7778				
bis(2,3-dibromopropylether) of tetrabromobisphenol A	CC(c1cc(c(c(c1)Br)OCC(CBr)Br)Br)(c1cc(c(c(c1)Br)OCC(CBr)Br)Br)C	+	4.4711		2.7780			8.4862	0.4856				7.5552		-0.2552									
bis(2-ethylhexyl)isophthalate	O(C(=O)c1cccc(C(=O)OCC(CC)CCCC)c1)CC(CC)CCCC	-	8.5649		9.5823			6.6439	0.7892			-0.7519	0.8152											
bis(4-aminophenyl)sulfide [Thiodianiline, 4,4"-]	S(c1ccc(N)cc1)c2ccc(N)cc2	+						15.6580					3.9279				11.2284							
bis(dimethylamino-5,8-dihydroxyanthraquinone , 1:4-	O=C2c1c(N(C)C)ccc(N(C)C)c1C(=O)c3c(O)ccc(O)c23	+	7.1133					5.9715				-0.9437	0.7319											
bisacodyl	O=C(Oc1ccc(cc1)C(c1ccccn1)c1ccc(cc1)OC(=O)C)C	-	2.7462					22.2375	-0.1745			-0.7128	3.8890											
Bromazepam	C1=C(Br)C=C3C(=C1)NC(=O)CN=C3C2=CC=CC=N2	-			0.1933			13.5520				0.6155	3.3319							2.8472				4.3782
Bromoacrolein, 2-	C(=C)(Br)C=O	+		3.2222			0.6389					0.3866												
bromochlorobenzene, m- [Bromochlorobenzene, 3-]	Brc1cc(Cl)ccc1	-						7.5300					1.7818											
bromomethyl-12-methylbenz(a)anthracene, 7-	BrCc3c1c(c2c(cc1)cccc2)c(C)c4c3cccc4	+	2.2452		0.8776			21.8862					2.7631	8.1231										
Bunolol	O(c2c1c(C(=O)CCC1)ccc2)CC(O)CNC(C)(C)C	-	6.1660		3.7770			5.5831	-0.5725			0.1913	2.5169		-0.2846					3.2432				
Bupropion [anhydrous;]	C1=CC(Cl)=CC(C(=O)C(C)NC(C)(C)C)=C1	+	7.9790					7.4120	-0.2975			0.6762	1.2413		-0.7574					3.2442				
butane sultone, 1,4-	S1(=O)(=O)OCCCC1	+			2.2525																			
Butoconazole	Clc3ccc(CCC(Sc1c(Cl)cccc1Cl)Cn2ccnc2)cc3	-			2.8325			19.2450	0.3216				4.3548											
Butoxyethanol, 2- [Ethyleneglycol butyl ether]	O(CCCC)CCO	-	2.1134		3.6728																			

butter yellow [oil yellow; Dimethylaminoazobenzene, p-; Dimethyl-4-aminoazobenzene, N,N-]	CN(c1ccc(cc1)N=Nc1ccccc1)C	+	4.2876				17.6953				2.8818						8.3459
butyl formate, t-	O(C(C)(C)C)C=O	-	5.4626			0.4583						-0.3178					
butyl phenyl glycidyl ether, tert-	O2C(COc1ccc(C(C)(C)C)cc1)C2	+	6.6277		1.5228		8.3176	0.3262			2.2621		0.2648				
butylamine, t-	NC(C)(C)C	-	5.8958											5.3542			
butyl-N-(2-hydroxyethyl)nitrosamine, N- [Ethanol, 2-(butylnitrosoamine)]	O=NN(CCCC)CCO	+	2.4359		2.9888												2.7386
butylnitrosoamino)-butanoic acid, 4-(	O=NN(CCCC(=O)O)CCCC	+	2.2899		3.5577					-0.8329							2.8128
butyltoluene, p-tert- [component of butyltoluene, tert-p- mixture]	C(C)(C)(C)c1ccc(C)cc1	-	8.8189				8.7419				2.7371		0.2854				
butyrolactone, DL-3- [Butyrolactone, beta-]	O1C(=O)CC1C	+	1.8764		0.6111			0.1921		-0.6713							
camphene	CC1(C2CC(C1=C)CC2)C	-	4.7257	4.1896	4.3149			1.8519		1.5313			0.4751				
carbamazepine	C1=CC=C2C(=C1)N(C(N)=O)C3=C(C=C2)C=CC=C3	-				3.9943	15.4695			-0.4735	3.5893			5.5255			
carboquone [Carbazilquinone]	O=C1C(=C(C(=O)C(=C1C)N1CC1)C(COC(=O)N)OC)N1CC1	+	3.8112		2.7494			-0.8217		0.1525				4.9888			
Carvedilol	O(C3=C1C(nC2=C1C=CC=C2)=CC=C3)CC(O)CNCCOc4c(OC)cccc4	-	1.6167		1.6714		21.3270	-0.6382			2.1423	3.8873				3.1828	
Cefoperazone	S2C5N(C(C(=O)O)=C(CSC1[n+](C)N=NN=1)C2)C(=O)C5NC(=O)C(NC(=O)N3C(=O)C(=O)N(CC)C3)c4ccc(O)cc4	-	3.3314		0.4975	1.6200	5.3352	-3.3477		-5.5813	0.5648					5.3485	
Cerivastatin	Fc2ccc(-c1c(C=CC(O)CC(O)CC(=O)O)c(C(C)C)nc(C(C)C)c1COC)cc2	-	9.7845		-0.2311	3.2868	6.2299	-2.1465		-1.1277	4.7116						
Chloro-1,3-butadiene, 2- (Chloroprene)	C=C(Cl)C=C	+		6.6497		1.4877				0.4974							
chloro-3-nitro-alpha,alpha,alpha-trifluorotoluene , 4- [Chloro-3-nitrobenzotrifluoride, 4-]	Clc1c(N(=O)=O)cc(C(F)(F)F)cc1	-					1.9446				-2.1545		-4.6184				
chloro-4-nitrophenyl)azo)-5-((2-(2,5-dioxo-1-pyrrolidinyl)ethyl)ethylamino)phenyl)acetamide, N-(2-((3-	O=C(Nc1cc(ccc1N=Nc1cc(c(cc1)[N+](=O)[O-])Cl)N(CCN1C(=O)CCC1=O)CC)C	+	3.3194		1.8457		9.3494			-0.6190	1.7886					2.7368	8.2792
chlorobenzalmalonitrile, o- [Chlorobenzalmelanonitrile; Chlorobenzylidenemalononitrile, o-]	C1(C=C(C#N)C#N)=C(Cl)C=CC=C1	+				1.4665	7.4620		3.5376	0.4917	1.2155						16.9888
chlorobenzilate	Clc2ccc(C(O)(c1ccc(Cl)cc1)C(=O)OCC)cc2	-	1.6826		0.1690		12.7972			-0.7417	1.7940		-1.8976				
Chlorodibromomethane [Dibromochloromethane]	BrC(Br)Cl	-						-0.6944									
chloroethyl acrylate, 2-	ClCCOC(=O)C=C	+		3.1959	0.5893	1.1372				-0.4253							
chloroethyl)-3-cyclohexyl-1-nitrosourea , 1-(2- [Lomustine]	C1CCC(NC(=O)N(N=O)CCCl)CC1	+			5.8333			0.1859		-0.4328						2.7893	2.6330
chloroform	ClC(Cl)Cl	-						-0.7500									
chloro-N-(2,6-diethylphenyl)-N-(propionylamidomethyl)-acetamide, 2-	CCc1cccc(c1N(C(=O)CCl)CNC(=O)CC)CC	+	5.8742		2.6779		6.4400			-0.2935	3.4322					2.7563	
chloronaphthalene, 1-	Clc1c2c(ccc1)cccc2	-					14.1540				0.8223	2.3164					
chlorophenol, m-	Clc1cc(O)ccc1	-					6.4647				0.7662						
chlorotoluene, p-	Clc1ccc(C)cc1	-	2.3820				7.7485				2.4630						
chrysazin monoglucoside tetraacetate	O4C(COC(=O)C)C(OC(=O)C)C(OC(=O)C)C(OC(=O)C)C4Oc3c1c(C(=O)c2c(C1=O)c(O)ccc2)ccc3	+	4.3632		-0.4829		8.3115	-7.3754		-4.4369	-1.1996						
CI acid blue 9 [Food blue No. 1]	S(=O)(=O)(O)c5cccc(CN(c4ccc(C(c1c(S(=O)(=O)O)cccc1)=C3C=CC(=[N+](CC)Cc2cc(S(=O)(=O)O)ccc2)C=C3)cc4)CC)c5	-	3.9246		1.8690	7.4297	25.7667			2.3981	2.4956						
CI acid red 114	S(=O)(=O)(Oc5ccc(N=Nc4c(C)cc(-c3ccc(N=Nc1c(O)ccc2c1c(S(=O)(=O)O)cc(S(=O)(=O)O)c2)c(C)c3)cc4)cc5)c6ccc(C)cc6	+	5.4986				27.2624				3.2157	-0.3513					16.8818
CI acid red 92	[O-]c1c(c2c(cc1Br)C(=C1C(=C(C(=O)C(=C1)Br)Br)O2)c1c(c(c(c(c1C(=O)[O-])Cl)Cl)Cl)Cl)Br	+				1.4670	1.5129			-0.9724	-0.6183						
CI direct blue 2	S(=O)(=O)(O)c6cc(N)c5c(O)c(N=Nc4ccc(-c3ccc(N=Nc1c(S(=O)(=O)O)cc2c(c1O)cc(N)cc2)cc3)cc4)c(S(=O)(=O)O)cc5c6	+					2.8228				-2.9669	0.7163		11.6860			15.7615
CI direct blue 6	S(=O)(=O)(O)c6cc(N)c5c(O)c(N=Nc4ccc(-c3ccc(N=Nc2c(S(=O)(=O)O)cc1c(c(N)cc(S(=O)(=O)O)c1)c2O)cc3)cc4)c(S(=O)(=O)O)cc5c6	-					17.1688				-5.5849	-0.9645		11.7643			15.4890
CI direct green 1 (CI 30280)	[O-]S(=O)(=O)c1c(c(c2c(c(c(cc2c1)S(=O)(=O)[O-])N=Nc1ccc(cc1)c1ccc(cc1)N=Nc1ccc(cc1)O)N)O)N=Nc1ccccc1	+					29.9468				-0.7855	-0.5628		6.2916			24.1286
CI direct red 39 (CI 23630)	S(=O)(=O)(O)c5cc4c(c(N=Nc3c(C)cc(-c2ccc(N=Nc1ccc(OCC)cc1)c(C)c2)cc3)c(O)cc4)c(S(=O)(=O)O)c5	-	5.6523		0.5829		22.4679				3.5833	-0.3318					16.9721
CI pigment violet 1	O=C(c1c(cccc1)c1c2c([o+]c3cc(ccc13)N(CC)CC)cc(cc2)N(CC)CC)O	-	8.5418		3.5968		19.6227			-0.9378	4.5213	3.3832					
Cilastatin	S(CCCCC=C(NC(=O)C1C(C)(C)C1)C(=O)O)CC(N)C(=O)C	-	3.9629		4.3235	1.5312		-0.9671		-2.4400			-0.3996	5.3899		2.4991	
cinnamaldehyde	C1(C=CC=O)C=CC=CC=1	+				4.2315	9.7159				1.5560						
citral	O=CC=C(C)CCC=C(C)C	-	6.1436		2.3190	4.6517				2.4874							
citrus red [CI solvent red 80]	Oc1ccc2c(c1N=Nc1c(ccc(c1)OC)OC)cccc2	+	3.1483				16.4144				2.2617	1.8148					8.4545
Clopidogrel	Clc3c(C(N2CCC1=C(C=C1)C2)C(=O)OC)cccc3	-	1.4280		2.5923	4.2617	7.4681	-0.4336		2.4645	1.4168						
cresol, m-	Oc1cccc(C)c1	-	1.9442				7.1519				1.4259						
cresyl glycidyl ether, o-	O2C(COc1c(C)cccc1)C2	+	2.4473		1.5384		8.2542	0.3376			2.1446						
curcumin	O(C)c2c(O)ccc(C=CC(=O)CC(=O)C=Cc1ccc(O)c(OC)c1)c2	-	2.8658		-0.2664	5.7887	9.3413			-0.6945	1.9394						

cyclobenzaprine [anhydrous;]	C1(=CCCN(C)C)C3=C(C=CC2C1=CC=CC=2)C=CC=C3	-	4.2417		2.1312		6.8260	17.3200			1.3547	5.2542							
Cycloheximide [Actidione]	O=C2C(C)CC(C)CC2C(O)CC1CC(=O)NC(=O)C1	-	4.9460		2.4653				-0.8786		-0.4375					2.2585			
cyclohexylthio)phthalimide, N-(	O=C1c2c(cccc2)C(=O)N1SC1CCCCC1	-			5.9137			7.7497	0.4176		-0.2941	1.9490							
cyclopentaphenanthrene	c24c1c3c(ccc1ccc2)cccc3C4	+			1.1519			17.7990				2.9794	5.7140						
D&C red 10	S(=O)(=O)(O)c3c(N=Nc1c(O)ccc2c1cccc2)ccc4c3cccc4	-						2.5121				-0.1789	2.5314						8.1144
decabromodiphenyl oxide	Brc2c(Br)c(Br)c(Br)c(Br)c2Oc1c(Br)c(Br)c(Br)c(Br)c1Br	-										9.4284							
Delavirdine	S(=O)(=O)(C)NC4C=CC3nC(C(=O)N2CCN(c1ncccc1NC(C)C)CC2)=CC=3C=4	-	5.2892		2.5654			12.6439	0.3183		-0.6942	2.8616	1.5578			5.8896	3.1519		
Di(2-hydroxyethyl)amino)-6''-methyl-1''-phenylazo-3-pyridine, 4''-(N,N-[Ref50mol8]	OCCN(c2cc(C)c(N=Nc1cnccc1)cc2)CCO	-	1.9555		1.5172			12.7589				3.4339							8.3896
diaminobenzanilide, 4,4''-	Nc1ccc(cc1)C(=O)Nc1ccc(cc1)N	+						13.7282			-0.1716	2.5790			11.1913	2.7696			
diaminobiuret, 1,5-	O=C(NC(=O)NN)NN	+									-1.6427				9.1844	5.5667			
diamino-H-acid, 2,7-	Nc1c(c(cc2cc(c(c(c12)O)N)S(=O)(=O)[O-])S(=O)(=O)[O-])N	-						1.5917				-4.5245	-0.4227		16.5350				
Diaminotoluene, 3,4- [Methyl-o-phenylenediamine, 4-]	Nc1c(N)cc(C)cc1	+	1.9819					5.6287				2.4558			1.9594				
diazidodiphenyl, 4,4''-	[N-]=[N+]=Nc1ccc(cc1)c1ccc(cc1)N=[N+]=[N-]	+						14.8168				3.3642					13.2894		13.1964
Dibenz[a,c]anthracene [Benzotriphenylene; Dibenzanthracene, 1,2:3,4-; Dibenzanthracene, 1,2-]	c12c5c(c3c(c1cccc2)cccc3)cc4c(cccc4)c5	+						3.7160					1.6227						
dibenzyl ether	O(Cc1ccccc1)Cc1ccccc1	-			1.3527			2.4427				2.4323							
dibutylamine [Di-n-butylamine]	N(CCCC)CCCC	-	4.4474		7.6654											3.3872			
dichloro-1-butene, 3,4-	ClCC(Cl)C=C	+		3.4155	0.4495		1.6571		-0.6327										
dichloro-2-nitrobenzene, 1,4-	[O-][N+](=O)c1c(ccc(c1)Cl)Cl	+						4.2328				0.4494							
dichloroacetyl)-3,4-dihydro-3-methyl-2H-1,4-benzoxazine, 4-(	CC1N(c2ccccc2OC1)C(=O)C(Cl)Cl	-	1.8929		0.4477			7.3396	-1.1149		-0.3133	1.4323							
dichlorobenzaldehyde , 3,4-	Clc1c(Cl)cc(C=O)cc1	-					0.7244	4.7279				1.4112							
dichlorobenzoic acid, 3,4-	Clc1c(Cl)ccc(C(=O)O)c1	-						4.1629			-1.1590	0.7524							
dichloromethyl cyanide [Dichloroacetonitrile]	N#CC(Cl)Cl	+							-0.8657	1.5586								7.6296	
dichloronitrobenzene, 2,4-	Clc1cc(Cl)c(N(=O)=O)cc1	+						4.2528				0.3187							
dichlorophenol, 2,4-	C1=CC(Cl)=CC(Cl)=C1O	-						4.5583				0.8624							
dichloroquinoxaline, 2,3-	Clc1nc2c(nc1Cl)cccc2	-						7.4282				0.4914	1.5128						
Dicyclohexylcarbodiimide	N(C1CCCCC1)=C=NC2CCCCC2	-			13.2382				1.6683	2.9749									8.9212
didemethyl-1-deoxypyrromycin, N,N-	O(C4c3c(O)c2c(C(=O)C1C(C(O)=CC=C1)C2=O)cc3C(C(=O)OC)C(O)(CC)C4)C5OC(C)C(O)C(N)C5	+	4.4979		0.4164		4.3162	1.3488	-7.6852		-2.2332	-0.8316		-1.6911	6.6126				
diethyl phosphorodithioate, O,O- [anhydrous; sodium]	SP(=S)(OCC)OCC	+	3.7426		1.1443														
diethylamine [anhydrous; HCl]	N(CC)CC	-	4.2139		2.1875											3.1112			
Diethylene glycol	O(CCO)CCO	-			0.6956														
diethylhexylamine, 2,2''- [Bis(2-ethylhexyl)amine]	N(CC(CC)CCCC)CC(CC)CCCC	-	9.2389		13.4195				1.8325							3.7522			
Difluoroquinoline, 5,7-	Fc2cc1ncccc1c(F)c2	+						6.7414				-1.1696	0.6888						
diglycidyl ether of resorcinol [digylcidyl resorcinol ether]	O3C(COc2cccc(OCC1OC1)c2)C3	+			2.8698			7.6554	0.5638			1.6476							
dihydro-11-methoxy-7-methyl-17h-cyclopenta(a)phenanthren-17-one , 15,16-	O(C)c4c1c(c(C)cc2c1cccc2)c3c(C(=O)CC3)c4	+	3.8594		1.4567			12.4934			0.2344	4.5948	4.7478						
dihydro-3-methyl-5-oxo-(4-((2-sulfoxy)ethyl)sulfooxy)ethyl)sulfonyl)phenyl)-1H-pyrazol-4-yl)azo)-, 2-((4,5- [potassium; sodium]	O=S(=O)c1ccc(cc1)N1N=C(C(C1O)N=Nc1ccc2c(c1S(=O)(=O)O)cccc2S(=O)(=O)[O-])CCCCOS(=O)(=O)[O-]	-			0.5973			1.7760	-2.8129		0.1874	-1.6731	-0.5262						12.3239
dihydro-7-methyl-17H-cyclopenta(a)phenanthren-17-one, 15,16-	O=C4c2c(c1c(C)cc3c(c1cc2)cccc3)CC4	+	2.1564		1.5700			14.8415			0.2958	3.4693	5.1325						
dihydrofuro(2,3-b)benzofuran, 3a-8a-	O1c3c(C2C1OC=C2)cccc3	+					3.7518	8.5972	0.1978			2.1886							
dihydroxy-1,4-benzoxazinone, 2,4-	O=C1N(c2c(cccc2)OC1O)O	+						6.3878	-1.6259		-0.8993	0.5917							
dihydroxy-4-sulfonaphthalene-2,7-diyl)bis(azo-4,1-phenyleneazo))bis(1-hydroxy-2 naphthalenecarboxylic acid, 4,4''-((1,8-	S(=O)(=O)(O)c8c4c(c(O)c(N=Nc3ccc(N=Nc1c2c(c(O)c(C(=O)O)c1)cccc2)cc3)cc4)c(O)c(N=Nc7ccc(N=Nc5c6c(c(O)c(C(=O)O)c5)cccc6)cc7)c8	+						3.9416			-2.6820	-2.6323	0.8393						32.9213
Dihydroxycholecalciferol, 1,25- [D3; Calcitriol]	OC(C)(C)CCCC(C)C3C2(C)C(C(=C=C1C(=C)C(O)CC(O)C1)CCC2)CC3	-	8.7768	4.5944	1.5642		4.4343		1.2498		3.3480			-0.1885					
Diisopropylbenzene	C1=CC=C(C(C(C)C)=C1)C(C)C	-	9.4820					8.7246	1.2844			2.9862							
dimethyl methylphosphonate	P(=O)(C)(OC)OC	-	4.1126																
dimethyl-15H-cyclopenta(a)phenanthrene, 12,17-	C4(C)c3c(C)cc2c1c(cccc1)ccc2c3CC=4	+	4.4667		1.8142		2.3535	15.5793			1.4329	4.3946	5.5253						
dimethyl-1-dodecanamine, N,N-	CCCCCCCCCCCCN(C)C	-	6.6338		15.6141														
dimethyl-2[3-(4,6-dimethoxypyrimidin-2-yl)ureidosulfnyl] nicotinamide, N,N-	COc1cc(nc(n1)NC(=O)NS(=O)(=O)c1c(cccn1)C(=O)N(C)C)OC	+	5.6177					5.2558			-1.7596	-0.8518				3.9116			
dimethylaminopyridine, 4-	CN(c1ccncc1)C	-	4.1852					7.5185				1.1852							
dimethylaniline, 2,3- [Xylidine, 2,3-]	Nc1c(C)c(C)ccc1	+	4.9370					5.9590				3.3356			5.6265				
dimethylanthracene, 9,10-	c13c(c(C)c2c(c1C)cccc2)cccc3	+	4.4249					17.3900				2.7719	5.4952						
dimethylfuran, 2,5-	o1c(C)ccc1C	-	3.8750					3.9750				1.9676							
dimethylhydrazine, 1,2- [anhydrous; 2HCl]	N(C)NC	-	3.6389													5.3611			
dimethylindole, 2,3-	CC1=C(Nc2c1cccc2)C	+	4.2535					8.3788				2.6313	2.5764				3.3268		
dimethylmorpholine, 2,6-	CC1OC(CNC1)C	+	4.1719		2.8611				0.8324							3.2593			

dimethylsuccinate	O(C)C(=O)CCC(=O)OC	-	2.5548		0.1730					-0.7956							
dinitro-6-chloroaniline, 2,4-	Nc1c(cc(cc1[N+](=O)[O-])[N+](=O)[O-])Cl	+					1.9426				-1.3373			5.3168			
dinitrobenzene, 1,3- [Dinitrobenzene, m-]	O=N(=O)c1cccc(N(=O)=O)c1	+					4.5935				-0.5478						
dinitropyrene, 1,6-	O=N(=O)c1ccc2ccc3c(ccc4ccc1c2c34)N(=O)=O	+					13.2287				0.1557	4.7733					
dinitrotoluene, 2,3-	O=N(=O)c1c(N(=O)=O)cccc1C	+	1.4634				3.9968				-0.6142						
dipentaerythritol	OCC(COCC(CO)(O)O)(O)O	-			-3.2453								-4.8224				
di-sec-butyl-p-phenylenediamine, N,N''-	N(c1ccc(NC(C)CC)cc1)C(C)CC	-	8.7814		2.2915		8.5431	1.7160			2.3964					6.9166	
dodecanedioic acid	OC(=O)CCCCCCCCCCC(=O)O	-			8.5145					-1.4284							
dodecylaniline, n-	CCCCCCCCCCCCNc1ccccc1	+	2.2812		15.1670		1.5000				1.2485					3.4699	
dodecyl-N-methylnitrosamine, N- [Nitrosomethyl-n-dodecylamine, N-]	O=NN(C)CCCCCCCCCCCC	+	3.9921		14.1114												2.8475
domperidone	C1=CC=C5C(=C1)N(CCCN4CCC(N2C(=O)NC3=C2C=CC(Cl)=C3)CC4)C(=O)N5	-			6.3114		13.3415	0.1944		-0.1128	4.1754					5.8364	
Edetic acid [Ethylenediamine tetraacetic acid; EDTA; sodium; anhydrous]	O=C(O)CN(CCN(CC(=O)O)CC(=O)O)CC(=O)C	-			-2.2554					-4.9120							
endrin	C13C(C2(Cl)C(Cl)(Cl)C1(Cl)C(Cl)=C2Cl)C4CC3C5C4O5	-			1.6132			1.3478		0.6423			-3.5464				
epoxybutyric acid ethyl ester, 2,3-	CC1C(O1)C(=O)OCC	+	3.6315		0.4359			-0.2298		-0.2315							
epoxycyclohexane, 1,2-	O1C2C1CCCC2	+			5.4838			1.4590									
Eprosartan	s3c(CC(C(=O)O)=CC2[n+](Cc1ccc(C(=O)O)cc1)C(CCCC)=NC=2)ccc3	-	2.1134		3.6673	1.6959	14.2700			-1.6180	3.7863						
Estradiol mustard	C1CC6(C)C(C2C1C4=C(CC2)C=C(OC(=O)C3=CC=C(N(CCCl)CCCl)C=C3)C=C4)CCC6OC(=O)C5=CC=C(N(CCCl)CCCl)C=C5	-	2.3433		1.8430		21.1695	1.4141		-0.6247	6.2694		-0.3993				
ethion	S(P(=S)(OCC)OCC)CSP(=S)(OCC)OCC	-	7.6687		2.8836												
ethyl anthranilate	O(C(=O)c1c(N)cccc1)CC	-	1.7694		0.3682		6.8475			-0.3652	0.8845			5.5600			
ethyl linoleate	CCC=CCC=CCC=CCCCCCCCC(=O)OCC	-	4.8992		11.2752	13.3955				-0.5215							
ethyl N-2-acetoxyethylnitrosocarbamate	O(C(=O)C)CCN(N=O)C(=O)OCC	+	2.8294		-0.4145					-1.3386							2.4300
Ethyl propionate	O=C(OCC)CC	-	3.5749		0.9727					-0.1227							
ethyl-1-nitrosourea, 1- [Ethylnitrosourea; Ethyl-N-nitroourea, N-; Nitroso-n-ethylurea, N-]]	C(C)N(C(=O)N)N=O	+	1.6333		0.2216					-0.8171				4.6597			2.3148
ethylaniline, N-	N(c1ccccc1)CC	-	2.9286		0.9993		1.1844				1.1944					3.2750	
ethylcarbazole, 9-	CCn1c2c(c3c1cccc3)cccc2	+	2.1933		1.2185		17.2447					5.3818					
ethylene oxide	O1CC1	+			2.0000												
ethylhexenal, 2-	O=CC(CCC=C)CC	-	2.2992	3.5853	2.8731	2.8846		0.2528									
ethylidene norbornene [Etheylidene-2-norborene, 5-]	C1(=CC)C2C=CC(C1)C2	-	2.1566		2.7474	7.2315		1.7372		1.6690							
Ethylurea, N- [Ethylurea]	O=C(N)NCC	+	1.8128		0.6648					-0.4665				4.6529		2.3472	
Famotidine	S(=O)(=O)(N)NC(=N)CCSCC1nC(NC(=N)N)=SC=1	-			1.4552		1.8395			-0.3715	1.3895			9.9274	14.4298	4.4965	
fensulfothion	S(=O)(C)c1ccc(OP(=S)(OCC)OCC)cc1	-	5.3570		0.8777		6.9144				1.3362						
Fluorescent brightner 225	n2c(nc(nc2N3CCOCC3)Nc4ccc(c(c4)S(=O)(=O)O)C=Cc5ccc(cc5S(=O)(=O)O)Nc6nc(nc(n6)Nc7ccccc7C)N8CCOCC8)Nc1c(cccc1)C	-	3.8818		4.1196	2.6672	23.5339				4.3438					12.5513	
Fluoroquinoline, 8-	Fc2c1ncccc1ccc2	+					1.1515				-0.2612	1.2890					
Folpet [Trichloromethylthio)phthalimide, n-(]	O=C1N(C(=O)c2c1cccc2)SC(Cl)(Cl)Cl	+					6.4762			-0.9224	0.6562		-1.7427				
formanilide	O=CNc1ccccc1	-				0.6624	9.2881				0.8264					2.5269	
furfural alcohol	o1c(CO)ccc1	-			-0.6944		4.9971				0.6111						
Gallic acid [anhydrous; sodium]	OC1=CC(C(O)=O)=CC(O)=C1O	-					1.6893			-1.2911	-2.3393						
glipizide	S(=O)(=O)(NC(=O)NC1CCCCC1)c3ccc(CCNC(=O)c2ncc(C)nc2)cc3	-	1.7889		5.8453		9.1466	0.2766		-1.1595	1.8260					7.5556	
glycidol	O1C(CO)C1	+			0.9549			0.1898									
Glycidyl methacrylate [Epoxypropyl methacrylate, 2,3-]	O1C(COC(=O)C(=C)C)C1	+	1.6211	3.4385	1.7854			0.1419		0.9366							
Glycine	O=C(O)CN	-			-0.2778					-0.9676				4.5718			
Guanidine [anhydrous; HCl]	NC(N)=N	-								-0.3333				8.9444	6.5556		
harman [anhydrous; HCl; harmane]	n2c(C)c1nc3c(c1cc2)cccc3	+	1.9943				12.5414				0.9988	4.4939					
Heptamethylnonane, 2,2,4,4,6,8,8-	CC(C)(C)CC(C)CC(C)(C)CC(C)(C)C	-	21.3619		3.9966			0.8388					1.3939				
hexabromocyclododecane, mixed isomers	BrC1CCC(C(CCC(C(CCC1Br)Br)Br)Br)Br	-			7.2418			3.3620									
hexachloroethane	ClC(Cl)(Cl)C(Cl)(Cl)Cl	-											-3.6997				
hexahydrodibenz(a,,j)anthracene, 1,2,3,4,8,9-	c24c(c1c(cccc1)CC2)cc3c5c(ccc3c4)CCCC5	+			7.5848		18.6166				6.2486	5.8878					
hexamethylenediisocyanate	O=C=NCCCCCCN=C=O	-			4.9445				2.9681								6.8288
hexylbenzoate	O(C(=O)c1ccccc1)CCCCCC	-	2.1627		5.4983		9.1132			-0.2157	0.6324						
hydroxy-2-acetylaminofluorene, 1- [Hydroxy-2-acetylaminofluorene, n-]	O=C(Nc1ccc2c(c1O)cc1ccccc12)C	-	1.4218				13.5572			-0.1937	0.5733	3.9580				2.6262	
hydroxy-2-acetylaminofluorene, 7-	O=C(C)Nc3ccc2c1c(cc(O)cc1)Cc2c3	+	1.5114		0.7982		11.3583			-0.6657	3.4248	2.3438				2.7843	
hydroxybenz(de)anthracen-7-one, 3-	O=C2c4c1c(c(O)ccc1c3c2cccc3)ccc4	+					16.6649			0.2713	1.6140	3.5466					
hydroxybenzaldehyde , 2-	C1=CC=C(C(O)=C1)C=O	-				0.6237	6.4652				0.3657						
hydroxyellipticine, 9-	Cc1c2c(c(c3ccncc13)C)nc1c2cc(cc1)O	+	4.1873				11.9942				2.6760	6.4416					
hydroxyethylpiperazinyl)-7-nitrobenzofuroxan , 4-(4·	o1n(=O)c3c(n1)c(N(=O)=O)ccc3N2CCN(CCO)CC2	+			3.4949		2.8830				0.3162	0.2787					
hydroxymethylbiphenyl, 4-	C2(C1=CC=CC=C1)C=CC(CO)=CC=2	-			0.1622		18.1574				3.3375						

hydroxyphenacetin, N- [Hydroxyphenacetin]	O=C(N(c1ccc(cc1)OCC)O)C	+	3.1788		0.5922		6.6337			-0.4227	1.1474									
hydroxytryptophan, L-5-	O=C(O)C(N)CC1C2=C(nC=1)C=CC(O)=C2	-			0.2350		6.6139	-0.9294		-1.3288	0.9426	1.6547		5.4684			3.7956			
IA 4 N-oxide	C12C3C4=C(SC1=C(CO)C=CC=2N(CCN(CC)CC)[N+]=3O)C=C(Cl)C=C4	+	4.2587		3.2891		9.4858				1.4738	5.2838								
Indomethacin	Clc3ccc(C(=O)n1c2c(c(CC(=O)O)c1C)cc(OC)cc2)cc3	-	3.2999		-0.1724		11.8663			-1.1899	2.8274	1.3436								
iodinated glycerol	O1C(CO)COC1C(C)I	+	2.1884		0.5777			0.1566												
isoamyl cinnamate	O(C(=O)C=Cc1ccccc1)CCC(C)C	-	4.2970		1.4332	3.2295	9.6966	0.5613		-0.2737	1.3600									
Isobutyl-p-hydroxybenzoate	OC1=CC=C(C=C1)C(OCC(C)C)=O	-	3.9526		0.4164		6.7862	0.3297		-0.3484	0.6543									
isodecyl diphenyl ester of phosphorous acid	CC(CCCCCCCOP(Oc1ccccc1)Oc1ccccc1)C	+	4.5746		8.1413		19.3927	0.8122			1.5338									
isophorone diisocyanate	O=C=NC1CC(C)(CN=C=O)CC(C)(C)C1	-	6.3956		3.1253			0.7519	3.2176				0.5615							7.5186
isopropyl methacrylate	O(C(=O)C(=C)C)C(C)C	-	5.2425	3.4336				-0.4737		0.1336										
Isotretinoin [1,3-cis-retinoic acid; isomer of Retinoic acid]	C1(C=CC(C)=CC=CC(C)=CC(=O)O)=C(C)CCCC1(C)C	-	1.7183		3.7220	11.2920				3.9230			0.2597							
juglone	O=C2c1c(O)cccc1C(=O)C=C2	+				2.3834	4.4588			-0.5711	0.2386									
Labetalol	O=C(N)c2c(O)ccc(C(O)CNC(C)CCc1ccccc1)c2	-	2.7750		2.2856		14.6473	-0.5320		-0.7170	1.6731			5.2445		3.2857				
Letrozole	n3(C(c1ccc(C#N)cc1)c2ccc(C#N)cc2)ncnc3	-					17.8863	-0.1513	4.2238		3.2133							17.8352		
lindane [Hexachlorocyclohexane; Benzenehexachloride, lindane, gamma-]	ClC1C(Cl)C(Cl)C(Cl)C(Cl)C1Cl	-						-2.6237												
Lovastatin [Mevacor]	C1C(C)C=C3C(C1OC(=O)C(C)CC)C(CCC2OC(=O)CC(O)C2)C(C)C=C3	-	8.3255		3.8558	6.7721		0.2362		0.8643										
Malathion [Carbophos]	S(P(=S)(OC)OC)C(C(=O)OCC)CC(=O)OCC	+	6.1940		0.3529			-0.7873		-1.8622										
maltol	O(C=CC1=O)C(C)=C1O	+	1.5245			2.4164				-0.4595										
mannide monooleate	O1C(CO)C(O)C(O)C(O)C1OC(=O)CCCCCCCC=CCCCCCCCC	-	2.2478		14.8938	4.5830		-6.9982		-0.5260										
Me2IQ, N-	N(C)(C)c1n(C)c3c(n1)c2c(nccc2)cc3	+	6.3787				9.9478				0.9550	4.2436								
menthane, p-	C1(C(C)C)CCC(C)CC1	-	7.1898		5.9276			2.9712												
Metformin HCl	CN(C)C(=N)NC(=N)N	-	3.3855							-0.1750				4.9358	13.7850	2.3125				
methoxy-2-propanol, 1-	OC(COC)C	-	3.2462		0.4356			-0.3247												
methoxy-4-aminoazobenzene, 3-	O(C)c2c(N)ccc(N=Nc1ccccc1)c2	+	1.5732				14.8347				2.7119			5.7995						8.2258
Methoxyacetaldehyde	O(C)CC=O	+	1.4856		0.2833	0.7833														
methoxyphenol, 4- [Hydroquinone monomethyl ether]	O(C)c1ccc(O)cc1	-	1.5897				6.5718				1.1722									
methyl 2-benzimidazolecarbamate [Carbendazim]	O=C(NC1=Nc2c(cccc2)N1)OC	+	1.3356				7.5656			-0.5379	0.3878	1.6785				2.4532	2.9377			
methyl anthranilate	O(C)C(=O)c1c(N)cccc1	-	1.3282				6.7895			-0.4000	0.8559			5.4963						
methyl furan	Cc1ccco1	-	1.9167				5.4497				0.9676									
methyl iodide	CI	+	1.9729																	
methyl methanesulfonate [MMS]	CS(=O)(=O)OC	+	2.1134																	
Methyl-2-amino-5chloro-be__, 1-	ClC2C=C1N=C(N)[n+](C)C1=CC=2	+	1.8736				5.5277				1.1878	1.8328		5.6114						
methyl-2-nitroaniline, 4-	O=N(=O)c1c(N)ccc(C)c1	+	1.7842				4.7273				1.2454			5.3487						
methyl-3-butyn-2-ol, 2-	OC(C)(C)C#C	-	3.1250			4.8556			2.1597				-0.9356							
methyl-3-nitroaniline , 4-	O=N(=O)c1c(C)ccc(N)c1	+	1.6782				4.6392				1.1218			5.3683						
methyl-5-nitrobenzimidazole, 2-	O=N(=O)C2C=C1N=C(C)nC1=CC=2	+	1.8113				4.5757				0.8282	1.4535					2.9986			
methyl-6-methoxy-2-amino-benzothiazolium chloride , 3-	COc1ccc2c(c1)CC(=[N+]2C)N	+	3.6539		0.8225		6.2149			0.8919	3.3590			5.8218						
methylbenz(a)anthracene, 12-	c14c(cccc1)cc2c(c3c(cc2)cccc3)c4C	+	2.2332				24.7000				1.3795	8.5321								
methylbenzoate	O(C)C(=O)c1ccccc1	-	1.3737				8.8776			-0.2911	0.5880									
methylbutyl-4-methoxybenzyladine-4''-aminocyannate, (+)-2-	O(C)c2ccc(C=Nc1ccc(C=CC(=O)OCC(C)CC)cc1)cc2	+	5.7775		1.4526	5.4440	15.3415	0.3844		-0.3135	3.5889									4.4451
methylene blue [anhydrous; trihydrate]	S1c3c(Nc2c1cc(N(C)C)cc2)ccc(N(C)C)c3	+	8.2873				13.6413				7.3870					3.5149				
methylene-bis(4-chlorophenol), 2,2''-	Clc1ccc(c(c1)Cc1c(ccc(c1)Cl)O)O	+			0.3738		9.6623				2.6725									
methylformamide, N-	O=CNC	-	1.5625			0.6250										2.2500				
methylolacrylamide, N-	O=C(NCO)C=C	-		3.1566	-0.3285	1.9347				-0.3588						2.9375				
methylpyrene, 1-	c24c1c3c(ccc1ccc2C)cccc3cc4	+	2.1864				19.8954				1.3572	8.2277								
methylquercetin, 3''-O-	O=C1C(=C(c2cc(c(cc2)O)OC)Oc2c1c(cc(c2)O)O)O	+	1.3526				6.2390			-1.7197	-0.8374									
methylquinoline, 8-	n2c1c(cccc1C)ccc2	+	2.7877				12.7980				1.2390	2.3218								
methyltetrahydrofuran, 2-	O1C(C)CCC1	-	2.1186		3.5163			0.5463												
Midodrine	O(C)c1ccc(OC)c(C(O)CNC(=O)CN)c1	-	3.4629		-0.4153		5.9131	-0.8838		-0.3232	1.6893			5.1629		2.5960				
Moexipril	O(C)c1c(OC)cc3c(c1)CC(C(=O)O)N(C(=O)C(C)NC(C(=O)OCC)CCc2ccccc2)C3	-	6.4521		1.5156		13.2623	-2.5646		-1.9421	3.6546					3.8976				
monocrotophos [anhydrous;]	P(=O)(OC(C)=CC(=O)NC)(OC)OC	-	5.3266			1.1435				-0.2152						2.3512				
Moricizine (Ethmozin)	S2c4c(N(C(=O)CCN1CCOCC1)c3c2cccc3)cc(NC(=O)OCC)cc4	-	1.7588		4.5326		13.4913			-0.4766	4.2565					2.7297				
Nafenopin	O(C(C)(C)C(=O)O)c3ccc(C2c1c(cccc1)CCC2)cc3	-	3.1123		3.5446		16.4963	0.4185		-0.9696	4.7578		-1.2233							
naphthylhydroxamic acid, 2-	O=C(NO)c2ccc1c(cccc1)c2	+					12.9913			-0.4943	0.4519	2.5147				1.6722				
Naratriptan	S(=O)(=O)(NC)CCC3C=C2C(nC=C2C1CCN(C)CC1)=CC=3	-	3.6336		5.3421		8.3722	0.5937			2.4551	2.3879				2.3723	3.3633			
Nicotinamide [Niacinamide]	O=C(N)c1cnccc1	-					6.3972			-0.4416	0.4421			4.9348						
nitrilotriacetic acid [Nitrilotriacetic acid, trisodium salt]	O=C(O)CN(CC(=O)O)CC(=O)O	-			-1.7958					-3.7847										
nitro-1-naphthalenecarbonitrile, 5-	N#Cc1c2c(ccc1)c(ccc2)[N+](=O)[O-]	+					9.8856		2.3391		0.6257	1.2236						8.8688		

nitro-2-furamidoxime, 5-	o1c(C(N)=NO)ccc1N(=O)=O	+					2.3617			-0.3268	-0.4854			5.9139					2.6947
nitro-2-furanyl)ethenyl)-2-thiazolyl)acetamide, N-(4-(2-(5-	s2c(NC(=O)C)nc(C=CC1oC(N(=O)=O)=CC=1)c2	+	1.4168			3.2123	4.5261			-0.1884	1.1833						2.5642		
nitro-2-thienyl)-2-thiazolylformamide, N-(4-(5-	S2=C(NC=O)nC(c1sc(N(=O)=O)cc1)=C2	+				0.5412	4.8156				1.8919						2.4248		
nitroacenaphthene, 5-	O=N(=O)C1C3C2C(=CC=1)CCC2C=CC=3	+			1.3150	11.6700		0.6669		2.3688									
nitro-alpha,alpha,alpha-trifluorotoluene, 3- [Nitrobenzotrifluoride, 3-]	FC(F)(F)c1cc(N(=O)=O)ccc1	-					3.2948				-1.5727		-4.5357						
Nitrobenzo(b)thien-3-yl)amino)phenol, 4-((2- [Ref117mol12]	s2c3c(c(Nc1ccc(O)cc1)c2N(=O)=O)cccc3	+					13.8122				1.4123	1.6785					3.6180		
nitrobenzofuroxan, 4-	o1n(=O)c2c(n1)c(N(=O)=O)ccc2	+					4.4442				-0.2400	0.1833							
nitrobenzyl chloride, p-	ClCc1ccc(N(=O)=O)cc1	+			0.3869		6.1724				0.9825								
Nitro-h6-benzanthracene, 3-	O=N(=O)c4cc3c(c1c(cc2c(c1)CCCC2)CC3)cc4	+			6.8549		1.3533				5.7326	2.4880							
nitro-N-methylphthalimide, 4-	CN1C(=O)c2cc(ccc2C1=O)[N+](=O)[O-]	+	1.3594				3.8333			-0.8794	0.2993								
nitro-o-phenylenediamine HCl, 4-	[O-][N+](=O)c1ccc(c(c1)N)N	+					4.1179				0.7266			1.7184					
nitrophenol, 2-	O=N(=O)c1c(O)cccc1	-					5.5493				-0.5619								
nitrophthalhydrazide, 4-	O=N(=O)c2cc1c(c(O)nnc1O)cc2	+					3.6383				-1.1984	0.3124							
nitroso-1,1''-biphenyl, 4-	O=Nc2ccc(-c1ccccc1)cc2	+					17.2389				2.7160								2.8553
nitroso-1,2,3,6-tetrahydropyridine, N-	O=NN1CC=CCC1	+			2.4119	4.6530													2.7796
nitrosocarbaryl [Naphthyl N-nitroso-N-methylcarbamate]	O(c2c1c(cccc1)ccc2)C(=O)N(C)N=O	+	1.2366				12.8488			-0.8893	0.4611	1.7659							2.4735
nitroso-N-methyl-N-alpha-acetoxybenzylamine , N-	O(C(=O)C)C(N(C)N=O)c1ccccc1	+	2.7383				8.9466	-0.7628		-0.4589	0.7352								2.7243
nitrosophenol, 4-	O=Nc1ccc(cc1)O	+					5.7237				0.4678								2.6556
nonanal	O=CCCCCCCCC	-	2.2137		8.3788	1.1371													
octachlorodibenzo-p-dioxin	Clc2c(Cl)c(Cl)c(Cl)c3Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Oc23	-									0.2826								
octyl methacrylate	O=C(C(=C)C)OCCCCCCCC	-	3.8732	3.5199	7.7952					0.2172									
oleic acid [anhydrous; potassium; diethanolamine condensate]	O=C(O)CCCCCCCC=CCCCCCCCC	-	2.2588		16.5795	4.6626				-0.6642									
orotic acid	O=C(O)c1nc(O)nc(O)c1	-					0.8354			-1.3352	-1.7850								
oxazepam	Clc3ccc2NC(=O)C(O)N=C(c1ccccc1)c2c3	-					14.4671	-1.4339		-0.1995	2.6220						2.6369		4.1112
oxybis(2-chloroaniline), 4,4''- [Dichloro-4,4''-diaminodiphenyl ether, 3,3''-]	Clc1c(ccc(c1)Oc1ccc(c(c1)Cl)N)N	+					1.8970				3.8969			11.2190					
Oxybutynin	C(O)(C(=O)OCC#CCN(CC)CC)(C1=CC=CC=C1)C2CCCCC2	-	4.1852		7.4885		9.1937	-0.1252	5.9266	-0.5762	0.6185		-1.5811						
Pemirolast	O=C2N3C(=NC=C2C1nN=NN=1)C(C)=CC=C3	-	1.8924				6.7871				1.1813	0.6192							
pentabromotoluene	Brc1c(Br)c(Br)c(Br)c(Br)c1C	-	2.3782								6.3360								
pentachloroanisole	Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1OC	+	1.4137								0.9289								
pentachlorotoluene, 2,4,alpha,alpha,alpha-	Clc1ccc(C(Cl)(Cl)Cl)c(Cl)c1	+					4.7249				1.2980		-1.4983						
pentamidine [anhydrous, isethionate]	O(c1ccc(C(=N)N)cc1)CCCCCOc2ccc(C(=N)N)cc2	-			4.1932		14.4184			0.1158	2.9586			1.8242	14.6795				
pentylphenyl 4-methoxybenzoate, 4-	COC(=O)Oc1ccc(cc1)CCCCCc1ccccc1	-	1.2978		5.7986		18.1896			-0.6864	3.1837								
Peri acid: 1-naphthylamine-8-sulfonic acid	Nc1cccc2cccc(c12)S(=O)(=O)O	+					9.6826				0.1795	1.4873		5.6782					
phenesterine	ClCCN(c5ccc(CC(=O)OC4CC3C(C)(C2C(C1C(C)(C(C(C)CCCC(C)C)CC1)CC2)CC=3)CC4)cc5)CCCl	-	12.4769		15.6659	5.1318	8.1632	4.9230		1.4869	2.6360		0.6661						
phenobarbital [anhydrous; sodium]	C1(NC(NC(C1(C1=CC=CC=C1)CC)=O)=O)=O	-	1.7385		0.2936		8.7232			-1.9286	0.5880		-1.3135				4.2850		
Phentolamine	N1C(CN(C2=CC=C(C=C2)C)C2=CC(O)=CC=C2)=NCC1	-	2.7449		2.4352		15.6768			0.9852	3.5368						3.2985		4.4679
phenylene diisocyanate, p-	O=C=Nc1ccc(N=C=O)cc1	-					6.2265		2.8496		0.9627								6.7243
phenylenediamine, o-	Nc1c(N)cccc1	+					7.2524				1.2917			1.7896					
phenylpiperazinyl)-4-nitrobenzofuroxan, 7-(	o1n(=O)c4c(n1)c(N(=O)=O)ccc4N3CCN(c2ccccc2)CC3	+			2.9437		13.5719				1.5181	0.7440							
Phorbol diburate	C12C3(O)C(C=C(CO)CC1(O)C(=O)C(C)=C2)C1C(OC(=O)CCC)(C(OC(=O)CCC)C3C)C1(C)C	-	1.9600		1.6230	3.3850		-3.8679		-0.5285			-5.4867						
Pimozide	Fc5ccc(C(c1ccc(F)cc1)CCCN4CCC(N2c3c(NC2=O)cccc3)CC4)cc5	-			6.6484		21.1292	0.3145		-0.2678	3.4615						2.9672		
piperonyl sulfoxide	S(=O)(C(C)Cc2cc1OCOc1cc2)CCCCCCCC	-	4.3116		9.4574		6.7720	0.1975			2.7954								
Pravastatin	O(C(=O)C(C)CC)C2C1C(C=CC(C)C1CCC(O)CC(O)CC(=O)O)=CC(O)C2	-	5.8488		1.7239	5.8852		-2.9300		-0.3933									
prednisone	O=C4C2C1(C)C(=CC(=O)C=C1)CCC2C3C(C)(C(O)(C(=O)CO)CC3)C4	+	3.8884		1.9937	5.1318		-0.6169		0.5197			-2.8926						
propanediol (2,2-bis(benzoyloxyl)methyl)-dibenzoate	O(C(=O)c1ccccc1)CC(COC(=O)c2ccccc2)(COC(=O)c3ccccc3)COC(=O)c4ccccc4	-			-1.5283		33.2551			-2.5900	1.1868		-1.4268						
propyl gallate	O(C(=O)c1cc(O)c(O)c(O)c1)CCC	-	1.8463		0.9474		2.6954			-0.6559	-1.7683								
propyl)chlorothioformic acid, S-(N-	ClC(=O)SCCC	+	2.6770		1.8388					-0.3384									
Propylacrolein, 2-	O=CC(=C)CCC	+	2.2254	3.4949	1.8483	0.8928				0.6968									
quercetin pentaacetate	O2C(c1cc(OC(=O)C)c(OC(=O)C)cc1)=C(OC(=O)C)C(=O)c3c2cc(OC(=O)C)cc3OC(=O)C	+	5.5565				6.1820			-5.5137	-1.8127								
Quinapril	O(C(=O)C(NC(C)C(=O)N2C(C(=O)O)Cc1c(cccc1)C2)CCc3ccccc3)CC	-	3.4265		1.8460		17.3397	-2.3530		-1.7974	2.9672						3.9365		
Rabeprazole [anhydrous;]	C1=CC=C3C(=C1)NC(S(=O)CC2=NC=CC(OCCCOC)=C2C)=N3	+	3.6417		2.3445		11.1531				2.8925	1.6912						3.1138	
Repaglinide	O(c3c(C(=O)O)ccc(CC(=O)NC(c2c(N1CCCCC1)cccc2)CC(C)C)c3)CC	-	6.1435		7.1460		13.2690	0.3375		-1.1246	3.5115						3.2587		
Riboflavine tetrabutyrate	C12=C(C=C(C(C)=C2)C)N=C2C(NC(N=C2N1CC(C(C(COC(CCC)=O)OC(CCC)=O)OC(CCC)=O)OC(CCC)=O)=O)=O	-	1.8923		1.2237		3.5589	-4.1969		-4.4196	2.5837						2.1269		8.5124
Rivastigmine (Exelon)	C1(OC(=O)N(C)CC)=CC=CC(C(C)N(C)C)=C1	-	9.7797		0.6316		7.6476	0.2848		-0.3268	1.7185								
safrole	O1COC2=CC(CC=C)=CC=C12	-		3.6774	1.2118	1.8726	5.9448				2.8894								
Salicylamide [Hydroxybenzamide, 2-]	O=C(N)c1c(O)cccc1	-					6.1521			-0.6129	0.8119			4.9156					

siduron	O=C(NC1C(C)CCCC1)Nc2ccccc2	-	2.2149	4.8333		9.5533	0.9146		-0.8893	0.8412					5.9268		
Stearyl lactylate calcium	OC(=O)C(C)OC(=O)C(C)OC(=O)CCCCCCCCCCCCCCCCC	-	4.8979	19.1548			-2.3427		-2.5217								
sterigmatocystin	O(C)c5c2C(=O)c1c(O)cccc1Oc2c3c(OC4OC=CC34)c5	+	1.4745		3.4528	6.3971	-0.6482		-0.3376	2.6847							
streptomycin [anhydrous; sulfate]	N=C(NC1C(C(C(C(C1O)NC(=N)N)O)O)OC1C(C(C(O1)C)(C=O)O)OC1C(C(C(C(O1)CO)O)O)NC)N	-	2.7337	-0.7648	0.1357		######		-1.2875		-2.3878	1.7663	15.2623	7.4992			
sucrose	O2C(CO)C(O)C(O)C(O)C2OC1(CO)OC(CO)C(O)C1O	-		-2.3224			######				-2.2218						
sulfolene, 3-	S1(=O)(=O)CC=CC1	-		0.4861	3.3519												
Tenoxicam	C(=O)(NC1=NC=CC=C1)C2N(C)S(=O)(=O)C3=C(C=2O)SC=C3	-	1.1817			9.2758			-1.8724	0.2762					2.4238		
tetrabromodibenzo-p-dioxin, 1,3,6,8-	Brc1cc(c2c(c1)Oc1c(cc(cc1Br)Br)O2)Br	-				7.5788				6.2356							
tetrachloroazobenzene, 3,3",4,4"-	Clc1c(ccc(c1)N=Nc1cc(c(cc1)Cl)Cl)Cl	+				1.1440				3.3320							8.5878
tetrachlorobiphenyl, 3,4,3",4"-	Clc1c(ccc(c1)c1cc(c(cc1)Cl)Cl)Cl	-				1.8591				4.6822							
tetrachlorophthalic anhydride	Clc2c(Cl)c1c(C(=O)oC1=O)c(Cl)c2Cl	-							-1.7491	-0.6826							
tetraethylene glycol diacrylate	O(CCOCCOCCOC(=O)C=C)CCOC(=O)C=C	-		6.5458 2.6633	2.1973				-0.9338								
tetrahydrobenz(a)anthracene-3,4-epoxide , 1,2,3,4-	O1C2C1CCc1c2ccc2cc3c(cc12)cccc3	+		2.3434		17.8485	0.8935			2.9454	5.4441						
tetramethoxy-dibenzo(g,p)chrysene, 3,6,14,14-	O(C)c2ccc1c4c(c3c(c1c2)cc(OC)cc3)c6c(c5c4ccc(OC)c5)cc(OC)cc6	+	6.8777			25.2220				3.3545	11.6314						
tetramethyl-1,3-butanediamine, N,N,N",N"-	N(C)(C)C(C)CCN(C)C	-	1.7312	2.4300			0.6967										
Theanine, L-	NC(=O)CCC(C(=O)O)NCC	-	1.8576	0.9149			-0.6644		-1.4193			4.8775		2.7390			
thioglycolic acid [anhydrous; sodium]	SCC(=O)O	-		-0.8333					-0.8812								
Ticlopidine	Clc3c(CN2CCC1=C(C=C1)C2)cccc3	-		4.3898	4.4685	8.1191			3.6363	2.1138							
Tolcapone	O=C(c1ccc(C)cc1)c2cc(O)c(O)c(N(=O)=O)c2	-	1.8665			8.6358			-0.4697	-1.2314							
toluenediamine, 2,6- [anhydrous; 2HCl; Diaminotoluene, 2,6-]	CC1=C(C=CC=C1N)N	+	1.9741			5.5229				2.4884		11.8130					
tolunitrile, m-	N#Cc1cccc(C)c1	-	1.9736			7.5156		2.6778		1.8649						8.4124	
Tranexamic acid	C(=O)(O)C1CCC(CN)CC1	-		4.3350			0.4754		-0.6385			5.4774					
triaziquone [Trenimon]	C4(N1CC1)=C(N2CC2)C(=O)C=C(N3CC3)C4=C	+		5.4622	1.5238				1.9359								
tribromoacetic acid	BrC(Br)(Br)C(=O)O	+							-1.6947		-1.1458						
tribromsalan	Brc2ccc(NC(=O)c1c(O)c(Br)cc(Br)c1)cc2	-				1.4273			-0.3733	2.8659					2.7193		
trichloro-2,3-epoxypropane, 1,1,1-	ClC(Cl)(Cl)C1OC1	+		0.5799			-0.1559				-1.1944						
trichloroethane, 1,1,2-	ClC(Cl)CCl	-		0.3864			-0.4586										
trichlorophenol, 3,4,5-	Clc1c(Cl)cc(O)cc1Cl	-				2.6583				0.7962							
triethyl phosphate	P(=O)(OCC)(OCC)OCC	-	5.2223	0.9919													
triethylamine	N(CC)(CC)CC	-	6.5625	3.5625													
triethylene glycol	O(CCO)CCOCCO	+		1.7283													
triethylene glycol dimethyl ether	O(CCOC)CCOCCOC	+	3.3247	3.7684													
trimesoyltri[2-ethyl aziridine], 1,1",1"-	O=C(N1CC1CC)c1cc(cc(c1)C(=O)N1CC1CC)C(=O)N1CC1CC	+	6.1767	5.3845		4.9913	0.8453		-0.2466	1.3477							
Trimethoprin/Sulfamethoxazole B	O=S(=O)(c1ccc(cc1)N)Cc1noc(c1)C	-	1.7146	-0.1724		7.6864				1.7538		5.5369					
trimethylhexan-1-ol, 3,5,5-	OCCC(C)CC(C)(C)C	-	8.9684	2.4743			0.6575				0.4113						
triphenyl phosphine	P(c1ccccc1)(c2ccccc2)c3ccccc3	-				32.3259				4.1942							
tris(2-hydroxyethyl)triazine-2,4,6-trione, 1,3,5-	O=C1N(CCO)C(=O)N(CCO)C(=O)N1CCO	-		-2.8213					-2.6631								
valeronitrile	CCCCC#N	-	2.8690	2.9334				2.6870								7.9474	
versiconal acetate	O(C(=O)C)CCC(c3c(O)cc2C(=O)c1c(c(O)cc(O)c1)C(=O)c2c3O)C=O	+	1.1763	-0.2586	0.4600	2.8176	-1.1274		-2.2917	-4.2836							
Vigabatrin	O=C(O)CCC(N)C=C	-		3.4262 5.5894	1.5446		-0.1795		-0.8127			5.3399					
vinyl fluoride	C=CF	-		2.6944	0.2500												
Vitamin K1 [Phytonadione; K1]	O=C1c2c(C(=O)C(CC=C(C)CCCC(C)CCCC(C)CCCC(C)C)=C1C)cccc2	-	13.3871	12.2584	2.1542	7.1786	2.4713		2.5947	1.9779							
Xylidine, 3,4- [Dimethylaniline, 3,4-]	Nc1ccc(C)c(C)c1	+	4.1393			5.9329				3.4280		5.5275					
Ziprasidone [anhydrous;]	C1=CC=C5C(=C1)SN=C5N4CCN(CCC2=C(Cl)C=C3C(=C2)CC(=O)N3)CC4	+		6.3634		12.4362			0.4999	4.9212	2.5758				2.8573		
Zopiclone	N3(C1=CC=C(Cl)C=N1)C(OC(=O)N2CCN(C)CC2)C4=C(C3=O)N=CC=N4	-	1.9981	2.6392		7.5695	-1.2596		-0.9283	1.1784							

SaaN	SsssN	SddsN	SdaaN	SsssNp	SsOH	SdO	SssO	SaaO	SsF	SsPH2	SssPH	SsssP	SdsssP	SssssssP	SsSH	SdS	SssS	SaaS	SdssS	SddssS	SsssssssS	SsCl	SsBr	SsI	SsCH3_acnt	SdCH2_acnt	SssCH2_acnt	StCH_acnt	SdsCH_acnt	SaaCH_acnt	SsssCH_acnt	SddC_acnt	StsC_acnt	SdssC_acnt	SaasC_acnt	SaaaC_acnt	SsssssC_acnt	SsNH3p_acnt	SsNH2_acnt	SssNH2p_acnt	SdNH_acnt	SssNH_acnt	SaaNH_acnt
8.8199																														7.0000					1.0000	6.0000			1.0000				
							1.1200																		3.0000		2.0000				1.0000												
					7.4167	9.0000																			1.0000									1.0000									
3.7933						21.5942																			1.0000					4.0000				2.0000	1.0000							2.0000	
3.4665		-0.6325				3.7334																			1.0000					2.0000				1.0000	2.0000								
					8.6686	1.5573	5.3985																		6.0000				6.0000	1.0000				3.0000	5.0000								
																											4.0000						2.0000										
						24.3272	22.4730																		1.0000		4.0000			1.0000	2.0000			4.0000	5.0000								
																									1.0000	2.0000	6.0000		2.0000	1.0000	2.0000			4.0000	5.0000								
					49.6460	25.4847	1.6614																				1.0000			6.0000	5.0000			2.0000	6.0000								
						1.1826	4.4653																			2.0000	1.0000		2.0000					1.0000									
							9.9594																			1.0000	3.0000		1.0000		1.0000												
8.4994	1.8874		2.1463			12.9470																			2.0000		3.0000			5.0000				1.0000	4.0000	2.0000							
																									2.0000					2.0000					4.0000				2.0000				
							5.1657																		3.0000					1.0000					5.0000				2.0000				
		-0.6915				2.6244																5.5631								2.0000					4.0000				2.0000				
4.3771		-0.4128				2.8485												2.4173												3.0000					4.0000				1.0000				
		-1.7763			9.8492	41.2250																								2.0000					4.0000				1.0000				
		-0.5643			8.4752	2.7838	5.1812																				2.0000			3.0000					3.0000				1.0000				
																	1.6250										2.0000							1.0000					1.0000				
																														9.0000					1.0000	4.0000			1.0000				
						24.3697																								7.0000				2.0000	5.0000				1.0000				
					8.5393	2.9720														-4.1532										4.0000					2.0000				1.0000				
4.1944																		1.5188												4.0000					1.0000	2.0000			1.0000				
4.1534																														6.0000					1.0000	2.0000			1.0000				
4.1557																														6.0000					1.0000	2.0000			1.0000				
1.1413																														1.0000					1.0000				1.0000				
3.9769						11.9600																							2.0000	4.0000				3.0000	1.0000				1.0000			1.0000	
	3.4936					11.6342																			2.0000				1.0000	5.0000				2.0000	1.0000								
						22.1980	33.6957													-4.1373					4.0000		2.0000				3.0000						3.0000		1.0000				
	2.1856				8.2350																						4.0000																
	0.5768					11.8470	1.6471																		2.0000					8.0000					4.0000								
					17.4322	44.5698																					2.0000			7.0000				3.0000	5.0000							1.0000	
4.2500			1.3352			23.6798	4.5483																		2.0000		3.0000			4.0000				2.0000	1.0000	2.0000						2.0000	
																														8.0000					4.0000				2.0000				
					18.5679	45.8830														-9.3284										6.0000					6.0000				2.0000				
					2.6422		5.6672																							8.0000	4.0000				2.0000	6.0000							
					2.6422		5.6672																							8.0000	4.0000				2.0000	6.0000							
									35.3636																					5.0000					1.0000		1.0000						
					9.4773	11.6566	5.9622																				1.0000			9.0000				1.0000	3.0000								
3.5624	4.3814	-0.5636	0.2446			34.1917		4.6695																			5.0000			7.0000					3.0000	2.0000							
					3.1798	11.3563																			2.0000		8.0000		4.0000		5.0000			1.0000								1.0000	
							11.9873																28.8114		2.0000		4.0000			4.0000	2.0000				8.0000		1.0000						
						24.7400	1.9635																		4.0000		1.0000			4.0000	2.0000			2.0000	2.0000								
																	1.6939													8.0000					4.0000				2.0000				
	3.4887				2.1887	26.1164																			4.0000					4.0000				2.0000	8.0000								
4.5274						22.2339	1.2214																		2.0000					12.0000	1.0000			2.0000	5.0000								
4.3125						11.6573																	3.4430				1.0000			7.0000				2.0000	4.0000							1.0000	
						9.3582																	2.8176			1.0000			1.0000					1.0000									
																						5.6150	3.2776							4.0000					2.0000									
																							3.6884		1.0000		1.0000			1.0000					2.0000	6.0000								
					9.9754	11.8738	5.7375																		3.0000		5.0000			3.0000	1.0000			1.0000	3.0000		1.0000						1.0000	
						12.5344																5.8547			4.0000					4.0000	1.0000			1.0000	2.0000		1.0000						1.0000	
						2.8568	4.4375													-3.8276							4.0000																
4.1323			2.8758														1.7242					18.6696					3.0000			1.0000	1.0000				5.0000								
					8.2460		4.9732																		1.0000		5.0000																

	2.5369												2.0000				9.0000				3.0000				
					9.5983	4.5486							3.0000			1.0000							1.0000		
						1.6558							3.0000		2.0000		4.0000	1.0000			2.0000		1.0000		
													3.0000										1.0000	1.0000	
	1.3369			8.4266	9.9656								1.0000		5.0000										
	1.3814			8.3479	2.3713								1.0000		6.0000					1.0000					
													4.0000				4.0000				2.0000		1.0000		
					9.8875	4.5000							1.0000		1.0000			1.0000		1.0000					
													2.0000	1.0000	3.0000			2.0000		1.0000			1.0000		
			1.5464		11.7533											2.0000	8.0000			1.0000	4.0000			1.0000	
	3.6851				36.5614	1.1570							2.0000		5.0000			1.0000		7.0000				1.0000	
4.6326				1.2811		16.8987							1.0000		4.0000		11.0000	1.0000			3.0000	4.0000			1.0000
11.1194	4.5132			19.6570	76.9490				2.3299				2.0000		4.0000	1.0000	4.0000	3.0000		8.0000	3.0000				2.0000
4.9582				29.9270	1.7951	5.4989		13.6828					5.0000		3.0000	2.0000	4.0000	4.0000		1.0000	7.0000				
											5.1497			2.0000		1.0000				1.0000					
		-0.9675			2.5940			36.2920			5.3323						3.0000				3.0000		1.0000		
	2.9150			8.9996	46.5456						5.9612		2.0000		5.0000		6.0000			3.0000	6.0000				1.0000
											5.8189					1.0000	4.0000		2.0000	1.0000	2.0000				
				1.9746	12.2975	5.2143					11.7818		1.0000		1.0000		8.0000			1.0000	4.0000		1.0000		
											5.1820	5.9586						1.0000							
					1.1718	4.4514					5.1917			1.0000	2.0000	1.0000				1.0000					
	0.8349				21.8294						5.4414				7.0000			1.0000		1.0000					1.0000
											14.4167							1.0000							
	1.5816				23.6777						5.7330		3.0000		5.0000		3.0000			2.0000	3.0000				1.0000
											5.9574						7.0000				1.0000	2.0000			
				8.7286							5.4850						4.0000				2.0000				
											5.6117		1.0000				4.0000				2.0000				
				1.3546	74.3524	33.1341							4.0000		1.0000		6.0000	5.0000		6.0000	6.0000				
	4.2477			29.1387	71.7426					######			2.0000		4.0000	4.0000	16.0000			3.0000	8.0000				
				29.9265	73.1170	5.2444				######			3.0000				18.0000				14.0000	2.0000			
				2.4165	24.8498	5.9883					25.2787	13.2354				1.0000	1.0000			7.0000	11.0000				
				5.6443	71.7243					######							15.0000				13.0000	4.0000		2.0000	
				6.2390	95.2448					######							14.0000				14.0000	4.0000		2.0000	
				4.5168	49.3630					-1.6530							19.0000				13.0000	2.0000		1.0000	
				29.8237	47.7670	5.4529				-9.8294			3.0000		1.0000		14.0000				12.0000	2.0000			
	4.5484			9.8958	12.7270		6.4676						4.0000		4.0000		1.0000			1.0000	5.0000	4.0000			
				17.7990	33.6867				1.4648				2.0000		6.0000	1.0000		2.0000		4.0000			1.0000	1.0000	1.0000
					9.8914											3.0000	5.0000				1.0000				
					1.2518								3.0000		2.0000	3.0000				2.0000					
				1.1412		1.4729							2.0000				9.0000				5.0000	2.0000			
	2.1343				12.2135	4.9818					6.2579		1.0000		3.0000	2.0000	4.0000	1.0000		3.0000	2.0000				
				8.8136									1.0000				4.0000				2.0000				
						1.5886							1.0000		2.0000		4.0000	1.0000			2.0000				
				19.8490	23.8589	9.9964							2.0000		1.0000	4.0000	6.0000			2.0000	6.0000				

	2.2262															2.0000		2.0000	3.0000	8.0000				1.0000	4.0000						
			1.3483	34.8356												2.0000		5.0000			5.0000			3.0000						1.0000	
	1.3618			24.3322							1.4352							5.0000		4.0000	1.0000			2.0000	2.0000						
																		1.0000		8.0000					2.0000	4.0000					
			19.8787	23.9257									-4.5333							12.0000					4.0000	4.0000					
					6.1856										35.3862										12.0000						
4.5589	4.2600			36.9616									-3.3624			3.0000		4.0000		7.0000	1.0000			1.0000	4.0000	2.0000				2.0000	1.0000
3.9899	1.9256		18.1922													1.0000		4.0000		7.0000					4.0000						
				11.8280																8.0000				1.0000	4.0000			2.0000		1.0000	
				2.2356																				2.0000				2.0000		3.0000	
			28.1634	44.9453									-9.5364							2.0000					6.0000	2.0000		3.0000			
																1.0000				3.0000					3.0000			2.0000			
																				8.0000					4.0000				2.0000		
																				14.0000						8.0000					
					5.6575													2.0000		1.0000					2.0000						
																2.0000		6.0000												1.0000	
														1.6486			1.0000	1.0000	1.0000		1.0000										
	-0.3252		8.4637	1.3476										11.5654						3.0000					3.0000						
	1.5869			11.8775	5.5158									11.2536		1.0000		1.0000		4.0000	2.0000			1.0000	2.0000						
				1.1683										11.1915					1.0000	3.0000					3.0000						
			8.4984	1.3627										11.1231						3.0000				1.0000	3.0000						
														9.7332							1.0000		1.0000								
		-0.5569		2.4222										11.1300						3.0000					3.0000						
			8.8531											11.9269						3.0000					3.0000						
8.9236														11.3642						4.0000					2.0000	2.0000					
																		1.0000			2.0000	1.0000									
			43.8962	4.1695	17.4999											3.0000		3.0000	3.0000	1.0000	8.0000			4.0000	5.0000		1.0000	1.0000			
					1.7529			-2.1647	4.2833	4.8725						2.0000		2.0000													
																2.0000		2.0000												1.0000	
			16.1726		4.6319													4.0000													
																4.0000		1.0000			2.0000									1.0000	
3.8229							25.5845													5.0000					2.0000	2.0000					
					21.2633													4.0000		4.0000	2.0000				2.0000						
				12.9670	5.6119											2.0000		2.0000		6.0000				1.0000	4.0000	4.0000					
	1.1484		39.3654	92.3963	4.2798							-2.5147	######					4.0000		9.0000	2.0000			1.0000	5.0000	2.0000					
				11.8850												1.0000		2.0000		7.0000				1.0000	3.0000	4.0000					
					1.8274														2.0000	4.0000	2.0000				2.0000						
	0.3785		18.2655	1.9888	4.8188															4.0000	1.0000			1.0000	2.0000						
			72.4956	48.3494									-4.9418							21.0000				2.0000	15.0000	6.0000					
			3.1978													4.0000	1.0000	1.0000	2.0000		5.0000			3.0000			2.0000				
																4.0000				4.0000	2.0000				2.0000						
				1.5690	8.8428			-2.6543								3.0000															
																2.0000		1.0000	1.0000	7.0000				1.0000	3.0000	4.0000					
	2.2825															3.0000		11.0000													
11.4296	1.1870			49.3678	9.8886								-4.4589			4.0000				4.0000				2.0000	5.0000					2.0000	
3.9120	2.4333															2.0000				4.0000					1.0000						
																2.0000				3.0000					3.0000			1.0000			
																2.0000				8.0000					2.0000	4.0000					
						5.8333										2.0000				2.0000					2.0000						
																2.0000														2.0000	
																2.0000				4.0000					2.0000	2.0000					1.0000
					5.4236											2.0000		2.0000			2.0000									1.0000	

						2.8440	8.5968																		2.0000		2.0000							2.0000								
	-1.4976				17.9351	2.9790																5.5288								2.0000					4.0000				1.0000			
		-1.3472				4.6348																								4.0000					2.0000							
		-0.8653				44.8788																								8.0000					2.0000	6.0000						
		-1.5139				41.6554																			1.0000					3.0000					3.0000							
					51.6427		4.4252																				4.0000										2.0000					
																									4.0000		2.0000			4.0000	2.0000				2.0000							2.0000
					16.8230	2.4275																					1.0000							2.0000								
																									1.0000		11.0000			5.0000					1.0000							1.0000
	1.4769					1.7300																			2.0000		11.0000															
	6.1253					24.6942																6.5135					7.0000			7.0000	1.0000			2.0000	5.0000							2.0000
	2.1416				34.4658	42.2212																					6.0000							4.0000								
							5.7212															39.5238					1.0000				6.0000			2.0000			3.0000					
						1.6685	9.5289																		2.0000		1.0000				2.0000			1.0000								
							5.2778																				4.0000				2.0000											
4.5390			2.1666		18.7925	22.9245												1.5314							1.0000		5.0000		1.0000	8.0000				3.0000	5.0000							
	4.2177					26.4268	12.1417															23.8760			1.0000		14.0000			11.0000	4.0000			2.0000	7.0000		1.0000					
							22.2184						-4.5752			1.8615	2.9944								4.0000		5.0000															
						11.1633	4.7898																		1.0000		1.0000			4.0000				1.0000	2.0000				1.0000			
						11.1364	4.9373																		2.0000		11.0000		6.0000					1.0000								
	0.5486					31.3946	9.2427																		2.0000		3.0000							2.0000								
						1.1896	4.5528																		2.0000		2.0000							1.0000								
	0.6250					19.5686																			1.0000		1.0000							1.0000					1.0000			
																									1.0000		1.0000			5.0000					1.0000							1.0000
			2.3657																						1.0000		1.0000			8.0000						4.0000						
							4.5000																				2.0000															
						1.2770																			1.0000	1.0000	3.0000		2.0000		1.0000											
																									1.0000		2.0000		3.0000		2.0000			1.0000								
						9.7142																			1.0000		1.0000							1.0000					1.0000			1.0000
4.2740						21.3252											1.5788	1.3433		-3.8556							3.0000			1.0000				2.0000	2.0000				2.0000		2.0000	2.0000
						11.2542	16.3467						-2.7226			5.2513			-1.2170						3.0000		2.0000			4.0000					2.0000							
27.4820	3.8827				2.7290	51.1275	1.9964													-9.6864					2.0000		8.0000		2.0000	14.0000					16.0000							4.0000
3.9574									12.9237																					6.0000					1.0000	2.0000						
	0.8588					23.5864											0.5677					16.6339								4.0000				2.0000	2.0000		1.0000					
						9.8631																							1.0000	5.0000					1.0000							1.0000
					8.3327			4.7326																			1.0000			3.0000					1.0000							
					34.9533	1.3128																								2.0000				1.0000	4.0000							
8.5945						48.9780														-3.9476					1.0000		7.0000			6.0000	1.0000			2.0000	4.0000							3.0000
					8.8124		4.6764																				2.0000				1.0000											
						1.6977	9.5956																		1.0000	1.0000	2.0000				1.0000			2.0000								
					7.5972	9.2436																					1.0000							1.0000					1.0000			
																																		1.0000					2.0000		1.0000	
8.7923																									1.0000					6.0000					1.0000	4.0000						
																									9.0000		3.0000				1.0000						3.0000					
																							22.8962				6.0000				6.0000											
																						3.8657															2.0000					
																											6.0000			8.0000					4.0000	4.0000						
						19.2585																					6.0000					2.0000										
						11.4552	5.1357																		1.0000		5.0000			5.0000				1.0000	1.0000							
					1.1847	11.5142																			1.0000					7.0000				1.0000	2.0000	4.0000						1.0000
					9.4919	11.3300																			1.0000		1.0000			6.0000				1.0000	4.0000	2.0000						1.0000
					9.9627	12.5241																								9.0000				1.0000	3.0000	4.0000						
					8.8793	1.6730																							1.0000	4.0000					2.0000							
8.9692					9.7414																				2.0000					6.0000					3.0000	6.0000						
3.5298	4.7300	-0.5895	0.2612		8.9496	33.7692		4.5335																			6.0000			2.0000					2.0000	2.0000						
					8.8995																						1.0000			9.0000					3.0000							

	0.5930			9.2615	1.7995	5.2160										2.0000		1.0000			4.0000				1.0000	2.0000						
				18.7788	1.6439													1.0000			4.0000	1.0000			1.0000	2.0000	2.0000		1.0000			1.0000
	4.1568		1.1913	9.8485	13.2984							1.5754		6.1832		2.0000		5.0000			5.0000					2.0000	6.0000					
			1.5380	9.2326	24.2528	5.2335								5.8862		2.0000		1.0000			7.0000				2.0000	5.0000	2.0000					
				8.6581		1.5245									2.2393	1.0000		2.0000				3.0000										
					11.2888	5.4883										2.0000		2.0000		2.0000	5.0000	1.0000			1.0000	1.0000						
				9.4463	11.3566	5.8792										2.0000		1.0000			4.0000	1.0000			1.0000	2.0000						
						17.7356		-1.4494								2.0000		7.0000			1.0000	1.0000				2.0000						
					2.5126											3.0000		4.0000				1.0000	2.0000					2.0000				
					1.6315	4.7731										3.0000	1.0000					1.0000			2.0000							
				8.6528	1.5344											5.0000		3.0000		6.0000					5.0000			1.0000				
				9.3376	22.4866															2.0000	3.0000				2.0000	3.0000						
				19.8494	11.2476											1.0000		3.0000			8.0000	2.0000			1.0000	4.0000			1.0000		1.0000	
8.2388			1.7527																		1.0000	1.0000		2.0000		4.0000						
														35.2870								6.0000										
				9.8934	24.2132	11.5600										4.0000		6.0000		3.0000		8.0000			3.0000							
					23.2900	19.9180			-2.6486	5.1712	1.4900					4.0000		3.0000				1.0000			2.0000							
				8.8498	1.5298	4.6887										1.0000				2.0000					3.0000							
				38.4546	11.9448	1.2414										1.0000		15.0000		2.0000		5.0000			1.0000							
9.4150	2.1670		2.9898													3.0000					5.0000					1.0000	4.0000					
																3.0000		4.0000				3.0000										
	1.5153															2.0000									2.0000				1.0000	2.0000	1.0000	
				8.4274		4.5532										2.0000		1.0000				1.0000										
						5.1116										1.0000					8.0000					4.0000			1.0000			
					9.2799	4.3229										1.0000		1.0000		1.0000												
				8.7966		4.8586										1.0000					4.0000					2.0000						
4.1332					1.8647	4.4492										1.0000					4.0000				1.0000	1.0000	2.0000				1.0000	1.0000
					1.9322	4.4981										1.0000					4.0000				1.0000	2.0000			1.0000			
							4.8333									1.0000					3.0000					1.0000						
															2.1595	1.0000																
					19.5556	3.9972							-3.1624			2.0000																
4.1299			1.8257											5.7922		1.0000					3.0000					2.0000	2.0000		1.0000			
		-0.4838			2.5991											1.0000					3.0000					3.0000			1.0000			
				8.5928												2.0000			1.0000					1.0000				1.0000				
		-0.4388			2.6487											1.0000					3.0000					3.0000			1.0000			
4.9620		-0.4271			2.8380											1.0000					3.0000					2.0000	2.0000					1.0000
	2.8700					5.1413										2.0000		1.0000			3.0000				1.0000	3.0000			1.0000			
																1.0000					11.0000					1.0000	6.0000					
					1.7912	4.4973										1.0000					5.0000				1.0000	1.0000						
					11.6673	1.3196										3.0000		2.0000		3.0000	8.0000	1.0000			1.0000	4.0000						
	4.2631										1.8298					4.0000					6.0000					6.0000					1.0000	
				19.3664										11.7895				1.0000			6.0000					6.0000						
					9.6250											1.0000				1.0000											1.0000	
				7.9886	1.2262												1.0000	1.0000		1.0000					1.0000						1.0000	
																1.0000					9.0000					1.0000	6.0000					
				38.9637	12.2437	1.4248										1.0000					5.0000				3.0000	7.0000						
4.2874																1.0000					6.0000					1.0000	2.0000					
						5.1528										1.0000		3.0000				1.0000										
				1.5711	11.2231	1.2234										2.0000		2.0000			3.0000	1.0000			1.0000	3.0000			1.0000		1.0000	
	1.3493			9.8982	38.2290	15.9468										4.0000		5.0000			7.0000	3.0000			3.0000	5.0000					1.0000	
					22.2376	13.8429			-3.5523							4.0000				1.0000					2.0000						1.0000	
	2.2556		1.7757		25.1868	1.3681					1.6229					1.0000		7.0000			7.0000				2.0000	5.0000					1.0000	
				9.1453	11.1524	5.5755										2.0000		3.0000			8.0000	1.0000			1.0000	4.0000		1.0000				
				8.4675	11.9600																7.0000				1.0000	1.0000	2.0000				1.0000	
	2.3744				23.2186								-3.1577			2.0000		6.0000			4.0000	1.0000				2.0000	2.0000				1.0000	1.0000
3.7595					1.3840																4.0000				1.0000	1.0000			1.0000			
	0.7986			24.8464	3.4355													3.0000							3.0000							
	-0.1998			8.8819	1.8483																6.0000			1.0000		2.0000	2.0000					

		-0.7141		8.1692	2.1876		4.5829												2.0000			1.0000	2.0000			1.0000			
4.1317		-0.6212			31.6898		4.9582			1.2900					1.0000			2.0000	3.0000			1.0000	4.0000					1.0000	
4.1687		-0.4394			31.1680					2.3244								1.0000	3.0000				4.0000					1.0000	
		-0.2847			21.7517												1.0000	6.0000		2.0000		3.0000							
		-0.8658			2.2367			36.2612											4.0000				2.0000		1.0000				
		-0.3815		9.2634	22.3434					1.1434									8.0000				4.0000	2.0000				1.0000	
3.2732		-0.6219	0.1273		31.6919		4.2125												3.0000				1.0000	2.0000					
		-0.4325			2.3463								5.4890				1.0000		4.0000				2.0000						
		-0.3292			21.8589												6.0000		5.0000				5.0000	2.0000					
	0.6845			8.6498	33.5999										1.0000				3.0000			2.0000	3.0000						
	-0.2686			8.4245	1.2847														3.0000				3.0000			2.0000			
		-0.6296		8.8393	2.1346														4.0000				2.0000						
6.5733		-0.6837		18.5660	2.9326														3.0000				3.0000	2.0000					
					1.2430														9.0000				3.0000						
	1.5000				9.8194												3.0000	2.0000											
	0.5990				21.5723	5.7357									1.0000				7.0000			1.0000	1.0000	2.0000					
	1.5240				21.2500	4.9824									2.0000				5.0000	1.0000		1.0000	1.0000						
				8.7848	9.7861														4.0000				2.0000						
					9.8937										1.0000		7.0000	1.0000											
						11.2567							48.3495										12.0000						
					1.9562	4.9716									2.0000	1.0000	7.0000					2.0000							
				8.5819	1.3250										1.0000		14.0000	2.0000				1.0000							
6.1718				25.5868	1.1929														1.0000			1.0000	3.0000						
				9.7984	11.7375								6.2528						8.0000	1.0000		2.0000	4.0000					1.0000	
						5.5717							11.7800						6.0000				6.0000			2.0000			
	2.1916			11.3658	12.8237	5.3829									2.0000		9.0000		5.0000	1.0000	2.0000	1.0000	1.0000		1.0000				
18.2274			1.4593		12.1666										1.0000				4.0000				4.0000	1.0000					
														17.3762	1.0000								6.0000						
						4.9999							28.8153		1.0000								6.0000						
													28.2882						3.0000				3.0000		1.0000				
						11.3142											5.0000		8.0000			2.0000	4.0000			2.0000	2.0000		
					1.9826	9.4880									1.0000		5.0000		9.0000			1.0000	3.0000						
				9.2820	22.1982							-4.2319							6.0000				2.0000	2.0000		1.0000			
	2.1734				13.1643	6.9644							11.9490		5.0000		15.0000	2.0000	4.0000	7.0000		2.0000	2.0000		2.0000				
					35.6599										1.0000		1.0000		5.0000			3.0000	1.0000		1.0000			2.0000	
			2.1491	9.7413											1.0000		3.0000		8.0000			1.0000	4.0000					1.0000	
					19.6150														4.0000		2.0000		2.0000						
																			4.0000				2.0000			2.0000			
3.5542	4.2868	-0.5675	0.2373		34.1385		4.5973										4.0000		7.0000				3.0000	2.0000					
				34.4530	38.8244	12.2152									6.0000		6.0000	2.0000		5.0000		5.0000			4.0000				
	4.3835				12.5248			26.9312									7.0000		12.0000	2.0000		1.0000	6.0000					1.0000	
					12.3253	1.7117					-0.7428				2.0000		9.0000		3.0000	1.0000			3.0000						
				39.6623	23.1299	5.8362									3.0000		6.0000	3.0000		8.0000		3.0000							
				2.4625	37.3926										2.0000		6.0000	3.0000		3.0000		4.0000			3.0000				
					51.2988	22.3792											4.0000		2.0000			4.0000	4.0000		1.0000				
				27.3114	11.2932	4.7843									1.0000		2.0000		2.0000			1.0000	4.0000						
					9.9313				1.1578				4.9860		1.0000		2.0000					1.0000							
					9.7952										1.0000	1.0000	2.0000	1.0000				1.0000							
					71.5870	31.3496									5.0000				5.0000			8.0000	7.0000						
	1.3962			9.7269	37.6848	5.2395									2.0000		5.0000		9.0000	3.0000		3.0000	3.0000					1.0000	
8.7657					12.6666	1.7897					-1.2996				2.0000		4.0000		6.0000				4.0000	2.0000					1.0000
	2.4418			9.3641	24.5560	5.4884									3.0000		8.0000		7.0000	2.0000		2.0000	5.0000					1.0000	
	1.4993				76.7313	23.1599									6.0000		1.0000		2.0000	3.0000		8.0000	4.0000					1.0000	
	3.6430				11.6518	5.3690									5.0000		1.0000		4.0000	1.0000		1.0000	2.0000						
						1.4124										1.0000	2.0000	1.0000	3.0000				3.0000						
				8.9891	1.4843														4.0000			1.0000	2.0000			1.0000			

				11.8400											1.0000		4.0000		5.0000	2.0000		1.0000	1.0000					2.0000
			8.7118	34.7140	9.6953										3.0000		16.0000			2.0000		3.0000						
			1.6214	12.9943	22.5522										1.0000			2.0000	4.0000	2.0000		1.0000	8.0000					
			73.9344	12.6400	22.9322										2.0000		1.0000	1.0000		14.0000		2.0000			1.0000	2.0000	2.0000	3.0000
			76.6668		15.4463												3.0000			8.0000					1.0000			
				2.7370								-2.6575					2.0000	2.0000										
3.9123	0.7197			49.3750							0.9934	-3.8922			1.0000				6.0000			3.0000	3.0000					1.0000
					11.7443									13.7796					4.0000				8.0000					
													23.3382						6.0000				6.0000					
													23.5786						6.0000				6.0000					
				22.4494	4.3393								22.9246									2.0000	6.0000					
				21.3632	24.9977											2.0000	8.0000	2.0000				2.0000						
					5.7467												2.0000		8.0000	2.0000			2.0000	4.0000				
					22.3668										4.0000				12.0000				4.0000	1.0000				
	4.4757														5.0000		2.0000			1.0000								
			8.6263	2.8195											1.0000		3.0000			1.0000		2.0000				1.0000		1.0000
			7.6458	9.2917						3.4159							1.0000					1.0000						
	2.4618												6.1698				4.0000	2.0000	4.0000			2.0000	2.0000					
		-0.8614	18.8412	33.6868											1.0000				6.0000			1.0000	6.0000					
															1.0000				3.0000				3.0000			2.0000		
															1.0000				4.0000		1.0000		2.0000					
			8.6660	1.5190													5.0000			2.0000		1.0000				1.0000		
	5.9549			24.5133													6.0000	1.0000				5.0000						
			8.1938	9.8830										8.3299								1.0000			1.0000			
			9.8785	12.9982										9.7993					6.0000			1.0000	6.0000					1.0000
					4.6778								16.9323				1.0000			1.0000					1.0000			
													15.2639				1.0000			1.0000								
			8.8985										16.6630						2.0000				4.0000					
				11.3465	14.4642				-3.2193						3.0000		3.0000											
	2.3750														3.0000		3.0000											
			16.5263		9.7455												6.0000											
					19.9291										2.0000		6.0000											
	5.4583			38.4419											3.0000		6.0000		3.0000	3.0000		3.0000	3.0000					
3.6652				23.9993		4.8392						-3.3949			1.0000		1.0000		5.0000				4.0000			1.0000		
			8.6336												4.0000		3.0000			1.0000					1.0000			
								-0.4460											15.0000				3.0000					
	2.6168		26.3563	35.3244													6.0000					3.0000						
															1.0000		3.0000				1.0000							
			4.6780	48.2922	4.7679										1.0000		2.0000	1.0000	3.0000	1.0000		3.0000	9.0000					
			8.1683	9.9298												1.0000	2.0000	1.0000		1.0000		1.0000				1.0000		
							1.5562									1.0000		1.0000										
				25.5259											6.0000		1.0000	1.0000	4.0000	3.0000		5.0000	2.0000					
															2.0000				3.0000				3.0000			1.0000		
4.6867	4.8819			11.5663							1.5783		6.4344				7.0000		6.0000			1.0000	5.0000	2.0000				1.0000
12.4866	5.2268			25.4980	5.6783								5.8913		1.0000		4.0000		5.0000	1.0000		2.0000	4.0000					

StN _acnt	SsssNHp _acnt	SdsN _acnt	SaaN _acnt	SssN _acnt	SddsN _acnt	SdaaN _acnt	SssssNp _acnt	SsOH _acnt	SdO _acnt	SssO _acnt	SaaO _acnt	SsF _acnt	SsPH2 _acnt	SssPH _acnt	SssP _acnt	SdsssP _acnt	SssssssP _acnt	SsSH _acnt	SdS _acnt	SssS _acnt	SaaS _acnt	SdssS _acnt	SddssS _acnt	SsssssssS _acnt	SsCl _acnt	SsBr _acnt	SsI _acnt
			2.0000																								
										2.0000																	
								1.0000	1.0000																		
			1.0000						2.0000																		
			1.0000		1.0000				3.0000																		
								1.0000	1.0000	1.0000																	
2.0000																											
									2.0000	4.0000																	
								5.0000	2.0000	2.0000																	
									1.0000	1.0000																	
										2.0000																	
			2.0000	1.0000		1.0000			1.0000																		
										1.0000																	
					1.0000				2.0000																1.0000		
			1.0000		1.0000				2.0000												2.0000						
					2.0000			1.0000	4.0000																		
					1.0000			1.0000	2.0000	1.0000																	
		1.0000																		1.0000							
									2.0000																		
								1.0000	2.0000														1.0000				
			1.0000																		1.0000						
			1.0000																								
			1.0000																								
			3.0000																								
			1.0000						1.0000																		
				2.0000					1.0000																		
									2.0000	6.0000													1.0000				
				1.0000				1.0000																			
		1.0000		1.0000					1.0000	2.0000																	
		2.0000						2.0000	4.0000																		
			1.0000			1.0000			2.0000	1.0000																	
								2.0000	4.0000														2.0000				
								2.0000		1.0000																	
								2.0000		1.0000																	
												3.0000															
								1.0000	1.0000	1.0000																	
			1.0000	2.0000	1.0000	1.0000			3.0000		1.0000																
								3.0000	1.0000																		
										2.0000																8.0000	
									2.0000	2.0000																	
																				1.0000							
				2.0000				2.0000	2.0000																		
			1.0000						2.0000	2.0000																	
		1.0000	1.0000						1.0000																	1.0000	
									1.0000																	1.0000	
																									1.0000	1.0000	
																										1.0000	
								1.0000	1.0000	1.0000																	
									1.0000																1.0000		
									2.0000	1.0000													1.0000				
			1.0000			1.0000														1.0000					3.0000		
								1.0000		1.0000																	

	2.0000		1.0000											
							1.0000	1.0000						
								2.0000						
	1.0000		1.0000			1.0000	1.0000							
	1.0000		1.0000			1.0000	2.0000							
							1.0000	1.0000						
					1.0000		1.0000							
			2.0000				3.0000	2.0000						
		1.0000				1.0000		3.0000						
		3.0000	4.0000			2.0000	6.0000				2.0000			
		1.0000				3.0000	1.0000	1.0000		1.0000				
													1.0000	
				1.0000			2.0000			3.0000			1.0000	
	2.0000		3.0000			1.0000	4.0000						1.0000	
2.0000													1.0000	
						1.0000	1.0000	1.0000					2.0000	
													1.0000	2.0000
							1.0000	1.0000					1.0000	
	1.0000		1.0000				2.0000						1.0000	
													3.0000	
			1.0000				2.0000						1.0000	
													1.0000	
						1.0000							1.0000	
													1.0000	
						1.0000	6.0000	6.0000						
			2.0000			3.0000	6.0000					3.0000		
	4.0000					3.0000	6.0000	1.0000				3.0000		
						2.0000	2.0000	1.0000					4.0000	4.0000
	4.0000					5.0000	6.0000					3.0000		
	4.0000					6.0000	8.0000					4.0000		
	6.0000					4.0000	4.0000					2.0000		
	4.0000					3.0000	4.0000	1.0000				2.0000		
			2.0000			1.0000	1.0000		1.0000					
						2.0000	3.0000				1.0000			
							1.0000							
							1.0000							
	2.0000					1.0000		2.0000						
			1.0000				1.0000	1.0000					1.0000	
						1.0000								
								2.0000						
						2.0000	2.0000	2.0000						

				1.0000																						
								1.0000	3.0000																	
				1.0000					2.0000											1.0000						
		2.0000						2.0000	2.0000														1.0000			
										1.0000																1.0000
			1.0000	2.0000					3.0000														1.0000			
		2.0000	1.0000	1.0000				2.0000																		
									1.0000																	
									2.0000																	
								3.0000	4.0000														2.0000			
		4.0000																								
										1.0000																
																									2.0000	
				1.0000				1.0000	1.0000																2.0000	
				1.0000					1.0000	1.0000															2.0000	
									1.0000																2.0000	
								1.0000	1.0000																2.0000	
1.0000																									2.0000	
					1.0000				2.0000																2.0000	
								1.0000																	2.0000	
			2.0000																						2.0000	
		2.0000																								
								4.0000	3.0000	3.0000																
										2.0000						1.0000		1.0000	1.0000							
								2.0000		1.0000																
			1.0000									2.0000														
										4.0000																
									1.0000	1.0000																
		3.0000		1.0000				4.0000	8.0000	1.0000												1.0000	3.0000			
									1.0000																	
										2.0000																
				1.0000				2.0000	1.0000	1.0000																
		8.0000						7.0000	4.0000														1.0000			
								3.0000																		
									1.0000	2.0000						1.0000										
				1.0000																						
			3.0000	1.0000					4.0000	2.0000													1.0000			
			1.0000	1.0000																						
											1.0000															
										1.0000																

							2.0000	2.0000																
		2.0000				2.0000	2.0000																1.0000	
			2.0000				4.0000																	
			2.0000				4.0000																	
			2.0000				4.0000																	
						6.0000		1.0000																
						2.0000	2.0000																	
1.0000		1.0000					1.0000																	
		3.0000					2.0000																1.0000	
		2.0000				4.0000	4.0000																	
								1.0000															6.0000	
							1.0000	2.0000																
								1.0000																
	1.0000			1.0000		2.0000	2.0000												1.0000					
		2.0000					2.0000	2.0000															4.0000	
								4.0000						2.0000			2.0000	2.0000						
							1.0000	1.0000																
							1.0000	1.0000																
1.0000		1.0000					3.0000	2.0000																
							1.0000	1.0000																
1.0000		1.0000					2.0000																	
				1.0000																				
								1.0000																
							1.0000																	
							1.0000																	
	1.0000						2.0000											1.0000	1.0000		1.0000			
							1.0000	3.0000						1.0000			1.0000			1.0000				
	6.0000	2.0000				2.0000	4.0000	2.0000													2.0000			
	1.0000									1.0000														
		1.0000					2.0000											1.0000					3.0000	
							1.0000																	
						1.0000			1.0000															
						4.0000	1.0000																	
	2.0000						4.0000														1.0000			
						1.0000		1.0000																
							1.0000	2.0000																
						1.0000	1.0000																	
	2.0000																							
																								6.0000
																							6.0000	
2.0000							2.0000																	
							1.0000	1.0000																
						1.0000	1.0000																	
						1.0000	1.0000																	
						1.0000	1.0000																	
						1.0000	1.0000																	
	2.0000					1.0000																		
	1.0000	2.0000	1.0000	1.0000		1.0000	3.0000		1.0000															
						1.0000																		

			1.0000			1.0000	1.0000	1.0000															
						2.0000	1.0000																
			2.0000		1.0000	1.0000	1.0000										1.0000			1.0000			
					1.0000	1.0000	2.0000	1.0000												1.0000			
						1.0000		2.0000														1.0000	
							1.0000	1.0000															
						1.0000	1.0000	1.0000															
								3.0000				1.0000											
		2.0000					2.0000																
							1.0000	1.0000															
						1.0000	1.0000																
						1.0000	2.0000																
						2.0000	1.0000																
2.0000		2.0000		1.0000																			
																				6.0000			
						1.0000	2.0000	2.0000															
							2.0000	4.0000				1.0000		1.0000	1.0000								
						1.0000	1.0000	1.0000															
						4.0000	1.0000	2.0000															
		2.0000	1.0000	1.0000																			
			1.0000																				
						1.0000		1.0000															
		2.0000						1.0000															
							1.0000	1.0000															
						1.0000		1.0000															
		1.0000					1.0000	1.0000															
							1.0000	1.0000															
									1.0000														
																							1.0000
							2.0000	1.0000											1.0000				
		1.0000		1.0000																1.0000			
					1.0000		2.0000																
						1.0000																	
					1.0000		2.0000																
		1.0000			1.0000		2.0000																
			1.0000					1.0000															
							1.0000	1.0000															
	1.0000						1.0000	2.0000															
			2.0000												1.0000								
						2.0000														2.0000			
							1.0000																
						1.0000	1.0000																
						4.0000	1.0000	2.0000															
		1.0000																					
								1.0000															
						1.0000	1.0000	2.0000															
			1.0000			1.0000	3.0000	3.0000															
							2.0000	3.0000				1.0000											
			1.0000		1.0000		2.0000	2.0000							1.0000								
						1.0000	1.0000	1.0000															
						1.0000	1.0000																
			1.0000				2.0000												1.0000				
		1.0000					1.0000																
			1.0000			3.0000	3.0000																
1.0000			1.0000			1.0000	1.0000																

1.0000			1.0000		1.0000	2.0000		1.0000							
	1.0000		1.0000			3.0000		1.0000			1.0000				
	1.0000		1.0000			3.0000					2.0000				
			1.0000			2.0000									
			1.0000			2.0000			3.0000						
			1.0000		1.0000	2.0000					1.0000				
	1.0000		1.0000	1.0000		3.0000		1.0000							
			1.0000			2.0000								1.0000	
			1.0000			2.0000									
		2.0000			1.0000	3.0000									
		1.0000			1.0000	1.0000									
			1.0000		1.0000	2.0000									
	2.0000		1.0000		2.0000	2.0000									
1.0000						1.0000									
1.0000		1.0000				1.0000									
1.0000		1.0000				2.0000	1.0000								
1.0000		1.0000				2.0000	1.0000								
1.0000					1.0000	1.0000									
						1.0000									
							2.0000							8.0000	
						1.0000	1.0000								
					1.0000	1.0000									
	2.0000				3.0000	1.0000									
1.0000					1.0000	1.0000								1.0000	
							1.0000							2.0000	
		1.0000			1.0000	1.0000	1.0000								
	5.0000			1.0000		1.0000									
															5.0000
							1.0000							5.0000	
														5.0000	
							2.0000								
						1.0000	2.0000								
					1.0000	2.0000							1.0000		
		1.0000				1.0000	1.0000							2.0000	
						3.0000									
1.0000				1.0000	1.0000										
2.0000						2.0000									
	1.0000	2.0000	1.0000	1.0000		3.0000		1.0000							
					3.0000	3.0000	2.0000								
		2.0000				1.0000			2.0000						
						1.0000	2.0000					1.0000			
					4.0000	2.0000	1.0000								
					2.0000	3.0000									
						4.0000	4.0000								
					3.0000	1.0000	1.0000								
						1.0000				1.0000				1.0000	
						1.0000									
						6.0000	6.0000								
		1.0000			1.0000	3.0000	1.0000								
	2.0000					1.0000	2.0000					1.0000			
		1.0000			1.0000	2.0000	1.0000								
2.0000		1.0000				6.0000	4.0000								
		2.0000				1.0000	1.0000								
							2.0000								
					1.0000	1.0000									

						1.0000										
					1.0000	3.0000	2.0000									
					1.0000	1.0000	4.0000									
					7.0000	1.0000	4.0000									
					8.0000		3.0000									
						2.0000								1.0000		
		1.0000	1.0000			4.0000							1.0000	1.0000		
							2.0000									4.0000
	2.0000														4.0000	
															4.0000	
						2.0000	1.0000								4.0000	
						2.0000	5.0000									
							1.0000									
							4.0000									
			2.0000													
					1.0000	2.0000										
					1.0000	1.0000						1.0000				
			1.0000												1.0000	
				1.0000	2.0000	3.0000										
1.0000																
					1.0000	1.0000										
			3.0000			2.0000										
					1.0000	1.0000										3.0000
					1.0000	1.0000										3.0000
							1.0000								3.0000	
															3.0000	
					1.0000										3.0000	
						1.0000	3.0000				1.0000					
			1.0000													
					2.0000		2.0000									
							4.0000									
			3.0000			3.0000										
		1.0000				2.0000		1.0000						1.0000		
					1.0000											
										1.0000						
			3.0000		3.0000	3.0000										
1.0000																
					4.0000	4.0000	1.0000									
					1.0000	1.0000										
									1.0000							
						2.0000										
		1.0000	2.0000			1.0000							1.0000		1.0000	
		3.0000	3.0000			2.0000	1.0000								1.0000	