Supporting Information

Toxic pressures of currently used chemicals from screening-level estimates of environmental release rates.

Blanked for double-blind reviewing

Table SI-2. Input and output of SimpleBoxTreat4Solutions calculations of Toxic Pressures in EU fresh waters, applied to 6409 'REACH chemicals', pharmaceuticals and pesticides currently used in Europe

Model SimpleBoxTreat, vs 4Solutions
Scenario 4REACH settings
Case calculation of expected toxic pressures on aquatic ecosystems from estimated emissions of chemical substances currently used in Europe

SUBSTANCE IDENTITIES			PHYS/CHEM PROPERTIES									TONNAGES		ESTIMATED EMISSIONS			EXPOSURE CONCENTRATIONS			ECOTOXICITIES		CALCULATED TOXIC PRESSURES		
SBT #	Name	CAS	MW	Tm	Pvap25	Sol25	Kow	pKα	kdeg(air)	kdeg(wat)	kdeg(soil)	EU tonnage	Manuf EU	E.air	E.water	E.soil	logC.wL	logC.w1R	logC.w2R	μ(logEC50	σ(logEC50	TP.wL	TP.w1R	TP.w2R
			g.mol^{-1}	°C	Pa	mg.L^{-1}	-	-	s^{-1}	s^{-1}	s^{-1}	tpa	tpa	tpa	tpa	tpa	g.L-1	g.L-1	g.L-1	g/L	g/L	-	-	-
REACH mono constituent organicsubstances																						***9.3%***	***3.6%***	***0.4%***
n			*3940*	*3940*	*3940*	*3940*	*3940*	*3940*	*3940*	*3940*	*3940*	*3940*	*3940*	*3940*	*3940*	*3940*	*3940*	*3940*	*3940*	*3940*	*3940*	*3940*	*3940*	*3940*
sum												***2.7E+08***		***2.4E+07***	***3.4E+05***	***1.2E+07***								
av												*6.8E+04*	*4.1E+04*	*6.2E+03*	*8.6E+01*	*3.1E+03*				*-1.85*	*0.71*			
std												*8.2E+05*	*5.4E+05*	*7.5E+04*	*1.0E+03*	*3.7E+04*				*1.35*	*0.50*			
2.5-p			*58*	*-119*	*6.7E-23*	*6.2E-09*	*8.4E-04*	*-1.2*	*3.5E-06*	*2.2E-09*	*6.6E-10*	*1.0E+00*	*5.8E-01*	*9.1E-02*	*1.3E-03*	*4.6E-02*	*-12.64*	*-12.52*	*-14.16*	*-6.54*	*0.08*	*4.9E-57*	*8.3E-58*	*2.6E-75*
50-p			*204*	*87*	*1.0E-02*	*1.2E+03*	*3.0E+02*	*14.0*	*3.5E-06*	*6.4E-07*	*3.5E-07*	*7.1E+02*	*4.5E+02*	*6.4E+01*	*9.0E-01*	*3.2E+01*	*-8.63*	*-8.89*	*-10.49*	*-1.83*	*0.64*	*8.9E-23*	*6.7E-25*	*1.8E-36*
97.5-p			*951*	*350*	*2.1E+05*	*1.7E+06*	*1.9E+13*	*14.0*	*3.5E-06*	*4.5E-06*	*3.5E-06*	*1.1E+06*	*7.1E+05*	*1.0E+05*	*1.4E+03*	*5.1E+04*	*-5.17*	*-5.67*	*-7.06*	*0.88*	*2.87*	*3.5E-06*	*3.9E-07*	*2.0E-11*
3	74-85-1	ethylene	28	-151	4.2E+06	3.6E+03	1.9E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.8E+06	3.9E+04	1.4E+06	-6.21	-5.56	-7.98	-1.15	0.24	0.0%	0.0%	9.0E-23
4	115-07-1	propene	42	-135	9.4E+05	2.1E+03	4.8E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+06	2.4E+04	8.7E+05	-6.37	-5.82	-8.47	-1.58	0.32	0.0%	0.0%	4.0E-23
5	71-43-2	benzene	78	-78	1.2E+04	1.1E+03	9.8E+01	14.0	3.5E-06	2.2E-08	1.1E-07	conf	conf	1.3E+06	1.9E+04	6.5E+05	-5.96	-5.51	-7.81	-1.12	0.84	0.0%	0.0%	5.8E-22
6	57-13-6	urea	60	29	2.8E+01	4.2E+05	2.8E-02	0	3.5E-06	7.0E-07	1.1E-06	conf	conf	1.6E+06	2.2E+04	7.9E+05	-2.84	-4.00	-5.83	0.56	0.97	0.0%	0.0%	3.7E-20
7	67-56-1	methanol	32	-101	1.6E+04	8.0E+05	2.3E-01	14.0	3.5E-06	4.7E-06	3.5E-06	conf	conf	1.4E+06	1.9E+04	7.1E+05	-5.49	-5.39	-6.71	0.29	0.89	0.0%	0.0%	8.1E-24
8	75-01-4	chloroethylene	62	-122	3.6E+05	4.8E+03	4.2E+01	14.0	3.5E-06	9.7E-09	1.1E-07	conf	conf	7.0E+05	9.8E+03	3.4E+05	-6.47	-5.83	-8.29	-0.55	0.70	0.0%	0.0%	8.9E-29
9	64-17-5	ethanol	46	-88	8.1E+03	6.3E+05	7.2E-01	14.0	3.5E-06	4.3E-06	3.5E-06	conf	conf	1.0E+06	1.4E+04	5.3E+05	-5.61	-5.50	-6.82	0.36	0.74	0.0%	0.0%	5.1E-25
10	107-06-2	1,2-dichloroethane	99	-77	1.0E+04	9.9E+03	6.8E+01	14.0	3.5E-06	1.4E-08	1.1E-07	conf	conf	6.0E+05	8.3E+03	2.9E+05	-5.75	-5.42	-7.34	-0.77	0.51	0.0%	0.0%	3.1E-21
11	74-98-6	propane	44	-134	8.2E+05	1.5E+03	6.5E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.9E+05	8.3E+03	2.9E+05	-6.84	-6.32	-9.05	-1.58	0.38	0.0%	0.0%	6.8E-27
12	106-97-8	butane	58	-120	2.4E+05	5.6E+02	2.0E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	5.4E+05	7.5E+03	2.6E+05	-6.74	-6.33	-9.11	-1.58	0.38	0.0%	0.0%	2.5E-27
13	100-42-5	styrene	104	-48	6.7E+02	2.9E+02	7.8E+02	14.0	3.5E-06	7.3E-07	1.1E-07	conf	conf	6.4E+05	8.9E+03	3.2E+05	-6.29	-5.97	-7.94	-1.75	0.49	0.0%	0.0%	4.7E-19
14	100-41-4	ethylbenzene	106	-47	1.0E+03	1.7E+02	1.1E+03	14.0	3.5E-06	8.6E-07	1.1E-07	conf	conf	6.0E+05	8.4E+03	3.0E+05	-6.48	-6.13	-8.37	-1.76	0.71	0.0%	0.0%	1.9E-21
15	1634-04-4	tert-butyl methyl ether	88	-94	3.4E+04	5.9E+04	2.7E+01	14.0	3.5E-06	4.6E-09	3.5E-07	conf	conf	4.5E+05	6.2E+03	2.2E+05	-5.71	-5.41	-7.21	-0.13	0.70	0.0%	0.0%	2.2E-24
16	98-82-8	cumene	120	-46	4.8E+02	8.9E+01	2.8E+03	14.0	3.5E-06	4.9E-08	1.1E-07	conf	conf	3.5E+05	4.9E+03	1.7E+05	-6.51	-6.19	-8.27	-2.08	0.70	0.0%	0.0%	4.6E-19
17	637-92-3	2-ethoxy-2-methylpropane	102	-81	1.7E+04	5.6E+03	8.3E+01	14.0	3.5E-06	3.3E-09	3.5E-07	conf	conf	3.0E+05	4.2E+03	1.4E+05	-6.38	-6.06	-8.11	-0.69	0.64	0.0%	0.0%	1.4E-26
18	100-21-0	terephthalic acid	166	127	1.6E-03	2.8E+03	5.8E+01	3.5	3.5E-06	9.4E-07	1.1E-06	conf	conf	4.8E+05	6.7E+03	2.5E+05	-3.95	-4.76	-6.54	-0.43	0.88	0.0%	0.0%	1.4E-18
19	106-42-3	p-xylene	106	-41	9.2E+02	1.9E+02	1.2E+03	14.0	3.5E-06	4.9E-07	1.1E-07	conf	conf	2.8E+05	4.0E+03	1.4E+05	-6.70	-6.36	-8.49	-2.04	0.54	0.0%	0.0%	1.6E-20
20	106-99-0	buta-1,3-diene	54	-123	2.7E+05	1.1E+03	1.1E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.7E+05	3.8E+03	1.3E+05	-7.15	-6.67	-9.49	-1.54	0.23	0.0%	0.0%	3.3E-30
21	80-15-9	α,α-dimethylbenzyl hydroperoxide	152	39	9.3E+00	7.3E+04	1.4E+02	12.3	3.5E-06	1.2E-08	1.1E-07	conf	conf	2.3E+05	3.2E+03	1.1E+05	-4.11	-3.84	-4.90	-2.00	0.26	0.1%	0.4%	1.7E-05
22	108-95-2	phenol	94	-2	4.3E+01	3.5E+04	3.2E+01	10.0	3.5E-06	9.3E-07	1.1E-06	conf	conf	3.1E+05	4.4E+03	1.6E+05	-5.32	-5.10	-6.71	-1.25	0.79	0.0%	0.0%	3.1E-15
23	75-28-5	isobutane	58	-133	3.5E+05	8.6E+02	1.7E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.2E+05	3.1E+03	1.1E+05	-7.25	-6.90	-9.71	-1.58	0.38	0.0%	0.0%	1.6E-31
24	110-82-7	cyclohexane	84	-83	1.3E+04	1.1E+02	1.5E+03	14.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	1.8E+05	2.6E+03	8.9E+04	-7.10	-6.76	-9.39	-1.20	0.99	0.0%	0.0%	6.2E-32
25	50-00-0	formaldehyde	30	-111	4.7E+05	2.3E+05	2.2E+00	14.0	3.5E-06	4.6E-06	3.5E-06	conf	conf	3.1E+05	4.3E+03	1.6E+05	-7.10	-6.70	-7.85	-1.40	0.72	0.0%	0.0%	1.7E-20
26	74-84-0	ethane	30	-148	2.7E+06	3.4E+03	2.1E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.0E+05	2.8E+03	1.0E+05	-7.35	-6.90	-9.19	-1.58	0.38	0.0%	0.0%	7.1E-28
27	75-56-9	methyloxirane	58	-100	7.1E+04	5.8E+04	2.3E+00	14.0	3.5E-06	6.1E-07	3.5E-07	conf	conf	2.5E+05	3.5E+03	1.3E+05	-6.49	-6.09	-7.98	-1.10	0.61	0.0%	0.0%	4.4E-23
28	108-88-3	toluene	92	-59	3.2E+03	4.6E+02	3.5E+02	14.0	3.5E-06	9.3E-07	1.1E-07	conf	conf	1.9E+05	2.7E+03	9.6E+04	-6.97	-6.56	-8.88	-1.35	0.74	0.0%	0.0%	2.5E-27
29	105-60-2	ε-caprolactam	113	67	4.8E-01	3.7E+04	4.6E+00	0	3.5E-06	2.4E-07	1.1E-06	conf	conf	2.2E+05	3.1E+03	1.1E+05	-3.68	-4.43	-6.12	0.29	0.51	0.0%	0.0%	2.9E-20
30	75-21-8	ethylene oxide	44	-109	1.7E+05	2.7E+05	8.9E-01	14.0	3.5E-06	4.3E-06	3.5E-07	conf	conf	2.4E+05	3.4E+03	1.2E+05	-6.73	-6.28	-8.00	-0.83	0.70	0.0%	0.0%	6.5E-25
31	107-21-1	ethane-1,2-diol	62	-32	8.1E+00	7.3E+05	6.3E-02	14.0	3.5E-06	4.4E-06	3.5E-06	conf	conf	2.4E+05	3.4E+03	1.2E+05	-4.97	-5.68	-7.51	1.18	0.48	0.0%	0.0%	2.6E-16
32	67-64-1	acetone	58	-94	3.3E+04	1.3E+05	5.8E-01	14.0	3.5E-06	4.7E-06	1.1E-06	conf	conf	2.0E+05	2.8E+03	1.0E+05	-6.82	-6.57	-8.09	0.60	0.86	0.0%	0.0%	1.0E-35
33	107-13-1	acrylonitrile	53	-72	1.3E+04	6.9E+04	1.6E+00	14.0	3.5E-06	5.2E-07	3.5E-07	conf	conf	1.7E+05	2.4E+03	8.8E+04	-6.31	-6.02	-7.35	-1.80	0.32	0.0%	0.0%	1.1E-15
34	74-87-3	chloromethane	50	-125	5.4E+05	1.1E+04	1.2E+01	14.0	3.5E-06	4.3E-08	3.5E-08	conf	conf	1.1E+05	1.5E+03	5.3E+04	-7.17	-6.36	-8.72	-0.45	0.24	0.0%	0.0%	1.5E-32
35	80-05-7	4,4'-isopropylidenediphenol	228	132	3.0E-05	3.7E+02	4.4E+03	9.7	3.5E-06	1.3E-07	1.1E-07	conf	conf	1.2E+05	1.7E+03	6.0E+04	-3.99	-4.57	-6.08	-2.40	0.45	1.2%	0.1%	7.3E-08
36	115-11-7	2-methylpropene	56	-131	3.0E+05	1.2E+03	1.7E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.3E+05	1.8E+03	6.5E+04	-7.70	-7.33	-10.26	-1.87	0.25	0.0%	0.0%	1.9E-33
37	75-65-0	2-methylpropan-2-ol	74	-74	6.3E+03	2.0E+05	5.4E+00	14.0	3.5E-06	4.6E-08	1.1E-06	conf	conf	1.0E+05	1.5E+03	5.2E+04	-5.76	-5.49	-6.66	0.63	0.70	0.0%	0.0%	1.1E-25
38	75-78-5	dichloro(dimethyl)silane	129	-90	1.7E+04	7.1E+03	1.7E+02	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	8.9E+04	1.2E+03	4.3E+04	-6.69	-6.16	-8.49	-0.41	0.11	0.0%	0.0%	3.6E-31
39	62-53-3	aniline	93	-6	1.1E+02	1.7E+04	1.2E+01	5.0	3.5E-06	4.3E-07	1.1E-06	conf	conf	1.3E+05	1.8E+03	6.7E+04	-4.89	-4.95	-6.68	-1.18	0.99	0.0%	0.0%	1.9E-15
40	64-19-7	acetic acid	60	-21	2.3E+03	9.6E+05	1.2E+00	4.9	3.5E-06	4.7E-06	3.5E-07	conf	conf	1.5E+05	2.1E+03	7.7E+04	-4.95	-5.85	-7.74	-0.61	0.75	0.0%	0.0%	1.3E-24
41	108-94-1	cyclohexanone	98	-30	5.4E+02	1.5E+04	1.3E+01	14.0	3.5E-06	8.0E-07	1.1E-06	conf	conf	1.3E+05	1.8E+03	6.8E+04	-6.32	-6.11	-7.25	-0.42	0.70	0.0%	0.0%	8.5E-23
42	74-82-8	methane	16	-153	7.1E+07	2.6E+03	6.0E+00	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	8.0E+04	1.1E+03	3.8E+04	-7.65	-6.50	-9.07	-1.58	0.38	0.0%	0.0%	4.9E-27
43	108-05-4	vinyl acetate	86	-84	1.6E+04	2.8E+04	5.4E+00	14.0	3.5E-06	9.5E-07	1.1E-06	conf	conf	1.2E+05	1.7E+03	6.2E+04	-6.89	-6.61	-8.24	-1.39	0.56	0.0%	0.0%	6.5E-23
44	112-84-5	(Z)-docos-13-enamide	338	183	1.1E-05	4.6E-05	2.8E+08	-0.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.3E+04	1.0E+03	3.7E+04	-7.34	-7.34	-7.49	-5.60	0.75	0.7%	0.7%	3.5E-03
45	79-10-7	acrylic acid	72	-10	8.0E+02	1.5E+05	2.8E+00	4.6	3.5E-06	4.7E-06	1.1E-06	conf	conf	1.2E+05	1.6E+03	6.1E+04	-5.39	-6.21	-7.87	-0.98	0.68	0.0%	0.0%	3.6E-23
46	78-78-4	2-methylbutane	72	-119	9.2E+04	3.0E+02	5.2E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	7.3E+04	1.0E+03	3.6E+04	-7.71	-7.39	-10.34	-2.02	0.50	0.0%	0.0%	7.3E-33
47	95-47-6	o-xylene	106	-41	9.1E+02	1.9E+02	1.2E+03	14.0	3.5E-06	5.0E-07	1.1E-07	conf	conf	7.0E+04	9.8E+02	3.5E+04	-7.31	-6.97	-9.10	-1.97	0.62	0.0%	0.0%	1.1E-24
48	124-04-9	adipic acid	146	102	1.7E-03	6.5E+04	1.7E+00	4.5	3.5E-06	1.2E-06	1.1E-06	conf	conf	9.8E+04	1.4E+03	5.0E+04	-4.39	-5.51	-7.33	-1.04	0.30	0.0%	0.0%	1.2E-19
49	3323-53-3	adipic acid, compound with hexane-1,6-diamine (1:1)	262	87	9.9E-03	1.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.6E+04	9.2E+02	3.3E+04	-4.20	-4.51	-6.17	-0.11	1.03	0.0%	0.0%	2.4E-18
50	109-66-0	pentane	72	-107	6.8E+04	3.2E+02	6.3E+02	14.0	3.5E-06	1.6E-06	3.5E-07	conf	conf	6.0E+04	8.4E+02	3.0E+04	-7.84	-7.46	-10.45	-2.14	0.70	0.0%	0.0%	8.0E-33
51	123-72-8	butyraldehyde	72	-80	1.4E+04	5.0E+04	6.6E+00	14.0	3.5E-06	4.1E-06	3.5E-06	conf	conf	7.8E+04	1.1E+03	4.0E+04	-7.46	-7.27	-8.55	-0.88	0.63	0.0%	0.0%	3.1E-28
52	994-05-8	2-methoxy-2-methylbutane	102	-81	1.0E+04	2.5E+04	8.3E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	6.2E+04	8.6E+02	3.1E+04	-6.91	-6.63	-8.26	-0.67	0.58	0.0%	0.0%	1.1E-27
53	108-78-1	melamine	126	133	1.2E-05	9.1E+05	4.2E-01	5.3	3.5E-06	1.6E-07	1.1E-07	conf	conf	5.9E+04	8.2E+02	3.0E+04	-3.57	-4.61	-6.31	-0.01	0.77	0.0%	0.0%	1.2E-19
54	104-76-7	2-ethylhexan-1-ol	144	-14	5.9E+00	1.4E+02	1.7E+03	14.0	3.5E-06	2.9E-07	1.1E-06	conf	conf	5.9E+04	8.2E+02	3.0E+04	-6.50	-6.23	-7.42	-1.58	0.18	0.0%	0.0%	3.3E-17
55	28553-12-0	di-''isononyl'' phthalate	419	85	3.1E-05	2.7E-03	2.3E+09	14.0	3.5E-06	2.5E-07	3.5E-07	conf	conf	4.1E+04	5.7E+02	2.0E+04	-5.98	-6.22	-6.37	-3.26	0.65	0.0%	0.0%	4.5E-06
56	80-62-6	methyl methacrylate	100	-80	4.9E+03	3.6E+04	1.9E+01	14.0	3.5E-06	6.8E-07	1.1E-06	conf	conf	6.1E+04	8.5E+02	3.1E+04	-6.94	-6.70	-7.98	-0.47	0.30	0.0%	0.0%	3.8E-27
57	141-32-2	butyl acrylate	128	-46	6.7E+02	1.8E+03	1.6E+02	14.0	3.5E-06	4.4E-07	1.1E-06	conf	conf	5.5E+04	7.7E+02	2.8E+04	-7.05	-6.77	-8.34	-2.26	0.49	0.0%	0.0%	2.0E-18
58	141-43-5	2-aminoethanol	61	-28	5.5E+01	1.0E+06	2.5E-02	9.0	3.5E-06	4.1E-07	3.5E-06	conf	conf	5.9E+04	8.2E+02	3.0E+04	-5.13	-5.18	-6.95	-0.65	0.77	0.0%	0.0%	1.1E-19
59	85-44-9	phthalic anhydride	148	22	3.0E-02	5.3E+02	1.2E+02	14.0	3.5E-06	1.2E-06	3.5E-07	conf	conf	6.3E+04	8.8E+02	3.2E+04	-5.72	-5.73	-7.51	-0.84	0.94	0.0%	0.0%	8.0E-22
60	57-55-6	propane-1,2-diol	76	-33	1.5E+01	1.7E+06	1.7E-01	14.0	3.5E-06	5.5E-07	1.1E-06	conf	conf	5.8E+04	8.0E+02	2.9E+04	-4.64	-5.20	-7.09	0.63	0.70	0.0%	0.0%	1.4E-28
61	106-98-9	but-1-ene	56	-122	2.5E+05	1.1E+03	1.5E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.2E+04	5.9E+02	2.1E+04	-7.95	-7.50	-10.31	-1.96	0.23	0.0%	0.0%	3.9E-33
62	71-36-3	butan-1-ol	74	-62	1.0E+03	7.5E+04	6.9E+00	14.0	3.5E-06	4.0E-06	3.5E-06	conf	conf	6.1E+04	8.5E+02	3.1E+04	-6.96	-6.83	-8.08	0.11	0.70	0.0%	0.0%	6.6E-32
63	98-85-1	1-phenylethanol	122	-7	7.3E+00	1.1E+04	3.1E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.5E+04	7.7E+02	2.8E+04	-6.00	-5.79	-7.53	-0.73	0.28	0.0%	0.0%	1.2E-22
64	108-24-7	acetic anhydride	102	-95	8.7E+02	2.9E+04	2.6E-01	14.0	3.5E-06	4.5E-06	1.1E-06	conf	conf	5.0E+04	7.0E+02	2.6E+04	-6.97	-6.82	-8.31	-0.55	0.94	0.0%	0.0%	7.5E-29
65	111-66-0	oct-1-ene	112	-70	2.2E+03	1.0E+01	1.3E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.3E+04	4.6E+02	1.6E+04	-8.05	-7.73	-10.66	-2.68	1.28	0.0%	0.0%	2.2E-30
66	78-79-5	isoprene	68	-119	7.3E+04	5.5E+02	3.8E+02	14.0	3.5E-06	2.9E-08	3.5E-07	conf	conf	2.9E+04	4.0E+02	1.4E+04	-7.92	-7.55	-10.22	-1.44	0.65	0.0%	0.0%	2.0E-36
67	27458-94-2	isononyl alcohol	144	-14	2.6E+00	1.4E+02	1.7E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.6E+04	6.3E+02	2.3E+04	-6.82	-6.60	-7.81	-2.01	0.17	0.0%	0.0%	5.6E-17
68	112-53-8	dodecan-1-ol	186	29	2.4E-01	5.8E+00	5.9E+04	14.0	3.5E-06	3.6E-06	3.5E-07	conf	conf	4.1E+04	5.7E+02	2.1E+04	-7.48	-7.32	-8.45	-2.98	0.61	0.0%	0.0%	2.9E-15
69	111-46-6	2,2'-oxydiethanol	106	9	3.5E-01	4.4E+06	3.4E-02	14.0	3.5E-06	2.0E-06	1.1E-06	conf	conf	4.6E+04	6.4E+02	2.4E+04	-4.74	-5.81	-7.88	1.35	0.70	0.0%	0.0%	3.0E-18
70	88-72-2	2-nitrotoluene	137	38	1.6E+01	5.9E+02	2.3E+02	14.0	3.5E-06	8.0E-09	1.1E-07	conf	conf	2.7E+04	3.8E+02	1.3E+04	-6.20	-5.93	-7.16	-1.48	0.70	0.0%	0.0%	2.4E-16
71	75-79-6	trichloro(methyl)silane	149	-77	2.1E+04	3.4E+04	1.0E+02	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	2.6E+04	3.7E+02	1.3E+04	-6.90	-6.49	-8.59	1.27	0.86	0.0%	0.0%	2.6E-22
72	141-78-6	ethyl acetate	88	-82	1.3E+04	3.8E+04	7.2E+00	14.0	3.5E-06	9.1E-07	1.1E-06	conf	conf	4.1E+04	5.7E+02	2.1E+04	-7.30	-7.04	-8.53	-0.20	0.45	0.0%	0.0%	6.2E-33
73	25068-38-6	4,4'-Isopropylidenediphenol, oligomeric reaction products with 1-chloro-2,3-epoxypropane	321	87	9.9E-03	2.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.3E+04	4.6E+02	1.7E+04	-4.50	-4.81	-6.46	-2.34	0.43	0.1%	0.0%	1.9E-09
74	11071-47-9	isooctene	112	-82	3.3E+03	5.4E+00	1.1E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.8E+04	3.9E+02	1.4E+04	-8.12	-7.80	-10.79	-2.12	0.32	0.0%	0.0%	1.6E-35
75	75-91-2	tert-butyl hydroperoxide	90	-41	5.1E+03	2.7E+05	8.7E+00	12.7	3.5E-06	4.6E-08	1.1E-06	conf	conf	2.8E+04	3.9E+02	1.4E+04	-6.23	-5.96	-7.12	-2.08	0.65	0.0%	0.0%	3.0E-13
76	124-09-4	hexamethylenediamine	116	25	2.4E+01	1.1E+06	2.2E+00	10.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.0E+04	5.5E+02	2.0E+04	-5.58	-5.81	-7.68	-1.09	0.50	0.0%	0.0%	2.3E-21
77	112-72-1	tetradecanol	214	49	2.7E-02	5.2E-01	5.6E+05	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.9E+04	4.1E+02	1.5E+04	-7.42	-7.27	-8.31	-3.40	0.47	0.0%	0.0%	1.1E-12
78	110-63-4	butane-1,4-diol	90	-8	7.3E-01	1.5E+06	6.0E-01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.1E+04	5.7E+02	2.1E+04	-5.15	-6.22	-8.19	0.50	1.28	0.0%	0.0%	1.0E-35
79	112-92-5	octadecan-1-ol	271	87	2.4E-04	4.4E-03	5.2E+07	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.5E+04	3.4E+02	1.2E+04	-7.00	-7.25	-7.89	-0.81	1.82	0.0%	0.0%	2.1E-24
80	67-63-0	propan-2-ol	60	-89	6.6E+03	3.6E+05	1.9E+00	14.0	3.5E-06	4.9E-07	3.5E-06	conf	conf	3.5E+04	4.9E+02	1.8E+04	-6.55	-6.32	-7.46	0.65	0.42	0.0%	0.0%	2.2E-31
81	7446-81-3	sodium acrylate	94	87	9.9E-03	6.5E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E+04	3.9E+02	1.4E+04	-4.59	-4.89	-6.53	-2.01	1.56	0.0%	0.0%	5.7E-11
82	117-81-7	bis(2-ethylhexyl) phthalate	391	64	2.7E-03	1.9E-02	2.5E+08	14.0	3.5E-06	4.1E-07	3.5E-07	conf	conf	2.2E+04	3.1E+02	1.1E+04	-6.80	-7.01	-7.74	-2.37	1.28	0.0%	0.0%	8.7E-15
83	36653-82-4	hexadecan-1-ol	242	69	1.2E-03	2.1E-02	5.4E+06	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.5E+04	3.5E+02	1.2E+04	-7.71	-7.69	-8.69	-4.37	0.04	0.0%	0.0%	3.3E-10
84	99-99-0	4-nitrotoluene	137	38	3.7E+00	2.8E+02	2.3E+02	14.0	3.5E-06	1.3E-08	1.1E-07	conf	conf	2.2E+04	3.1E+02	1.1E+04	-6.05	-5.78	-6.94	-1.58	0.70	0.0%	0.0%	8.6E-15
85	101-68-8	4,4'-methylenediphenyl diisocyanate	250	99	2.5E-02	3.5E+01	1.7E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.8E+04	3.9E+02	1.4E+04	-6.69	-6.60	-8.00	0.37	0.26	0.0%	0.0%	3.2E-33
86	107-01-7	2-butene	56	-120	2.3E+05	9.3E+02	1.2E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.8E+04	3.9E+02	1.4E+04	-8.35	-7.97	-10.98	-1.83	0.27	0.0%	0.0%	2.3E-39
87	120-61-6	dimethyl terephthalate	194	-23	3.3E-02	2.0E+03	4.6E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.4E+04	4.7E+02	1.7E+04	-5.65	-5.92	-7.77	-1.55	0.34	0.0%	0.0%	3.2E-19
88	102-71-6	2,2',2''-nitrilotriethanol	149	83	4.5E-04	1.0E+06	3.3E-03	8.0	3.5E-06	6.7E-09	3.5E-06	conf	conf	2.1E+04	2.9E+02	1.0E+04	-4.23	-4.83	-5.84	0.18	0.70	0.0%	0.0%	4.2E-18
89	77-92-9	citric acid	192	169	7.5E-07	2.4E+05	2.1E-02	3.0	3.5E-06	8.4E-07	1.1E-06	conf	conf	3.3E+04	4.6E+02	1.7E+04	-4.37	-5.71	-7.57	-0.20	0.44	0.0%	0.0%	3.0E-26
90	25167-67-3	butene	56	-122	2.5E+05	1.1E+03	1.5E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.3E+04	3.3E+02	1.2E+04	-8.21	-7.76	-10.57	-1.95	0.20	0.0%	0.0%	3.7E-35
91	75-09-2	dichloromethane	85	-90	5.8E+04	1.8E+04	2.2E+01	14.0	3.5E-06	2.0E-08	3.5E-08	conf	conf	2.0E+04	2.7E+02	9.5E+03	-7.46	-6.95	-9.21	-0.60	0.57	0.0%	0.0%	4.2E-35
92	108-93-0	cyclohexanol	100	-33	8.7E+01	2.9E+04	4.4E+01	14.0	3.5E-06	8.0E-07	1.1E-06	conf	conf	3.1E+04	4.4E+02	1.6E+04	-6.38	-6.15	-7.65	-0.32	0.70	0.0%	0.0%	6.2E-26
93	107-31-3	methyl formate	60	-99	7.9E+04	2.0E+05	6.8E-01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	3.3E+04	4.5E+02	1.7E+04	-7.63	-7.35	-8.94	0.09	0.76	0.0%	0.0%	2.0E-38
94	110-65-6	but-2-yne-1,4-diol	86	29	3.3E-01	1.8E+05	1.2E-01	13.2	3.5E-06	1.7E-07	3.5E-06	conf	conf	2.6E+04	3.6E+02	1.3E+04	-4.65	-5.21	-6.83	-0.98	0.50	0.0%	0.0%	3.2E-17
95	91-20-3	naphthalene	128	5	5.4E+00	9.1E+01	1.5E+03	14.0	3.5E-06	1.2E-08	1.1E-07	conf	conf	1.9E+04	2.7E+02	9.5E+03	-6.58	-6.31	-7.58	-2.38	0.48	0.0%	0.0%	5.6E-14
96	108-31-6	maleic anhydride	98	-52	2.2E+01	9.7E+04	4.2E+01	14.0	3.5E-06	6.4E-07	1.1E-06	conf	conf	3.0E+04	4.2E+02	1.5E+04	-6.06	-5.84	-7.54	-0.94	0.75	0.0%	0.0%	1.9E-21
97	102-09-0	diphenyl carbonate	214	-2	5.3E-02	4.5E+01	1.6E+03	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.6E+04	3.7E+02	1.3E+04	-6.03	-5.78	-7.38	-2.38	0.46	0.0%	0.0%	4.5E-13
98	67-66-3	chloroform	119	-79	2.5E+04	6.6E+03	3.3E+01	14.0	3.5E-06	2.9E-08	3.5E-08	conf	conf	1.8E+04	2.6E+02	8.9E+03	-7.57	-7.02	-9.37	-1.16	0.58	0.0%	0.0%	4.5E-32
99	64-18-6	formic acid	46	-25	4.8E+03	2.1E+06	3.5E-01	3.8	3.5E-06	4.7E-06	1.1E-06	conf	conf	3.1E+04	4.3E+02	1.6E+04	-5.24	-6.73	-8.45	-0.25	0.59	0.0%	0.0%	5.5E-32
100	98-83-9	2-phenylpropene	118	-45	2.6E+02	2.7E+02	2.8E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.2E+04	3.1E+02	1.1E+04	-7.51	-7.23	-8.98	-2.17	0.55	0.0%	0.0%	1.3E-22
101	75-15-0	carbon disulphide	76	-77	4.6E+04	3.9E+03	8.7E+01	14.0	3.5E-06	2.9E-09	1.1E-06	conf	conf	1.7E+04	2.4E+02	8.3E+03	-7.91	-7.60	-9.80	-2.00	0.63	0.0%	0.0%	3.5E-29
102	75-54-7	dichloro(methyl)silane	114	-112	5.5E+04	4.9E+04	5.0E+01	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	1.7E+04	2.4E+02	8.4E+03	-7.19	-6.76	-8.93	-0.36	0.33	0.0%	0.0%	9.2E-35
103	79-06-1	acrylamide	71	22	1.7E+01	9.4E+05	1.5E-01	0	3.5E-06	3.5E-07	1.1E-06	conf	conf	2.6E+04	3.6E+02	1.3E+04	-4.48	-5.49	-7.24	-0.88	0.29	0.0%	0.0%	4.9E-20
104	78-93-3	butanone	72	-80	1.3E+04	2.0E+05	1.8E+00	14.0	3.5E-06	9.5E-07	1.1E-06	conf	conf	2.7E+04	3.7E+02	1.4E+04	-7.15	-6.94	-8.11	0.35	0.40	0.0%	0.0%	6.1E-34
105	123-86-4	n-butyl acetate	116	-57	1.6E+03	4.0E+03	7.1E+01	14.0	3.5E-06	9.2E-07	1.1E-06	conf	conf	2.5E+04	3.5E+02	1.3E+04	-7.59	-7.33	-8.85	-0.99	0.45	0.0%	0.0%	1.4E-29
106	556-67-2	octamethylcyclotetrasiloxane	297	2	1.6E+02	1.3E+00	6.2E+06	14.0	3.5E-06	7.9E-09	3.5E-09	conf	conf	1.6E+04	2.3E+02	7.9E+03	-8.02	-7.59	-10.06	-4.10	0.29	0.0%	0.0%	8.6E-18
107	110-88-3	1,3,5-trioxane	90	-54	1.4E+03	1.6E+05	2.8E-01	14.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	1.6E+04	2.2E+02	7.6E+03	-6.02	-5.74	-6.88	1.01	0.27	0.0%	0.0%	2.9E-13
108	106-89-8	1-chloro-2,3-epoxypropane	93	-66	2.4E+03	4.1E+04	4.3E+00	14.0	3.5E-06	7.7E-07	3.5E-07	conf	conf	2.5E+04	3.4E+02	1.3E+04	-7.04	-6.81	-8.09	-1.68	0.68	0.0%	0.0%	2.7E-20
109	584-84-9	4-methyl-m-phenylene diisocyanate	174	19	3.4E+00	1.3E+03	5.5E+03	14.0	3.5E-06	4.5E-08	3.5E-07	conf	conf	1.7E+04	2.4E+02	8.3E+03	-5.92	-5.67	-6.89	-0.74	0.96	0.0%	0.0%	7.5E-19
110	79-20-9	methyl acetate	74	-95	7.0E+03	1.7E+05	2.3E+00	14.0	3.5E-06	9.1E-07	1.1E-06	conf	conf	2.4E+04	3.4E+02	1.3E+04	-7.06	-6.86	-8.02	-0.33	0.21	0.0%	0.0%	2.2E-28
111	121-91-5	isophthalic acid	166	127	3.5E-06	2.8E+03	5.8E+01	3.5	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.6E+04	3.6E+02	1.3E+04	-5.58	-6.66	-8.39	-0.65	0.87	0.0%	0.0%	1.0E-28
112	872-05-9	dec-1-ene	140	-45	2.8E+02	6.4E-01	1.3E+05	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.5E+04	2.1E+02	7.5E+03	-8.31	-7.99	-10.79	-2.68	1.28	0.0%	0.0%	2.4E-31
113	111-42-2	2,2'-iminodiethanol	105	29	7.2E-02	3.2E+05	1.9E-02	9.0	3.5E-06	5.0E-07	3.5E-06	conf	conf	2.3E+04	3.2E+02	1.2E+04	-4.80	-5.67	-7.49	-0.79	0.77	0.0%	0.0%	5.5E-22
114	592-41-6	hex-1-ene	84	-95	2.5E+04	1.5E+02	1.4E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.7E+04	2.3E+02	8.2E+03	-8.33	-7.98	-10.88	-2.68	1.28	0.0%	0.0%	4.8E-32
115	127-18-4	tetrachloroethylene	166	-61	2.4E+03	4.6E+02	9.3E+02	14.0	3.5E-06	3.9E-08	1.1E-07	conf	conf	1.4E+04	1.9E+02	6.7E+03	-7.91	-7.56	-9.78	-1.72	0.66	0.0%	0.0%	5.8E-31
116	108-38-3	m-xylene	106	-41	8.8E+02	1.9E+02	1.2E+03	14.0	3.5E-06	5.7E-07	1.1E-07	conf	conf	1.6E+04	2.3E+02	8.0E+03	-7.96	-7.62	-9.75	-2.01	0.48	0.0%	0.0%	1.1E-28
117	109-99-9	tetrahydrofuran	72	-85	2.3E+04	5.1E+04	8.7E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.1E+04	3.0E+02	1.1E+04	-7.58	-7.27	-8.87	0.58	0.30	0.0%	0.0%	8.1E-42
118	107-15-3	ethylenediamine	60	-24	2.4E+03	1.0E+06	2.4E-02	10.0	3.5E-06	4.5E-07	1.1E-06	conf	conf	1.9E+04	2.7E+02	9.7E+03	-6.09	-5.89	-7.48	-0.83	0.74	0.0%	0.0%	1.1E-21
119	74-86-2	acetylene	26	-154	2.4E+06	6.2E+03	3.2E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.5E+04	2.0E+02	7.2E+03	-8.47	-7.68	-9.99	-0.71	0.50	0.0%	0.0%	1.8E-40
120	124-40-3	dimethylamine	45	-106	2.0E+05	1.0E+06	6.8E-01	10.7	3.5E-06	5.1E-07	3.5E-07	conf	conf	1.8E+04	2.5E+02	9.3E+03	-7.29	-6.87	-8.11	-1.11	0.52	0.0%	0.0%	8.0E-24
121	75-76-3	tetramethylsilane	88	-117	9.5E+04	2.7E+02	5.2E+02	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	1.2E+04	1.6E+02	5.6E+03	-8.24	-7.24	-10.02	-2.93	1.46	0.0%	0.0%	2.2E-24
122	107-98-2	1-methoxypropan-2-ol	90	-58	9.8E+02	1.0E+06	3.2E-01	14.0	3.5E-06	6.4E-07	1.1E-06	conf	conf	1.8E+04	2.6E+02	9.4E+03	-6.18	-5.99	-7.69	0.70	0.70	0.0%	0.0%	2.0E-33
123	79-11-8	chloroacetic acid	94	11	3.3E+01	7.0E+05	2.2E+00	2.9	3.5E-06	6.9E-07	3.5E-07	conf	conf	1.8E+04	2.5E+02	9.0E+03	-4.76	-5.83	-7.75	-2.10	1.70	0.0%	0.0%	3.4E-16
124	78-84-2	isobutyraldehyde	72	-92	2.2E+04	7.5E+04	5.5E+00	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.8E+04	2.6E+02	9.5E+03	-8.05	-7.85	-9.14	-1.05	0.45	0.0%	0.0%	3.3E-31
125	75-45-6	chlorodifluoromethane	86	-139	8.8E+05	1.9E+03	7.8E+00	14.0	3.5E-06	3.5E-08	1.1E-08	conf	conf	1.1E+04	1.5E+02	5.2E+03	-8.29	-7.23	-9.98	-0.33	0.18	0.0%	0.0%	1.6E-43
126	111-76-2	2-butoxyethanol	118	-20	6.3E+01	7.1E+04	3.7E+00	14.0	3.5E-06	1.0E-06	1.1E-06	conf	conf	1.8E+04	2.5E+02	9.1E+03	-6.49	-6.28	-7.97	0.10	0.25	0.0%	0.0%	4.5E-31
127	103-11-7	2-ethylhexyl acrylate	184	-10	2.4E+01	5.7E+01	1.2E+04	14.0	3.5E-06	2.6E-07	1.1E-06	conf	conf	1.3E+04	1.8E+02	6.3E+03	-7.66	-7.38	-8.99	-1.87	0.58	0.0%	0.0%	1.2E-24
128	115-77-5	pentaerythritol	136	89	3.4E-06	1.0E+06	1.7E-02	14.0	3.5E-06	3.9E-08	1.1E-06	conf	conf	1.1E+04	1.6E+02	5.5E+03	-4.32	-5.12	-6.41	0.95	0.56	0.0%	0.0%	3.7E-26
129	77-73-6	3a,4,7,7a-tetrahydro-4,7-methanoindene	132	-17	2.2E+02	9.1E+02	1.4E+03	14.0	3.5E-06	9.0E-08	3.5E-07	conf	conf	1.1E+04	1.5E+02	5.4E+03	-7.36	-7.08	-8.63	-1.93	0.43	0.0%	0.0%	5.4E-22
130	77-99-6	propylidynetrimethanol	134	60	5.6E-03	1.9E+05	1.5E+00	14.0	3.5E-06	3.0E-08	3.5E-06	conf	conf	1.0E+04	1.4E+02	5.0E+03	-4.91	-5.28	-6.50	0.97	0.43	0.0%	0.0%	7.0E-27
131	156-62-7	calcium cyanamide	80	87	9.9E-03	5.5E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+04	1.7E+02	5.9E+03	-4.97	-5.26	-6.90	-0.54	1.36	0.0%	0.0%	4.7E-20
132	27247-96-7	2-ethylhexyl nitrate	175	-15	3.5E+01	1.7E+02	1.3E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.3E+04	1.8E+02	6.7E+03	-7.92	-7.67	-9.00	-1.89	0.17	0.0%	0.0%	1.5E-24
133	78-92-2	butan-2-ol	74	-76	2.7E+03	8.5E+04	5.9E+00	14.0	3.5E-06	4.2E-07	1.1E-06	conf	conf	1.4E+04	1.9E+02	7.0E+03	-7.07	-6.84	-7.97	0.39	0.26	0.0%	0.0%	3.3E-33
134	110-54-3	n-hexane	86	-94	2.0E+04	9.1E+01	1.9E+03	14.0	3.5E-06	1.6E-06	1.1E-07	conf	conf	1.1E+04	1.5E+02	5.3E+03	-8.58	-8.13	-11.15	-1.04	0.78	0.0%	0.0%	1.4E-47
135	124-41-4	sodium methanolate	54	87	9.9E-03	3.7E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+04	1.5E+02	5.5E+03	-5.01	-5.30	-6.93	0.82	0.70	0.0%	0.0%	9.0E-29
136	44992-01-0	[2-(acryloyloxy)ethyl]trimethylammonium chloride	194	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+04	1.5E+02	5.5E+03	-4.99	-5.29	-6.94	-1.30	1.05	0.0%	0.0%	3.7E-16
137	10042-59-8	2-propylheptan-1-ol	158	-3	3.4E+00	4.9E+01	5.1E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.3E+04	1.8E+02	6.6E+03	-7.68	-7.46	-8.59	-2.59	0.23	0.0%	0.0%	4.7E-18
138	65-85-0	benzoic acid	122	49	4.0E-01	3.5E+03	7.4E+01	4.1	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.4E+04	1.9E+02	7.1E+03	-5.55	-6.38	-8.14	-1.04	0.66	0.0%	0.0%	1.9E-24
139	74-93-1	methanethiol	48	-115	2.0E+05	2.3E+04	6.0E+00	10.7	3.5E-06	1.1E-07	3.5E-07	conf	conf	8.7E+03	1.2E+02	4.2E+03	-8.10	-7.65	-9.63	-2.42	0.39	0.0%	0.0%	3.5E-25
140	126-30-7	2,2-dimethylpropane-1,3-diol	104	-1	3.3E-01	3.3E+05	1.4E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.4E+04	1.9E+02	7.0E+03	-5.30	-6.24	-8.14	-0.21	0.81	0.0%	0.0%	4.9E-30
141	140-88-5	ethyl acrylate	100	-71	5.1E+03	1.6E+04	1.7E+01	14.0	3.5E-06	3.2E-07	1.1E-06	conf	conf	1.1E+04	1.6E+02	5.7E+03	-7.60	-7.33	-8.88	-2.36	0.43	0.0%	0.0%	6.1E-21
142	75-77-4	chlorotrimethylsilane	109	-103	2.6E+04	1.4E+03	3.0E+02	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	8.0E+03	1.1E+02	3.9E+03	-8.10	-7.33	-9.97	-0.51	0.25	0.0%	0.0%	6.2E-42
143	3268-49-3	3-(methylthio)propionaldehyde	104	-44	2.6E+02	2.3E+04	2.6E+00	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.3E+04	1.9E+02	6.9E+03	-7.53	-7.40	-8.70	-2.10	0.42	0.0%	0.0%	1.9E-21
144	78-87-5	1,2-dichloropropane	113	-80	6.1E+03	3.1E+03	1.8E+02	14.0	3.5E-06	1.0E-08	3.5E-08	conf	conf	7.5E+03	1.1E+02	3.6E+03	-7.81	-7.40	-9.50	-1.00	0.63	0.0%	0.0%	2.8E-34
145	74-90-8	hydrogen cyanide	27	-88	9.9E+04	3.4E+04	2.0E-01	14.0	3.5E-06	6.9E-07	3.5E-07	conf	conf	1.0E+04	1.4E+02	5.2E+03	-7.95	-7.47	-9.40	-3.28	0.88	0.0%	0.0%	1.1E-18
146	53306-54-0	bis(2-propylheptyl) phthalate	447	106	4.9E-06	5.7E-04	2.3E+10	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.0E+03	9.8E+01	3.4E+03	-6.69	-6.75	-6.88	-0.13	1.42	0.0%	0.0%	2.7E-22
147	79-00-5	1,1,2-trichloroethane	133	-63	2.7E+03	5.0E+03	1.0E+02	14.0	3.5E-06	2.2E-08	3.5E-08	conf	conf	7.2E+03	1.0E+02	3.5E+03	-7.52	-7.17	-9.08	-1.05	0.34	0.0%	0.0%	8.9E-31
148	75-07-0	acetaldehyde	44	-106	1.2E+05	5.7E+05	6.8E-01	14.0	3.5E-06	4.5E-06	3.5E-06	conf	conf	1.2E+04	1.7E+02	6.2E+03	-8.13	-7.93	-9.11	-1.05	0.82	0.0%	0.0%	5.4E-31
149	616-38-6	dimethyl carbonate	90	-120	7.5E+03	1.2E+05	1.7E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.1E+04	1.6E+02	5.9E+03	-7.57	-7.36	-8.59	-0.54	0.30	0.0%	0.0%	7.5E-31
150	149-57-5	2-ethylhexanoic acid	144	38	8.3E+00	5.1E+03	9.1E+02	4.9	3.5E-06	6.0E-07	3.5E-07	conf	conf	1.1E+04	1.5E+02	5.5E+03	-5.94	-6.15	-7.99	-0.87	0.47	0.0%	0.0%	1.4E-24
151	25265-71-8	oxydipropanol	134	31	2.0E-01	2.3E+06	3.2E-01	14.0	3.5E-06	9.2E-08	3.5E-07	conf	conf	8.3E+03	1.2E+02	4.1E+03	-4.61	-5.38	-6.92	0.70	0.53	0.0%	0.0%	7.3E-28
152	126-99-8	2-chlorobuta-1,3-diene	89	-106	2.9E+04	2.2E+03	3.4E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	8.1E+03	1.1E+02	4.0E+03	-8.50	-8.15	-10.59	-1.94	0.45	0.0%	0.0%	2.3E-35
153	79-09-4	propionic acid	74	-9	8.1E+02	3.5E+05	3.8E+00	4.9	3.5E-06	4.7E-06	1.1E-06	conf	conf	1.1E+04	1.6E+02	5.9E+03	-6.41	-7.22	-8.89	-1.03	0.37	0.0%	0.0%	1.4E-29
154	68-04-2	trisodium citrate	258	87	9.9E-03	1.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.4E+03	1.2E+02	4.2E+03	-5.10	-5.41	-7.06	0.16	0.37	0.0%	0.0%	3.0E-25
155	2809-21-4	etidronic acid	206	88	1.7E-08	1.0E+06	9.8E-01	1.9	3.5E-06	8.4E-09	1.1E-06	conf	conf	6.6E+03	9.3E+01	3.2E+03	-4.66	-5.34	-6.35	-0.36	0.62	0.0%	0.0%	5.7E-18
156	3164-34-9	calcium tartrate	188	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.2E+03	1.1E+02	4.1E+03	-5.11	-5.42	-7.07	-1.00	0.64	0.0%	0.0%	2.2E-18
157	108-90-7	chlorobenzene	113	-46	1.2E+03	2.0E+02	4.4E+02	14.0	3.5E-06	2.2E-09	3.5E-08	conf	conf	6.1E+03	8.5E+01	2.9E+03	-8.20	-7.72	-9.99	-1.83	0.74	0.0%	0.0%	1.0E-31
158	78-59-1	3,5,5-trimethylcyclohex-2-enone	138	17	3.3E+01	2.0E+03	4.2E+02	14.0	3.5E-06	2.1E-07	1.1E-06	conf	conf	8.1E+03	1.1E+02	4.1E+03	-7.02	-6.75	-7.96	-0.70	0.70	0.0%	0.0%	1.5E-25

159	96-33-3	methyl acrylate	86	-84	1.2E+04	3.3E+04	5.4E+00	14.0	3.5E-06	3.2E-07	1.1E-06	conf	conf	8.0E+03	1.1E+02	4.0E+03	-7.75	-7.47	-9.02	-2.26	0.40	0.0%	0.0%	2.2E-22
160	107-02-8	acrylaldehyde	56	-95	3.5E+04	2.5E+05	1.5E+00	14.0	3.5E-06	4.5E-06	3.5E-06	conf	conf	9.9E+03	1.4E+02	5.1E+03	-8.18	-8.03	-9.20	-4.03	0.59	0.0%	0.0%	7.5E-14
161	75-35-4	1,1-dichloroethylene	97	-104	8.0E+04	3.5E+03	1.3E+02	14.0	3.5E-06	1.9E-08	1.1E-07	conf	conf	5.7E+03	7.9E+01	2.7E+03	-8.46	-7.96	-10.48	-0.81	0.49	0.0%	0.0%	1.0E-43
162	116-14-3	tetrafluoroethylene	100	-162	1.9E+06	2.8E+01	1.6E+01	14.0	3.5E-06	3.5E-08	3.5E-08	conf	conf	5.6E+03	7.8E+01	2.7E+03	-8.63	-8.10	-10.88	-0.64	0.41	0.0%	0.0%	8.8E-49
163	108-80-5	cyanuric acid	129	120	3.2E-03	1.7E+05	4.1E+00	6.8	3.5E-06	2.2E-09	3.5E-07	conf	conf	5.6E+03	7.8E+01	2.7E+03	-4.77	-5.34	-6.28	-0.88	2.00	0.0%	0.0%	6.1E-15
164	811-97-2	norflurane	102	-151	5.3E+05	3.2E+03	4.8E+01	14.0	3.5E-06	3.5E-08	3.5E-08	conf	conf	5.5E+03	7.7E+01	2.7E+03	-8.56	-7.70	-10.38	-0.40	0.27	0.0%	0.0%	1.9E-46
165	79-41-4	methacrylic acid	86	-7	2.9E+02	9.7E+04	9.8E+00	4.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.5E+03	1.3E+02	4.9E+03	-6.35	-7.18	-8.86	-1.03	0.67	0.0%	0.0%	2.6E-29
166	112-41-4	dodec-1-ene	168	-22	3.6E+01	5.3E-02	1.3E+06	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	5.5E+03	7.7E+01	2.7E+03	-8.77	-8.49	-11.26	-2.68	1.28	0.0%	0.0%	7.9E-35
167	78-83-1	2-methylpropan-1-ol	74	-74	1.8E+03	1.0E+05	5.9E+00	14.0	3.5E-06	4.3E-06	3.5E-06	conf	conf	8.9E+03	1.2E+02	4.6E+03	-7.86	-7.73	-8.96	0.04	0.42	0.0%	0.0%	4.1E-38
168	64-02-8	tetrasodium ethylenediaminetetraacetate	380	87	9.9E-03	2.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.6E+03	9.2E+01	3.3E+03	-5.20	-5.51	-7.17	-0.78	0.72	0.0%	0.0%	3.5E-20
169	111-40-0	2,2'-iminodi(ethylamine)	103	18	3.4E+01	1.0E+06	7.4E-03	10.0	3.5E-06	2.9E-09	3.5E-06	conf	conf	5.1E+03	7.2E+01	2.5E+03	-5.55	-5.43	-6.39	-0.54	0.67	0.0%	0.0%	3.2E-17
170	84852-15-3	Phenol, 4-nonyl-, branched	220	90	8.0E-03	2.5E-01	8.3E+05	10.0	3.5E-06	9.9E-09	3.5E-07	conf	conf	5.1E+03	7.1E+01	2.5E+03	-7.44	-7.27	-8.31	-3.60	0.84	0.0%	0.0%	8.6E-12
171	544-17-2	calcium diformate	130	87	9.9E-03	9.0E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.3E+03	8.8E+01	3.2E+03	-5.24	-5.54	-7.18	0.54	1.38	0.0%	0.0%	1.4E-28
172	103-67-3	benzyl(methyl)amine	121	-9	1.3E+02	1.3E+04	3.5E+01	9.7	3.5E-06	3.5E-07	1.1E-07	conf	conf	7.0E+03	9.8E+01	3.6E+03	-6.91	-6.67	-8.00	-2.13	0.78	0.0%	0.0%	2.4E-17
173	123-38-6	propionaldehyde	58	-93	4.2E+04	2.0E+05	2.1E+00	14.0	3.5E-06	4.5E-06	3.5E-06	conf	conf	8.0E+03	1.1E+02	4.1E+03	-8.36	-8.20	-9.42	-1.14	0.41	0.0%	0.0%	1.6E-32
174	108-65-6	2-methoxy-1-methylethyl acetate	132	-50	6.7E+02	6.9E+04	3.3E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	8.0E+03	1.1E+02	4.1E+03	-7.64	-7.52	-8.94	-0.06	0.49	0.0%	0.0%	3.5E-37
175	541-02-6	decamethylcyclopentasiloxane	371	-5	2.9E+01	4.8E-02	8.5E+07	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	4.5E+03	6.3E+01	2.2E+03	-7.99	-7.71	-9.56	-3.52	2.14	0.0%	0.0%	3.1E-18
176	112-34-5	2-(2-butoxyethoxy)ethanol	162	19	1.5E+00	5.3E+05	1.9E+00	14.0	3.5E-06	7.7E-07	3.5E-07	conf	conf	7.3E+03	1.0E+02	3.7E+03	-5.45	-6.18	-8.19	0.25	0.70	0.0%	0.0%	9.7E-34
177	919-94-8	Butane, 2-ethoxy-2-methyl-	116	-68	5.3E+03	5.2E+03	2.6E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	6.6E+03	9.2E+01	3.3E+03	-8.31	-8.03	-9.86	-0.69	0.27	0.0%	0.0%	1.7E-39
178	100-44-7	α-chlorotoluene	127	-27	1.3E+02	6.6E+02	6.2E+02	14.0	3.5E-06	8.0E-07	1.1E-07	conf	conf	6.8E+03	9.5E+01	3.5E+03	-7.95	-7.70	-9.10	-2.21	0.70	0.0%	0.0%	3.7E-23
179	79-33-4	l-(+)-lactic acid	90	23	3.8E+00	7.7E+05	2.2E-01	3.8	3.5E-06	4.7E-07	3.5E-07	conf	conf	6.9E+03	9.6E+01	3.5E+03	-4.97	-6.05	-7.94	-0.44	0.46	0.0%	0.0%	4.6E-27
180	4904-61-4	cyclododeca-1,5,9-triene	162	-15	9.8E+00	7.5E-01	3.0E+05	14.0	3.5E-06	1.6E-08	3.5E-07	conf	conf	4.4E+03	6.2E+01	2.1E+03	-8.70	-8.44	-10.57	-2.31	0.77	0.0%	0.0%	2.2E-32
181	25167-70-8	2,4,4-trimethylpentene	112	-84	5.5E+03	4.3E+00	1.2E+04	14.0	3.5E-06	1.1E-07	1.1E-07	conf	conf	4.5E+03	6.3E+01	2.2E+03	-8.76	-8.41	-11.19	-2.98	0.21	0.0%	0.0%	4.1E-32
182	10543-57-4	N,N'-ethylenebis[N-acetylacetamide]	228	186	2.0E-06	1.0E+05	4.4E-03	-1.0	3.5E-06	4.5E-07	1.1E-06	conf	conf	6.8E+03	9.4E+01	3.4E+03	-4.86	-6.10	-7.92	0.21	0.42	0.0%	0.0%	1.8E-31
183	593-81-7	trimethylammonium chloride	96	87	9.9E-03	6.6E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.6E+03	7.8E+01	2.8E+03	-5.30	-5.59	-7.23	-2.63	1.58	0.0%	0.0%	2.4E-11
184	115-10-6	dimethyl ether	46	-128	5.1E+05	2.0E+05	1.2E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	6.2E+03	8.6E+01	3.2E+03	-8.30	-7.75	-9.32	-0.23	0.54	0.0%	0.0%	7.3E-39
185	83196-58-1	(8R,9S,10R,13S,14S,17R)-17-Hydroxy-10,13-dimethyl-1,2,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydrospiro[cyclop	358	191	1.2E-08	4.2E+00	1.5E+04	11.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	5.7E+03	8.0E+01	2.9E+03	-5.53	-6.35	-7.95	-2.94	0.17	0.0%	0.0%	4.1E-13
186	79-01-6	trichloroethylene	131	-77	9.7E+03	7.0E+02	3.0E+02	14.0	3.5E-06	2.6E-08	1.1E-07	conf	conf	4.2E+03	5.8E+01	2.0E+03	-8.54	-8.11	-10.54	-1.23	0.48	0.0%	0.0%	1.2E-40
187	106-46-7	1,4-dichlorobenzene	147	-14	8.8E+01	1.2E+02	1.9E+03	14.0	3.5E-06	2.3E-09	3.5E-08	conf	conf	4.1E+03	5.8E+01	2.0E+03	-7.88	-7.58	-9.40	-2.26	0.83	0.0%	0.0%	1.0E-24
188	107-18-6	allyl alcohol	58	-76	3.1E+03	4.5E+05	1.6E+00	14.0	3.5E-06	4.3E-06	1.1E-06	conf	conf	7.2E+03	1.0E+02	3.7E+03	-7.60	-7.48	-8.98	-2.72	0.66	0.0%	0.0%	2.0E-19
189	77-78-1	dimethyl sulphate	126	15	8.3E+01	1.2E+05	1.4E+00	14.0	3.5E-06	4.4E-07	3.5E-06	conf	conf	6.2E+03	8.6E+01	3.1E+03	-6.63	-6.39	-8.04	-1.76	0.26	0.0%	0.0%	1.4E-19
190	98-00-0	furfuryl alcohol	98	-12	5.5E+01	1.9E+05	2.8E+00	14.0	3.5E-06	3.1E-07	1.1E-06	conf	conf	5.8E+03	8.1E+01	2.9E+03	-6.36	-6.13	-7.82	-0.44	0.66	0.0%	0.0%	2.7E-26
191	94-28-0	2,2'-ethylenedioxydiethyl bis(2-ethylhexanoate)	403	48	5.6E-04	2.0E+00	4.0E+05	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	4.7E+03	6.5E+01	2.3E+03	-6.90	-6.88	-8.25	-3.10	0.29	0.0%	0.0%	9.4E-14
192	75-12-7	formamide	45	29	1.7E+01	1.0E+06	2.5E-02	0	3.5E-06	7.5E-07	3.5E-06	conf	conf	6.3E+03	8.8E+01	3.2E+03	-5.47	-6.57	-8.27	0.41	0.70	0.0%	0.0%	1.2E-35
193	68-12-2	N,N-dimethylformamide	73	-32	4.7E+02	3.4E+06	1.2E-01	0	3.5E-06	3.0E-07	3.5E-07	conf	conf	5.7E+03	7.9E+01	2.9E+03	-4.94	-5.96	-7.76	0.91	0.51	0.0%	0.0%	1.7E-35
194	822-06-0	hexamethylene diisocyanate	168	49	2.8E+00	3.3E+03	1.6E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	6.2E+03	8.6E+01	3.2E+03	-7.23	-7.02	-8.59	-0.94	0.43	0.0%	0.0%	4.2E-28
195	123-05-7	2-ethylhexanal	128	-42	2.9E+02	4.4E+02	5.1E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	5.0E+03	7.0E+01	2.5E+03	-8.10	-7.82	-9.51	-2.25	0.08	0.0%	0.0%	1.6E-25
196	2439-35-2	2-(dimethylamino)ethyl acrylate	143	-24	2.3E+02	3.0E+04	2.6E+00	8.2	3.5E-06	3.5E-06	1.1E-06	conf	conf	6.6E+03	9.2E+01	3.4E+03	-7.66	-7.55	-9.00	-2.42	0.87	0.0%	0.0%	2.6E-21
197	98-54-4	4-tert-butylphenol	150	37	6.0E-01	9.4E+02	2.6E+03	10.0	3.5E-06	2.2E-09	1.1E-06	conf	conf	3.8E+03	5.3E+01	1.8E+03	-6.07	-5.87	-6.89	-2.26	0.84	0.0%	0.0%	1.9E-11
198	14543-49-8	604-471-9	140	-40	2.7E+02	5.8E+01	1.4E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.7E+03	6.6E+01	2.3E+03	-8.66	-8.36	-10.54	-2.89	0.80	0.0%	0.0%	4.0E-28
199	96-76-4	2,4-di-tert-butylphenol	206	77	3.6E-01	1.3E+01	2.1E+05	10.8	3.5E-06	3.5E-06	1.1E-06	conf	conf	5.0E+03	6.9E+01	2.5E+03	-8.41	-8.27	-9.40	-2.79	0.70	0.0%	0.0%	1.8E-21
200	108-77-0	2,4,6-trichloro-1,3,5-triazine	184	69	3.1E+00	5.8E+02	5.4E+01	4.2	3.5E-06	1.1E-07	1.1E-07	conf	conf	4.6E+03	6.5E+01	2.3E+03	-5.38	-5.76	-7.34	-0.31	0.77	0.0%	0.0%	4.9E-24
201	26896-20-8	neodecanoic acid	172	48	2.0E+00	7.2E+01	6.8E+03	4.9	3.5E-06	3.5E-06	1.1E-06	conf	conf	6.2E+03	8.7E+01	3.2E+03	-7.67	-7.54	-9.11	-0.91	0.35	0.0%	0.0%	5.6E-32
202	629-59-4	tetradecane	198	1	4.9E+00	4.8E-03	1.7E+07	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.7E+03	5.2E+01	1.8E+03	-8.72	-8.60	-11.26	-0.07	2.47	0.0%	0.0%	9.2E-58
203	763-32-6	3-methylbut-3-en-1-ol	86	-60	4.9E+02	9.6E+03	1.8E+01	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	6.0E+03	8.4E+01	3.1E+03	-8.22	-8.06	-9.18	-0.03	0.37	0.0%	0.0%	2.6E-39
204	111-91-1	bis(2-chloroethoxy)methane	173	-6	1.9E+01	1.7E+04	2.0E+01	14.0	3.5E-06	1.8E-08	3.5E-07	conf	conf	3.6E+03	5.1E+01	1.8E+03	-6.20	-5.92	-7.06	-0.85	0.30	0.0%	0.0%	3.9E-19
205	2855-13-2	3-aminomethyl-3,5,5-trimethylcyclohexylamine	170	58	4.3E+00	1.4E+05	7.9E+01	10.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.6E+03	7.8E+01	2.9E+03	-6.71	-6.74	-8.55	-1.14	0.57	0.0%	0.0%	1.7E-26
206	947-04-6	dodecane-12-lactam	197	123	4.9E-04	4.8E+01	4.1E+03	-0.3	3.5E-06	3.5E-07	1.1E-07	conf	conf	4.7E+03	6.5E+01	2.4E+03	-5.63	-6.07	-7.93	-1.06	0.23	0.0%	0.0%	4.6E-23
207	793-24-8	N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine	268	122	6.6E-04	1.0E+00	4.8E+04	4.6	3.5E-06	3.5E-06	3.5E-07	conf	conf	5.6E+03	7.8E+01	2.9E+03	-6.64	-7.43	-9.17	-3.20	1.28	0.0%	0.0%	7.3E-18
208	95-53-4	o-toluidine	107	12	4.7E+01	7.6E+03	4.2E+01	4.0	3.5E-06	4.3E-07	3.5E-07	conf	conf	5.0E+03	6.9E+01	2.5E+03	-5.62	-6.28	-8.10	-1.37	0.80	0.0%	0.0%	3.6E-22
209	3327-22-8	(3-chloro-2-hydroxypropyl)trimethylammonium chloride	188	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.2E+03	5.8E+01	2.1E+03	-5.41	-5.71	-7.36	-0.53	0.87	0.0%	0.0%	8.5E-23
210	75-50-3	trimethylamine	59	-110	2.2E+05	4.2E+05	1.1E+00	10.0	3.5E-06	5.5E-07	3.5E-07	conf	conf	4.8E+03	6.7E+01	2.4E+03	-8.06	-7.64	-9.10	-0.55	0.58	0.0%	0.0%	1.3E-34
211	108-01-0	2-dimethylaminoethanol	89	-40	4.4E+02	1.0E+06	1.1E-01	9.0	3.5E-06	6.1E-07	3.5E-06	conf	conf	5.1E+03	7.1E+01	2.6E+03	-6.72	-6.52	-8.25	-0.95	0.75	0.0%	0.0%	9.0E-26
212	590-29-4	potassium formate	84	87	9.9E-03	5.8E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.0E+03	5.6E+01	2.0E+03	-5.45	-5.74	-7.38	-0.30	0.77	0.0%	0.0%	2.5E-24
213	97-88-1	butyl methacrylate	142	-43	3.3E+02	1.3E+03	5.6E+02	14.0	3.5E-06	7.5E-07	1.1E-06	conf	conf	4.6E+03	6.4E+01	2.3E+03	-8.24	-7.98	-9.41	-1.07	0.60	0.0%	0.0%	5.1E-33
214	107-22-2	glyoxal	58	-67	3.8E+04	4.7E+05	2.2E-02	14.0	3.5E-06	4.7E-06	3.5E-06	conf	conf	5.2E+03	7.2E+01	2.7E+03	-8.24	-8.09	-9.38	-0.73	0.34	0.0%	0.0%	1.9E-35
215	108-10-1	4-methylpentan-2-one	100	-67	2.9E+03	1.0E+04	1.4E+01	14.0	3.5E-06	9.4E-07	1.1E-06	conf	conf	4.7E+03	6.5E+01	2.4E+03	-8.24	-7.99	-9.42	0.02	0.39	0.0%	0.0%	9.6E-42
216	111-41-1	2-(2-aminoethylamino)ethanol	104	26	8.8E-01	1.0E+06	7.4E-03	9.7	3.5E-06	3.5E-06	3.5E-06	conf	conf	5.1E+03	7.2E+01	2.6E+03	-6.16	-7.20	-9.10	-0.64	0.51	0.0%	0.0%	6.0E-34
217	629-11-8	hexane-1,6-diol	118	14	1.7E-01	3.4E+05	5.8E+00	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	5.1E+03	7.1E+01	2.6E+03	-6.47	-7.52	-9.12	0.54	0.32	0.0%	0.0%	1.4E-43
218	112-18-5	dodecyldimethylamine	213	23	2.1E+00	1.3E-01	2.8E+05	10.0	3.5E-06	1.2E-07	1.1E-07	conf	conf	3.0E+03	4.1E+01	1.4E+03	-8.89	-8.61	-10.90	-3.85	0.75	0.0%	0.0%	3.6E-24
219	576-26-1	2,6-xylenol	122	25	1.4E+01	3.3E+03	4.1E+02	10.9	3.5E-06	3.4E-08	3.5E-07	conf	conf	3.2E+03	4.5E+01	1.6E+03	-6.63	-6.35	-7.52	-2.15	0.84	0.0%	0.0%	8.3E-15
220	624-92-0	dimethyl disulphide	94	-70	3.3E+03	5.1E+03	7.4E+01	14.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	2.8E+03	4.0E+01	1.4E+03	-7.94	-7.65	-9.42	-2.35	0.58	0.0%	0.0%	2.9E-24
221	1120-36-1	tetradec-1-ene	196	0	1.4E+01	6.7E-03	1.2E+07	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.9E+03	4.0E+01	1.4E+03	-8.82	-8.62	-11.18	-2.68	1.28	0.0%	0.0%	2.7E-34
222	109-55-7	3-aminopropyldimethylamine	102	-23	1.2E+03	4.4E+05	3.5E-01	10.3	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.8E+03	6.7E+01	2.5E+03	-7.55	-7.42	-9.09	-0.94	0.91	0.0%	0.0%	1.4E-31
223	31570-04-4	tris(2,4-ditert-butylphenyl) phosphite	647	269	6.3E-12	2.2E-11	1.2E+18	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.7E+03	3.8E+01	1.3E+03	-13.67	-13.67	-13.67	-0.46	0.16	0.0%	0.0%	1.0E-79
224	1738-25-6	3-dimethylaminopropiononitrile	98	-24	1.8E+02	4.4E+05	3.5E-01	7.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.6E+03	6.4E+01	2.4E+03	-6.66	-6.60	-8.55	-0.37	0.51	0.0%	0.0%	7.9E-32
225	98-01-1	2-furaldehyde	96	-29	3.1E+02	6.7E+04	6.8E+00	14.0	3.5E-06	3.1E-07	1.1E-06	conf	conf	4.0E+03	5.6E+01	2.0E+03	-6.98	-6.74	-8.10	-1.69	0.31	0.0%	0.0%	2.7E-20
226	107-45-9	1,1,3,3-tetramethylbutylamine	129	-20	9.7E+02	1.4E+00	3.8E+02	10.0	3.5E-06	6.6E-09	3.5E-07	conf	conf	2.7E+03	3.8E+01	1.3E+03	-8.90	-8.54	-11.27	-1.81	0.22	0.0%	0.0%	6.0E-42
227	112-30-1	decan-1-ol	158	8	1.5E+00	3.7E+01	6.2E+03	14.0	3.5E-06	3.7E-06	3.5E-07	conf	conf	4.3E+03	6.0E+01	2.2E+03	-8.38	-8.22	-9.38	-2.34	0.70	0.0%	0.0%	4.8E-24
228	5064-31-3	trisodium nitrilotriacetate	257	87	9.9E-03	1.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.5E+03	4.9E+01	1.7E+03	-5.48	-5.79	-7.44	0.26	0.66	0.0%	0.0%	1.8E-28
229	75-68-3	1-chloro-1,1-difluoroethane	101	-125	3.4E+05	2.0E+03	1.1E+02	14.0	3.5E-06	3.5E-08	1.1E-08	conf	conf	2.6E+03	3.7E+01	1.3E+03	-8.86	-7.91	-10.64	-0.85	0.23	0.0%	0.0%	9.2E-45
230	111-87-5	octan-1-ol	130	-14	1.3E+01	6.2E+02	6.5E+02	14.0	3.5E-06	3.8E-06	1.1E-06	conf	conf	4.4E+03	6.2E+01	2.3E+03	-8.26	-8.10	-9.30	-1.50	0.40	0.0%	0.0%	3.7E-29
231	6422-86-2	bis(2-ethylhexyl) terephthalate	391	64	2.9E-03	1.0E-02	2.5E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.7E+03	3.8E+01	1.3E+03	-7.84	-8.01	-8.95	-2.13	2.07	0.0%	0.0%	9.8E-23
232	56-23-5	carbon tetrachloride	154	-58	1.3E+04	3.9E+02	2.8E+02	14.0	3.5E-06	3.9E-08	3.5E-08	conf	conf	2.6E+03	3.7E+01	1.3E+03	-8.78	-8.12	-10.77	-1.53	0.85	0.0%	0.0%	4.0E-40
233	74-89-5	methylamine	31	-98	3.1E+05	1.0E+06	2.3E-01	11.0	3.5E-06	4.2E-07	1.1E-06	conf	conf	3.9E+03	5.4E+01	2.0E+03	-8.04	-7.56	-8.64	-0.78	0.70	0.0%	0.0%	1.4E-29
234	96-18-4	1,2,3-trichloropropane	147	-47	3.9E+02	1.8E+03	3.2E+02	14.0	3.5E-06	1.5E-08	3.5E-08	conf	conf	2.7E+03	3.7E+01	1.3E+03	-7.75	-7.45	-9.12	-1.35	0.70	0.0%	0.0%	5.6E-29
235	5216-25-1	α,α,α,4-tetrachlorotoluene	230	40	3.3E+00	3.6E+00	3.5E+04	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	2.7E+03	3.8E+01	1.3E+03	-8.37	-8.10	-9.88	-1.12	0.64	0.0%	0.0%	3.0E-36
236	143-28-2	(Z)-octadec-9-enol	268	85	2.0E-03	2.7E-03	3.2E+07	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.7E+03	3.8E+01	1.3E+03	-8.47	-8.50	-9.81	-1.52	2.00	0.0%	0.0%	1.1E-32
237	16219-75-3	5-ethylidene-8,9,10-trinorborn-2-ene	120	-30	8.2E+02	3.0E+02	4.7E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.3E+03	4.7E+01	1.7E+03	-8.78	-8.50	-10.47	-2.35	0.23	0.0%	0.0%	2.0E-31
238	112-27-6	2,2'-(ethylenedioxy)diethanol	150	47	2.7E-02	9.4E+06	1.8E-02	14.0	3.5E-06	1.7E-06	1.1E-06	conf	conf	4.3E+03	6.0E+01	2.2E+03	-5.62	-6.73	-8.81	1.08	0.73	0.0%	0.0%	1.1E-23
239	80-56-8	pin-2(3)-ene	136	-14	5.4E+02	2.8E+01	1.9E+04	14.0	3.5E-06	9.7E-08	1.1E-07	conf	conf	2.6E+03	3.6E+01	1.2E+03	-8.88	-8.57	-10.93	-2.06	1.14	0.0%	0.0%	4.2E-37
240	2492-26-4	sodium benzothiazol-2-yl sulphide	189	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.3E+03	4.5E+01	1.6E+03	-5.52	-5.82	-7.47	-2.75	0.51	0.0%	0.0%	7.5E-12
241	140-66-9	4-(1,1,3,3-tetramethylbutyl)phenol	206	73	6.9E-02	1.6E+01	1.9E+05	10.0	3.5E-06	4.5E-09	1.1E-06	conf	conf	2.5E+03	3.5E+01	1.2E+03	-6.99	-6.91	-7.95	-3.68	0.84	0.0%	0.0%	5.3E-10
242	103-23-1	bis(2-ethylhexyl) adipate	371	9	4.3E-04	1.5E-02	1.3E+08	14.0	3.5E-06	4.3E-07	3.5E-07	conf	conf	2.5E+03	3.5E+01	1.2E+03	-7.59	-7.91	-8.39	-2.51	1.35	0.0%	0.0%	2.2E-17
243	101-54-2	N-(4-aminophenyl)aniline	184	105	5.8E-03	1.8E+03	6.6E+01	4.6	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.1E+03	5.7E+01	2.1E+03	-6.10	-6.94	-8.71	-2.91	0.46	0.0%	0.0%	5.9E-17
244	100-51-6	benzyl alcohol	108	-5	7.1E+00	2.4E+04	1.2E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.0E+03	5.6E+01	2.1E+03	-7.14	-6.94	-8.67	-0.91	0.64	0.0%	0.0%	7.3E-29
245	506-59-2	dimethylammonium chloride	82	87	9.9E-03	5.6E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.1E+03	4.3E+01	1.5E+03	-5.56	-5.85	-7.49	-1.68	0.64	0.0%	0.0%	5.6E-17
246	611-19-8	α,2-dichlorotoluene	161	3	2.0E+01	5.1E+01	2.8E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	2.7E+03	3.8E+01	1.3E+03	-8.06	-7.77	-9.45	-3.27	0.21	0.0%	0.0%	5.9E-19
247	532-32-1	sodium benzoate	144	87	9.9E-03	1.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.1E+03	4.3E+01	1.5E+03	-5.55	-5.85	-7.50	-0.87	0.48	0.0%	0.0%	1.4E-21
248	830-13-7	cyclododecanone	182	30	6.7E-01	3.5E-01	1.2E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.0E+03	4.2E+01	1.5E+03	-8.79	-8.52	-10.36	-2.20	0.24	0.0%	0.0%	1.1E-31
249	143-07-7	lauric acid	200	82	1.9E-01	2.7E+01	1.0E+05	4.9	3.5E-06	3.7E-06	3.5E-07	conf	conf	4.0E+03	5.6E+01	2.1E+03	-7.65	-7.71	-9.35	-1.63	0.57	0.0%	0.0%	1.4E-28
250	124-18-5	decane	142	-44	2.3E+02	4.0E-01	1.8E+05	14.0	3.5E-06	3.1E-07	1.1E-07	conf	conf	2.4E+03	3.3E+01	1.2E+03	-9.12	-8.81	-11.60	-1.05	0.70	0.0%	0.0%	1.3E-51
251	354-33-6	pentafluoroethane	120	-162	9.5E+05	8.0E+01	3.5E+01	14.0	3.5E-06	3.5E-08	3.5E-08	conf	conf	2.3E+03	3.2E+01	1.1E+03	-9.00	-8.33	-11.10	-0.40	0.26	0.0%	0.0%	4.7E-53
252	294-62-2	cyclododecane	168	-18	3.1E+00	1.4E-01	1.3E+06	14.0	3.5E-06	7.2E-09	3.5E-07	conf	conf	2.3E+03	3.2E+01	1.1E+03	-9.05	-8.81	-11.01	-1.67	0.70	0.0%	0.0%	6.2E-41
253	71-23-8	propan-1-ol	60	-75	3.1E+03	1.7E+05	2.2E+00	14.0	3.5E-06	4.3E-06	3.5E-06	conf	conf	4.0E+03	5.5E+01	2.0E+03	-8.16	-8.04	-9.28	0.54	0.26	0.0%	0.0%	5.7E-45
254	287-92-3	cyclopentane	70	-95	4.2E+04	3.5E+02	4.8E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.4E+03	3.4E+01	1.2E+03	-9.05	-8.69	-11.41	-1.98	0.55	0.0%	0.0%	1.1E-41
255	120-18-3	naphthalene-2-sulphonic acid	208	139	1.0E-05	2.7E+03	1.0E+00	0.7	3.5E-06	1.0E-08	3.5E-07	conf	conf	2.3E+03	3.2E+01	1.1E+03	-4.93	-5.73	-6.77	-0.72	0.69	0.0%	0.0%	2.5E-18
256	106-47-8	4-chloroaniline	128	24	3.2E+00	1.7E+03	5.2E+01	4.0	3.5E-06	5.1E-09	3.5E-07	conf	conf	2.3E+03	3.2E+01	1.1E+03	-5.36	-5.78	-6.77	-2.08	0.78	0.0%	0.0%	9.9E-12
257	629-73-2	hexadec-1-ene	224	21	1.0E+00	8.1E-03	1.1E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.3E+03	3.2E+01	1.1E+03	-8.35	-8.40	-10.49	-2.68	1.28	0.0%	0.0%	3.1E-29
258	872-50-4	1-methyl-2-pyrrolidone	99	26	4.3E+01	4.4E+06	7.8E-01	0	3.5E-06	2.0E-07	3.5E-06	conf	conf	3.1E+03	4.3E+01	1.6E+03	-5.59	-6.27	-7.89	-0.09	0.13	0.0%	0.0%	3.4E-29
259	112-75-4	dimethyl(tetradecyl)amine	241	43	2.7E-01	1.4E-02	2.6E+06	10.1	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.4E+03	3.3E+01	1.2E+03	-9.14	-8.92	-11.34	-4.01	0.89	0.0%	0.0%	6.1E-26
260	122-39-4	diphenylamine	169	54	1.3E-01	7.3E+01	1.9E+03	1.0	3.5E-06	4.1E-09	3.5E-07	conf	conf	2.2E+03	3.1E+01	1.1E+03	-5.66	-5.79	-6.75	-2.92	0.52	0.0%	0.0%	2.1E-08
261	128-37-0	2,6-di-tert-butyl-p-cresol	220	83	2.4E-01	1.6E+00	1.1E+05	12.1	3.5E-06	2.4E-09	1.1E-06	conf	conf	2.2E+03	3.1E+01	1.1E+03	-8.01	-7.75	-9.19	-2.96	0.84	0.0%	0.0%	2.8E-19
262	4098-71-9	3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	222	87	1.5E-01	4.5E+02	5.6E+04	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	3.1E+03	4.3E+01	1.6E+03	-7.58	-7.47	-8.92	-1.74	0.68	0.0%	0.0%	6.1E-25
263	25322-69-4	Propane-1,2-diol, propoxylated	308	113	9.5E-06	9.5E+02	6.2E-01	14.0	3.5E-06	1.8E-07	3.5E-07	conf	conf	2.9E+03	4.0E+01	1.5E+03	-5.14	-6.01	-7.73	0.68	0.74	0.0%	0.0%	1.5E-33
264	111-20-6	sebacic acid	202	127	8.9E-04	1.1E+03	1.5E+02	4.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.5E+03	4.9E+01	1.8E+03	-6.03	-6.84	-8.75	-1.93	0.25	0.0%	0.0%	9.8E-23
265	106-44-5	p-cresol	108	16	1.7E+01	1.6E+04	1.1E+02	10.0	3.5E-06	7.1E-07	3.5E-06	conf	conf	3.3E+03	4.6E+01	1.7E+03	-7.24	-7.01	-8.61	-1.91	0.41	0.0%	0.0%	5.1E-22
266	75-05-8	acetonitrile	41	-84	2.7E+04	1.8E+05	7.1E-01	14.0	3.5E-06	8.3E-07	3.5E-07	conf	conf	3.3E+03	4.6E+01	1.7E+03	-8.04	-7.75	-9.03	-0.34	0.72	0.0%	0.0%	1.1E-35
267	108-91-8	cyclohexylamine	99	-27	1.1E+03	9.1E+03	4.3E+01	10.0	3.5E-06	3.2E-07	1.1E-06	conf	conf	2.9E+03	4.1E+01	1.5E+03	-8.04	-7.78	-9.06	-1.17	0.70	0.0%	0.0%	8.3E-30
268	112-88-9	octadec-1-ene	252	30	3.5E-01	6.8E-04	1.1E+09	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.0E+03	2.9E+01	9.9E+02	-7.87	-7.98	-9.51	-2.68	1.28	0.0%	0.0%	8.5E-23
269	55542-26-2	17β-hydroxy-17-(3-hydroxy-1-propynyl)androst-4-ene-3-one	342	196	1.6E-09	4.6E-01	8.5E+02	13.2	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.2E+03	4.5E+01	1.7E+03	-6.09	-7.11	-8.78	-1.83	0.43	0.0%	0.0%	1.6E-23
270	552-30-7	benzene-1,2,4-tricarboxylic acid 1,2-anhydride	192	118	7.6E-05	4.1E+02	8.9E+01	3.4	3.5E-06	3.5E-06	1.1E-06	conf	conf	3.5E+03	4.8E+01	1.8E+03	-6.61	-7.58	-9.30	-0.50	0.31	0.0%	0.0%	1.6E-36
271	75-31-0	isopropylamine	59	-84	7.9E+04	2.1E+05	1.9E+00	10.0	3.5E-06	4.1E-07	1.1E-06	conf	conf	2.9E+03	4.1E+01	1.5E+03	-8.23	-7.95	-9.42	-0.76	0.70	0.0%	0.0%	1.7E-35
272	106-43-4	4-chlorotoluene	127	-27	3.0E+02	6.1E+01	1.5E+03	14.0	3.5E-06	1.3E-08	1.1E-07	conf	conf	2.0E+03	2.8E+01	9.6E+02	-8.72	-8.40	-10.47	-2.14	0.70	0.0%	0.0%	6.6E-33
273	95-48-7	o-cresol	108	16	3.3E+01	1.7E+04	1.1E+02	10.0	3.5E-06	6.7E-07	3.5E-06	conf	conf	3.1E+03	4.4E+01	1.6E+03	-7.30	-7.06	-8.61	-1.52	0.40	0.0%	0.0%	2.1E-24
274	100-00-5	1-chloro-4-nitrobenzene	158	49	1.5E+00	4.0E+02	2.9E+02	14.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	2.0E+03	2.8E+01	9.6E+02	-6.70	-6.42	-7.52	-2.07	0.70	0.0%	0.0%	3.4E-15
275	102-76-1	triacetin	218	-37	7.0E-01	2.5E+04	2.3E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	3.4E+03	4.8E+01	1.8E+03	-7.26	-7.41	-9.29	-0.34	0.45	0.0%	0.0%	9.2E-38
276	81-11-8	4,4'-diaminostilbene-2,2'-disulphonic acid	370	283	1.4E-16	6.4E-01	3.8E-02	-1.2	3.5E-06	3.5E-06	3.5E-07	conf	conf	3.4E+03	4.8E+01	1.8E+03	-5.74	-7.10	-9.22	-1.24	0.98	0.0%	0.0%	2.0E-30
277	57-10-3	palmitic acid	256	116	7.4E-03	4.3E-01	9.1E+06	4.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.9E+03	4.0E+01	1.5E+03	-7.41	-7.35	-8.99	-4.25	0.10	0.0%	0.0%	6.6E-12
278	111-69-3	adiponitrile	108	21	3.4E-01	2.5E+04	2.2E+00	14.0	3.5E-06	4.4E-07	3.5E-07	conf	conf	2.9E+03	4.1E+01	1.5E+03	-5.95	-6.36	-8.26	-0.07	0.26	0.0%	0.0%	6.5E-32
279	112-35-6	2-(2-(2-methoxyethoxy)ethoxy)ethanol	164	25	4.6E-01	3.3E+06	3.5E-02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	3.2E+03	4.4E+01	1.6E+03	-5.69	-6.72	-8.75	1.50	0.74	0.0%	0.0%	2.5E-23
280	71-55-6	1,1,1-trichloroethane	133	-72	1.5E+04	2.3E+03	4.8E+02	14.0	3.5E-06	4.8E-08	3.5E-08	conf	conf	1.9E+03	2.7E+01	9.3E+02	-8.74	-8.24	-10.62	-1.01	0.61	0.0%	0.0%	3.1E-43
281	123-42-2	4-hydroxy-4-methylpentan-2-one	116	-11	6.5E+01	3.3E+05	4.6E-01	14.0	3.5E-06	9.4E-07	1.1E-06	conf	conf	3.1E+03	4.3E+01	1.6E+03	-6.95	-6.79	-8.66	0.48	0.56	0.0%	0.0%	3.0E-39
282	109-67-1	pent-1-ene	70	-108	7.1E+04	5.0E+02	4.6E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.2E+03	3.1E+01	1.1E+03	-9.21	-8.83	-11.71	-2.05	0.28	0.0%	0.0%	1.2E-43
283	55542-27-3	17β-hydroxy-17-(3-hydroxypropyl)androst-4-ene-4-one	347	192	3.2E-09	3.5E+01	4.5E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.9E+03	4.1E+01	1.5E+03	-6.20	-7.24	-8.81	-1.97	0.45	0.0%	0.0%	7.0E-23
284	96-48-0	γ-butyrolactone	86	-42	3.9E+01	8.3E+04	4.9E-01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	3.2E+03	4.5E+01	1.7E+03	-7.56	-7.41	-9.26	-0.41	0.62	0.0%	0.0%	6.7E-37
285	107-07-3	2-chloroethanol	81	-54	5.9E+02	2.6E+05	1.3E+00	14.0	3.5E-06	4.3E-07	1.1E-07	conf	conf	2.8E+03	3.9E+01	1.4E+03	-6.88	-6.60	-8.28	-1.12	0.63	0.0%	0.0%	7.0E-25
286	461-58-5	cyanoguanidine	84	45	5.1E+00	2.6E+05	4.6E-02	-0.9	3.5E-06	1.1E-06	1.1E-06	conf	conf	3.0E+03	4.2E+01	1.5E+03	-5.65	-6.94	-8.79	0.56	0.82	0.0%	0.0%	5.8E-41
287	120-82-1	1,2,4-trichlorobenzene	181	16	2.4E+01	3.0E+01	8.5E+03	14.0	3.5E-06	2.4E-09	3.5E-08	conf	conf	1.8E+03	2.5E+01	8.7E+02	-8.34	-8.05	-9.85	-2.53	0.51	0.0%	0.0%	6.7E-26
288	3209-22-1	1,2-dichloro-3-nitrobenzene	192	66	1.1E+00	7.9E+01	1.3E+03	14.0	3.5E-06	2.3E-09	3.5E-08	conf	conf	1.8E+03	2.5E+01	8.7E+02	-7.19	-6.92	-8.13	-2.46	0.70	0.0%	0.0%	2.9E-16
289	120-83-2	2,4-dichlorophenol	163	47	8.8E+00	3.6E+03	6.3E+02	14.0	3.5E-06	2.2E-09	1.1E-07	conf	conf	1.8E+03	2.5E+01	8.7E+02	-6.65	-6.38	-7.45	-2.15	0.64	0.0%	0.0%	1.9E-14
290	1066-35-9	chlorodimethylsilane	94	-125	7.3E+04	9.6E+03	8.5E+01	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	1.8E+03	2.5E+01	8.5E+02	-8.58	-7.94	-10.46	-0.51	0.25	0.0%	0.0%	3.4E-46
291	89-98-5	2-chlorobenzaldehyde	141	9	2.6E+01	9.5E+02	2.2E+02	14.0	3.5E-06	4.9E-08	3.5E-07	conf	conf	2.0E+03	2.8E+01	9.9E+02	-7.48	-7.21	-8.43	-2.13	0.35	0.0%	0.0%	1.0E-19
292	6419-19-8	nitrilotrimethylenetris(phosphonic acid)	299	90	2.7E-09	1.0E+06	3.5E-06	2.3	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.6E+03	3.7E+01	1.3E+03	-5.03	-6.13	-8.06	-0.71	0.70	0.0%	0.0%	4.3E-26
293	1569-02-4	1-ethoxypropan-2-ol	104	-46	5.1E+02	2.3E+05	1.0E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.9E+03	4.1E+01	1.5E+03	-7.36	-7.18	-8.79	0.01	0.64	0.0%	0.0%	1.6E-36
294	826-36-8	2,2,6,6-tetramethyl-4-piperidone	155	53	2.7E+01	3.2E+03	2.7E+00	9.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.9E+03	4.0E+01	1.5E+03	-7.69	-7.51	-8.90	-0.72	0.52	0.0%	0.0%	7.5E-32
295	98-07-7	α,α,α-trichlorotoluene	195	10	1.7E+01	2.9E+01	7.9E+03	14.0	3.5E-06	3.9E-08	1.1E-07	conf	conf	1.8E+03	2.5E+01	8.8E+02	-8.33	-8.04	-9.77	-0.66	1.11	0.0%	0.0%	5.3E-39
296	712-50-5	cyclohexyl phenyl ketone	188	50	2.7E-01	1.0E+01	8.7E+03	14.0	3.5E-06	1.8E-08	1.1E-06	conf	conf	1.8E+03	2.5E+01	8.8E+02	-7.50	-7.23	-8.48	-2.29	0.23	0.0%	0.0%	4.6E-19
297	17773-41-0	2-hydroxy-4-(methylthio)butyronitrile	131	27	2.9E-01	2.7E+04	2.4E-01	10.6	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.9E+03	4.0E+01	1.5E+03	-6.31	-6.82	-8.80	-3.11	0.41	0.0%	0.0%	2.1E-16
298	104-15-4	toluene-4-sulphonic acid	172	102	3.9E-04	2.8E+03	2.4E-01	0.7	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.5E+03	3.5E+01	1.3E+03	-5.14	-6.22	-8.13	-1.25	1.21	0.0%	0.0%	4.5E-23
299	88-12-0	1-vinyl-2-pyrrolidone	111	29	1.8E+01	3.7E+05	1.8E+00	-0.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.8E+03	3.9E+01	1.5E+03	-5.69	-6.83	-8.81	-0.52	1.07	0.0%	0.0%	1.2E-32
300	111-77-3	2-(2-methoxyethoxy)ethanol	120	-15	1.5E+01	1.5E+06	6.6E-02	14.0	3.5E-06	8.3E-07	1.1E-06	conf	conf	2.7E+03	3.8E+01	1.4E+03	-6.21	-6.67	-8.65	0.55	0.70	0.0%	0.0%	9.9E-40
301	75-04-7	ethylamine	45	-85	2.0E+04	1.0E+06	7.1E-01	10.0	3.5E-06	4.1E-07	1.1E-06	conf	conf	2.5E+03	3.5E+01	1.3E+03	-7.56	-7.34	-8.50	-0.74	0.67	0.0%	0.0%	7.8E-29
302	75-64-9	tert-butylamine	73	-65	4.7E+04	5.7E+05	5.2E+00	10.0	3.5E-06	8.3E-09	1.1E-06	conf	conf	1.7E+03	2.3E+01	8.1E+02	-7.74	-7.46	-8.80	-1.24	0.53	0.0%	0.0%	1.6E-27
303	111-27-3	hexan-1-ol	102	-38	1.2E+02	1.1E+04	6.6E+01	14.0	3.5E-06	3.9E-06	3.5E-06	conf	conf	2.8E+03	3.9E+01	1.4E+03	-8.35	-8.18	-9.46	-0.74	0.42	0.0%	0.0%	6.4E-36
304	2403-88-5	2,2,6,6-tetramethylpiperidin-4-ol	157	53	4.2E-01	2.3E+03	8.7E+00	9.6	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.7E+03	3.8E+01	1.4E+03	-7.28	-7.10	-8.87	-0.73	0.27	0.0%	0.0%	1.4E-31
305	502-44-3	hexan-6-olide	114	-22	2.3E+01	2.4E+04	4.8E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.8E+03	3.9E+01	1.4E+03	-7.86	-7.69	-9.35	-0.25	0.39	0.0%	0.0%	6.0E-39
306	95-49-8	2-chlorotoluene	127	-27	3.5E+02	5.6E+01	1.5E+03	14.0	3.5E-06	3.5E-09	1.1E-07	conf	conf	1.6E+03	2.2E+01	7.8E+02	-8.85	-8.52	-10.65	-1.81	0.70	0.0%	0.0%	8.4E-37
307	1570-64-5	4-chloro-o-cresol	143	36	3.8E+00	1.1E+03	5.0E+02	9.6	3.5E-06	3.9E-09	1.1E-06	conf	conf	1.6E+03	2.3E+01	7.9E+02	-6.80	-6.53	-7.64	-2.54	0.84	0.0%	0.0%	1.7E-13
308	25265-77-4	isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-diol	216	25	6.4E-01	1.1E+03	1.0E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.7E+03	3.8E+01	1.4E+03	-8.18	-8.00	-9.47	-1.40	0.48	0.0%	0.0%	4.3E-31
309	121-44-8	triethylamine	101	-71	7.9E+03	4.8E+04	3.2E+01	11.0	3.5E-06	1.5E-08	1.1E-06	conf	conf	1.6E+03	2.3E+01	8.0E+02	-7.93	-7.64	-9.18	-1.17	0.70	0.0%	0.0%	1.4E-30
310	124-10-7	methyl myristate	242	36	3.4E-01	6.0E-01	1.9E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+03	2.5E+01	9.0E+02	-9.02	-8.82	-10.21	-4.14	0.30	0.0%	0.0%	2.1E-18
311	3926-62-3	sodium chloroacetate	116	87	9.9E-03	8.0E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+03	2.8E+01	1.0E+03	-5.73	-6.03	-7.67	-1.80	1.96	0.0%	0.0%	2.6E-17
312	298-12-4	glyoxylic acid	74	16	2.5E+01	2.5E+05	4.0E-02	3.5	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.7E+03	3.8E+01	1.4E+03	-6.17	-7.54	-9.37	-0.70	0.50	0.0%	0.0%	1.5E-35
313	95-33-0	N-cyclohexylbenzothiazole-2-sulfenamide	264	151	2.4E-04	1.7E+00	3.0E+03	10.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.5E+03	3.4E+01	1.3E+03	-7.51	-7.33	-8.97	-2.19	0.83	0.0%	0.0%	1.8E-22
314	110-91-8	morpholine	87	-15	1.5E+03	3.6E+06	2.8E-01	8.0	3.5E-06	3.5E-09	3.5E-07	conf	conf	1.5E+03	2.1E+01	7.4E+02	-6.23	-5.98	-6.92	-1.01	0.67	0.0%	0.0%	1.7E-17
315	661-19-8	docosan-1-ol	327	123	8.2E-06	2.8E-04	4.8E+09	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.5E+03	2.1E+01	7.4E+02	-7.42	-7.65	-7.77	-6.15	0.62	0.0%	0.0%	1.1E-17
316	111-81-9	methyl undec-10-enoate	198	11	4.0E+00	1.1E+01	4.6E+04	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.9E+03	2.6E+01	9.2E+02	-8.57	-8.30	-9.80	-2.91	0.49	0.0%	0.0%	3.6E-23
317	105-59-9	2,2'-methyliminodiethanol	119	25	3.3E-01	1.0E+06	3.2E-02	9.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	2.6E+03	3.7E+01	1.4E+03	-6.43	-7.52	-9.40	-0.53	0.59	0.0%	0.0%	4.9E-37
318	142-90-5	dodecyl methacrylate	254	34	1.9E-01	1.1E-01	4.8E+06	14.0	3.5E-06	8.4E-07	3.5E-07	conf	conf	1.6E+03	2.3E+01	7.9E+02	-9.07	-8.90	-10.54	-2.47	2.44	0.0%	0.0%	4.4E-31
319	16470-24-9	tetrasodium 4,4'-bis[[4-[bis(2-hydroxyethyl)amino]-6-(4-sulphonatoanilino)-1,3,5-triazin-2-yl]amino]stilbene-2,2'-dis	1165	87	9.9E-03	8.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.9E+03	2.7E+01	9.7E+02	-5.71	-6.04	-7.71	-0.61	0.64	0.0%	0.0%	1.9E-24
320	110-86-1	pyridine	79	-45	2.6E+03	1.3E+06	6.3E+00	5.0	3.5E-06	7.0E-07	1.1E-07	conf	conf	2.4E+03	3.3E+01	1.2E+03	-6.10	-6.67	-8.60	-0.79	0.86	0.0%	0.0%	3.2E-29
321	75-38-7	1,1-difluoroethylene	64	-156	2.5E+06	2.2E+03	1.7E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.7E+03	2.4E+01	8.6E+02	-9.34	-8.70	-11.51	-0.68	0.13	0.0%	0.0%	2.4E-54
322	868-85-9	dimethyl phosphonate	110	-52	2.0E+02	1.9E+05	7.4E-02	14.0	3.5E-06	2.4E-08	1.1E-06	conf	conf	1.6E+03	2.2E+01	7.8E+02	-6.49	-6.23	-7.38	-0.95	0.42	0.0%	0.0%	2.1E-20
323	868-77-9	2-hydroxyethyl methacrylate	130	-13	1.1E+01	5.3E+04	2.0E+00	14.0	3.5E-06	6.8E-07	1.1E-06	conf	conf	2.4E+03	3.3E+01	1.2E+03	-7.02	-6.83	-8.64	-0.69	0.39	0.0%	0.0%	3.3E-30
324	79-04-9	chloroacetyl chloride	113	-46	3.9E+03	1.5E+04	6.0E-01	14.0	3.5E-06	8.1E-07	1.1E-07	conf	conf	2.3E+03	3.2E+01	1.2E+03	-8.24	-7.83	-9.66	-2.24	0.75	0.0%	0.0%	1.6E-26
325	3319-31-1	tris(2-ethylhexyl) benzene-1,2,4-tricarboxylate	547	197	7.8E-06	3.2E-05	3.9E+11	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.4E+03	2.0E+01	7.0E+02	-7.50	-7.50	-7.50	-6.55	1.62	0.0%	0.0%	2.9E-16
326	100-97-0	methenamine	140	65	1.2E+01	1.0E+06	7.1E-05	4.9	3.5E-06	3.7E-07	3.5E-07	conf	conf	2.2E+03	3.0E+01	1.1E+03	-5.36	-6.38	-8.27	1.59	0.70	0.0%	0.0%	1.9E-20
327	140-01-2	pentasodium (carboxylatomethyl)iminobis(ethylenenitrilo)tetraacetate	503	87	9.9E-03	3.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+03	2.6E+01	9.2E+02	-5.75	-6.07	-7.73	-0.65	1.00	0.0%	0.0%	2.3E-24
328	628-96-6	ethylene dinitrate	152	-10	5.2E+01	5.4E+04	1.5E+01	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	2.3E+03	3.3E+01	1.2E+03	-7.26	-7.04	-8.88	-1.69	1.13	0.0%	0.0%	4.3E-25
329	88-73-3	1-chloro-2-nitrobenzene	158	49	3.8E+00	3.8E+02	2.9E+02	14.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	1.4E+03	2.0E+01	6.8E+02	-7.19	-6.91	-8.07	-1.80	0.70	0.0%	0.0%	1.5E-19
330	85-43-8	1,2,3,6-tetrahydrophthalic anhydride	152	-1	7.7E+00	1.0E+04	9.1E+01	14.0	3.5E-06	3.5E-06	3.5E-07	conf	conf	2.4E+03	3.4E+01	1.2E+03	-7.97	-7.80	-9.45	-0.64	0.30	0.0%	0.0%	1.4E-36
331	6683-19-8	pentaerythritol tetrakis(3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate)	1178	87	9.9E-03	8.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+03	2.5E+01	8.8E+02	-5.75	-6.08	-7.75	-0.67	0.29	0.0%	0.0%	2.5E-24
332	100-52-7	benzaldehyde	106	-22	1.3E+02	4.9E+03	5.1E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.2E+03	3.1E+01	1.1E+03	-8.14	-7.94	-9.09	-1.53	0.65	0.0%	0.0%	1.7E-27
333	556-82-1	3-methylbut-2-en-1-ol	86	-59	3.1E+02	4.9E+03	1.5E+01	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	2.3E+03	3.2E+01	1.2E+03	-8.66	-8.50	-9.62	-0.68	0.47	0.0%	0.0%	1.2E-37
334	95-63-6	1,2,4-trimethylbenzene	120	-22	2.2E+02	8.5E+01	4.3E+03	14.0	3.5E-06	1.4E-08	1.1E-07	conf	conf	1.4E+03	1.9E+01	6.5E+02	-8.75	-8.45	-10.36	-2.32	0.70	0.0%	0.0%	7.6E-31
335	123-77-3	C,C'-azodi(formamide)	116	117	1.4E-03	1.5E+05	1.3E-04	0.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.2E+03	3.1E+01	1.1E+03	-5.61	-6.94	-8.88	-1.37	0.37	0.0%	0.0%	3.7E-27
336	69-72-7	salicylic acid	138	94	4.3E-03	5.1E+03	1.7E+02	3.0	3.5E-06	1.6E-06	1.1E-06	conf	conf	2.2E+03	3.1E+01	1.1E+03	-6.55	-7.38	-9.12	-0.76	0.70	0.0%	0.0%	3.4E-33
337	2416-94-6	2,3,6-trimethylphenol	136	41	2.8E+00	9.5E+02	1.4E+03	10.9	3.5E-06	1.6E-08	1.1E-07	conf	conf	1.4E+03	1.9E+01	6.7E+02	-6.83	-6.56	-7.67	-1.96	0.84	0.0%	0.0%	1.8E-16
338	122-20-3	1,1',1''-nitrilotripropan-2-ol	191	79	2.5E-03	2.6E+06	6.0E-02	7.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.2E+03	3.0E+01	1.1E+03	-5.76	-6.88	-8.90	-0.14	0.72	0.0%	0.0%	3.0E-36
339	107-86-8	3-methyl-2-butenal	84	-77	1.1E+03	1.2E+04	1.4E+01	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	2.2E+03	3.1E+01	1.1E+03	-8.77	-8.60	-9.73	-1.81	0.14	0.0%	0.0%	5.6E-30
340	106-50-3	p-phenylenediamine	108	53	8.7E-02	2.0E+04	4.1E-01	6.0	3.5E-06	2.2E-09	1.1E-06	conf	conf	1.3E+03	1.8E+01	6.3E+02	-5.50	-6.01	-6.94	-2.55	0.90	0.0%	0.0%	1.8E-10
341	98-86-2	acetophenone	120	-10	4.3E+01	3.5E+03	4.7E+01	14.0	3.5E-06	7.4E-07	1.1E-06	conf	conf	2.1E+03	2.9E+01	1.1E+03	-7.85	-7.63	-8.89	-0.82	0.70	0.0%	0.0%	5.3E-31

342	5435-64-3	3,5,5-trimethylhexanal	142	-35	1.8E+02	7.3E+01	1.2E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.7E+03	2.4E+01	8.6E+02	-9.06	-8.77	-10.76	-1.61	0.34	0.0%	0.0%	2.5E-39
343	611-70-1	isobutyrophenone	148	2	1.7E+01	3.5E+02	3.8E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.8E+03	2.5E+01	9.3E+02	-8.07	-7.82	-9.03	-1.07	0.32	0.0%	0.0%	3.2E-30
344	1562-00-1	sodium 2-hydroxyethanesulphonate	148	87	9.9E-03	1.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+03	2.3E+01	8.1E+02	-5.82	-6.12	-7.77	-6.00	0.64	0.0%	0.0%	1.1E-17
345	106-14-9	12-hydroxystearic acid	300	153	4.5E-07	1.1E+00	2.6E+06	4.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.9E+03	2.7E+01	9.9E+02	-6.46	-7.43	-8.99	-3.91	0.19	0.0%	0.0%	1.8E-13
346	110-85-0	piperazine	86	7	9.5E+01	1.0E+06	1.6E-01	9.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.2E+03	3.0E+01	1.1E+03	-7.44	-7.45	-9.44	-1.47	1.02	0.0%	0.0%	2.5E-30
347	2402-79-1	2,3,5,6-tetrachloropyridine	217	55	8.1E-01	2.1E+01	2.4E+03	14.0	3.5E-06	3.5E-08	3.5E-08	conf	conf	1.3E+03	1.9E+01	6.6E+02	-7.74	-7.47	-8.79	-2.51	0.44	0.0%	0.0%	1.3E-19
348	112-07-2	2-butoxyethyl acetate	160	-15	7.2E+01	3.2E+03	3.7E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.0E+03	2.8E+01	1.0E+03	-8.19	-7.99	-9.20	-0.79	0.55	0.0%	0.0%	1.7E-33
349	101-77-9	4,4'-methylenedianiline	198	128	2.8E-04	4.9E+02	1.5E+02	5.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.0E+03	2.8E+01	1.0E+03	-6.26	-7.09	-8.99	-2.01	0.62	0.0%	0.0%	1.1E-23
350	615-16-7	2-hydroxybenzimidazole	134	96	4.9E-02	6.5E+02	1.6E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.8E+03	2.5E+01	9.3E+02	-6.71	-6.59	-8.37	-1.99	1.16	0.0%	0.0%	3.7E-20
351	108-39-4	m-cresol	108	16	2.2E+01	1.6E+04	1.1E+02	10.0	3.5E-06	2.8E-06	3.5E-06	conf	conf	2.1E+03	2.9E+01	1.1E+03	-8.16	-7.98	-9.44	-1.54	0.84	0.0%	0.0%	7.5E-30
352	5994-61-6	N-(carboxymethyl)-N-(phosphonomethyl)glycine	227	304	2.6E-11	1.1E+04	1.3E-05	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.8E+03	2.5E+01	9.3E+02	-5.24	-6.30	-8.23	-0.93	0.48	0.0%	0.0%	9.8E-26
353	110-17-8	fumaric acid	116	84	1.3E-09	5.5E+04	1.1E+00	3.0	3.5E-06	4.7E-06	1.1E-06	conf	conf	2.1E+03	3.0E+01	1.1E+03	-6.37	-7.77	-9.58	-0.97	0.95	0.0%	0.0%	4.2E-35
354	7659-86-1	2-ethylhexyl mercaptoacetate	204	16	1.1E+03	6.1E+01	4.8E+03	8.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.6E+03	2.3E+01	8.2E+02	-9.48	-9.19	-12.01	-3.18	0.61	0.0%	0.0%	8.8E-37
355	57-11-4	stearic acid	284	133	1.1E-03	2.4E-02	8.7E+07	4.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.6E+03	2.3E+01	8.2E+02	-7.73	-7.71	-9.23	-4.69	0.36	0.0%	0.0%	4.5E-11
356	420-46-2	1,1,1-trifluoroethane	84	-152	9.3E+05	3.2E+04	5.5E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.3E+03	1.8E+01	6.4E+02	-9.21	-8.76	-10.70	-1.36	0.21	0.0%	0.0%	7.1E-41
357	108-68-9	3,5-xylenol	122	25	3.1E+00	6.7E+03	4.1E+02	10.0	3.5E-06	4.5E-07	3.5E-07	conf	conf	1.8E+03	2.6E+01	9.3E+02	-7.16	-6.92	-8.59	-1.79	0.84	0.0%	0.0%	1.2E-22
358	80-07-9	bis(4-chlorophenyl) sulphone	287	146	1.1E-04	3.5E+00	7.9E+03	14.0	3.5E-06	1.1E-08	3.5E-09	conf	conf	1.2E+03	1.7E+01	6.0E+02	-6.17	-6.04	-7.10	-2.63	0.22	0.0%	0.0%	8.2E-11
359	6104-30-9	N,N''-(isobutylidene)diurea	174	141	7.8E-04	2.3E+01	2.1E-02	0.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.0E+03	2.8E+01	1.0E+03	-5.85	-7.12	-8.99	-1.28	1.27	0.0%	0.0%	1.6E-28
360	112-38-9	undec-10-enoic acid	184	71	9.3E-01	3.4E+01	2.3E+04	4.9	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.8E+03	2.5E+01	9.1E+02	-7.05	-6.78	-8.49	-1.93	0.79	0.0%	0.0%	3.4E-21
361	2487-90-3	trimethoxysilane	121	-81	1.1E+04	1.3E+05	6.0E-02	14.0	3.5E-06	4.5E-07	1.1E-06	conf	conf	1.8E+03	2.5E+01	9.2E+02	-8.18	-7.91	-9.32	-0.37	1.04	0.0%	0.0%	9.4E-38
362	7396-58-9	N-methyldidecylamine	312	90	2.8E-03	3.2E-04	7.6E+08	10.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+03	1.7E+01	5.9E+02	-8.12	-8.26	-9.66	-4.35	1.25	0.0%	0.0%	1.5E-14
363	116-15-4	hexafluoropropene	150	-153	5.9E+05	1.1E+00	1.3E+02	14.0	3.5E-06	3.5E-08	3.5E-08	conf	conf	1.2E+03	1.7E+01	5.8E+02	-9.26	-8.94	-11.69	-1.17	0.29	0.0%	0.0%	2.5E-51
364	3302-10-1	3,5,5-trimethylhexanoic acid	158	37	6.1E+00	4.9E+01	2.2E+03	4.9	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.1E+03	2.9E+01	1.1E+03	-8.26	-8.02	-9.53	-1.06	0.20	0.0%	0.0%	5.4E-34
365	839-90-7	tris(2-hydroxyethyl)-1,3,5-triazinetrione	261	241	1.2E-13	7.6E+05	1.2E+00	-0.6	3.5E-06	3.5E-06	3.5E-06	conf	conf	2.1E+03	2.9E+01	1.1E+03	-6.51	-7.87	-9.47	0.01	1.92	0.0%	0.0%	4.6E-42
366	80-54-6	2-(4-tert-butylbenzyl)propionaldehyde	204	46	4.8E-01	3.9E+00	2.3E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.5E+03	2.2E+01	7.7E+02	-8.41	-8.15	-9.43	-2.14	0.49	0.0%	0.0%	1.0E-25
367	124-28-7	dimantine	298	81	2.2E-02	7.5E-04	2.5E+08	10.1	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+03	1.7E+01	5.9E+02	-8.38	-8.49	-10.30	-3.88	0.66	0.0%	0.0%	2.6E-20
368	100-20-9	terephthaloyl dichloride	203	68	6.5E-01	7.1E+02	7.6E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.1E+03	2.9E+01	1.1E+03	-8.05	-7.89	-9.53	0.30	0.30	0.0%	0.0%	3.9E-45
369	3282-30-2	pivaloyl chloride	121	-48	4.3E+03	2.9E+03	7.8E+00	14.0	3.5E-06	3.2E-08	1.1E-06	conf	conf	1.2E+03	1.7E+01	5.9E+02	-8.63	-8.32	-10.27	-1.10	0.75	0.0%	0.0%	1.6E-39
370	144-62-7	oxalic acid	90	63	7.5E-01	7.3E+05	1.8E-02	1.2	3.5E-06	4.7E-06	1.1E-06	conf	conf	2.1E+03	2.9E+01	1.1E+03	-6.39	-7.78	-9.63	-0.17	0.69	0.0%	0.0%	6.6E-42
371	577-11-7	docusate sodium	445	87	9.9E-03	3.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+03	2.1E+01	7.4E+02	-5.84	-6.16	-7.82	-1.44	0.26	0.0%	0.0%	3.8E-20
372	120-80-9	pyrocatechol	110	46	1.5E-01	8.8E+04	1.1E+01	10.0	3.5E-06	4.1E-06	1.1E-06	conf	conf	2.0E+03	2.7E+01	1.0E+03	-6.87	-7.87	-9.60	-2.00	0.47	0.0%	0.0%	1.0E-27
373	2432-99-7	11-aminoundecanoic acid	201	304	2.1E-07	1.6E+01	6.9E-01	4.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.9E+03	2.6E+01	9.6E+02	-5.81	-6.98	-8.99	-2.52	1.47	0.0%	0.0%	1.1E-20
374	131-11-3	dimethyl phthalate	194	-23	6.2E-01	2.0E+03	4.6E+01	14.0	3.5E-06	7.9E-07	3.5E-07	conf	conf	1.8E+03	2.5E+01	9.3E+02	-7.31	-7.08	-8.87	-1.01	0.42	0.0%	0.0%	1.4E-29
375	26523-78-4	tris(nonylphenyl) phosphite	689	317	2.6E-15	2.8E-13	1.1E+20	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E+03	1.6E+01	5.4E+02	-15.55	-15.55	-15.55	-1.88	1.37	0.0%	0.0%	3.0E-85
376	2216-51-5	L-menthol	156	-6	1.0E+00	9.4E+02	2.4E+03	14.0	3.5E-06	3.2E-07	3.5E-07	conf	conf	1.6E+03	2.2E+01	8.0E+02	-7.21	-6.97	-8.53	-1.68	0.13	0.0%	0.0%	6.0E-23
377	540-97-6	dodecamethylcyclohexasiloxane	445	-9	4.7E+00	1.7E-03	1.2E+09	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	1.1E+03	1.5E+01	5.3E+02	-8.06	-7.83	-9.06	-4.55	0.59	0.0%	0.0%	5.9E-11
378	13674-84-5	tris(2-chloro-1-methylethyl) phosphate	328	72	7.5E-03	3.0E+01	7.8E+02	14.0	3.5E-06	1.5E-08	1.1E-07	conf	conf	1.1E+03	1.6E+01	5.6E+02	-6.52	-6.25	-7.35	-1.19	0.29	0.0%	0.0%	6.7E-19
379	29329-71-3	(1-hydroxyethylidene)bisphosphonic acid, sodium salt	229	87	9.9E-03	1.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+03	2.0E+01	7.1E+02	-5.87	-6.18	-7.83	-0.49	1.50	0.0%	0.0%	4.7E-26
380	112-39-0	methyl palmitate	270	63	6.3E-02	7.4E-02	1.8E+07	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+03	1.7E+01	5.8E+02	-8.98	-8.90	-10.32	-4.56	0.25	0.0%	0.0%	9.3E-17
381	95-51-2	2-chloroaniline	128	24	3.1E+01	1.8E+03	5.2E+01	3.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	1.1E+03	1.5E+01	5.3E+02	-5.65	-6.09	-7.04	-1.96	0.73	0.0%	0.0%	2.1E-13
382	108-46-3	resorcinol	110	46	1.6E-02	3.3E+05	1.1E+01	9.6	3.5E-06	5.1E-08	1.1E-06	conf	conf	1.2E+03	1.7E+01	6.2E+02	-5.81	-6.25	-7.58	-1.48	0.73	0.0%	0.0%	1.4E-18
383	25601-41-6	Methyl dec-9-enoate	184	0	1.1E+01	3.7E+01	1.5E+04	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	1.4E+03	1.9E+01	6.7E+02	-8.16	-7.75	-9.63	-2.53	0.45	0.0%	0.0%	1.9E-24
384	505-32-8	3,7,11,15-tetramethylhexadec-1-en-3-ol	297	70	1.9E-03	8.1E-02	1.7E+08	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.1E+03	1.5E+01	5.2E+02	-7.85	-8.06	-8.53	-4.27	0.94	0.0%	0.0%	5.9E-10
385	7680-73-1	1-methylpyridinium chloride	130	87	9.9E-03	9.0E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+03	1.9E+01	6.8E+02	-5.90	-6.20	-7.84	-1.84	0.64	0.0%	0.0%	4.6E-18
386	100-02-7	4-nitrophenol	139	71	3.9E-02	3.8E+04	8.1E+01	7.2	3.5E-06	1.1E-08	3.5E-07	conf	conf	1.1E+03	1.5E+01	5.3E+02	-5.82	-6.15	-7.20	-1.90	0.56	0.0%	0.0%	1.8E-14
387	629-96-9	icosan-1-ol	299	105	6.7E-05	9.4E-04	5.0E+08	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.1E+03	1.5E+01	5.2E+02	-7.90	-8.25	-8.63	-5.51	0.50	0.0%	0.0%	4.0E-06
388	75-00-3	chloroethane	65	-111	1.6E+05	1.2E+04	3.8E+01	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	1.1E+03	1.5E+01	5.2E+02	-9.04	-8.38	-10.79	-1.01	0.15	0.0%	0.0%	1.0E-44
389	22042-96-2	[[(phosphonomethyl)imino]bis[(ethylenenitrilo)bis(methylene)]]tetrakisphosphonic acid, sodium salt	595	87	9.9E-03	4.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+03	1.9E+01	6.7E+02	-5.88	-6.20	-7.86	-0.59	1.21	0.0%	0.0%	1.4E-25
390	5131-66-8	1-butoxypropan-2-ol	132	-22	5.3E+01	1.5E+04	9.5E+00	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.5E+03	2.1E+01	7.8E+02	-7.32	-7.10	-8.56	-0.03	0.22	0.0%	0.0%	2.1E-34
391	104-93-8	4-methylanisole	122	-23	1.6E+02	3.6E+02	4.2E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.7E+03	2.3E+01	8.6E+02	-9.20	-8.98	-10.43	-0.77	0.50	0.0%	0.0%	1.2E-43
392	108-20-3	diisopropyl ether	102	-99	2.0E+04	8.8E+03	7.6E+01	14.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	1.0E+03	1.4E+01	4.9E+02	-8.77	-8.45	-10.46	-0.15	0.70	0.0%	0.0%	2.1E-49
393	120-78-5	di(benzothiazol-2-yl) disulphide	332	213	8.3E-08	2.0E-03	4.6E+04	3.0	3.5E-06	4.7E-09	3.5E-07	conf	conf	1.0E+03	1.4E+01	5.0E+02	-6.05	-6.14	-7.12	-1.50	0.75	0.0%	0.0%	4.7E-16
394	22113-87-7	methylammonium nitrate	94	87	9.9E-03	6.5E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+03	1.8E+01	6.6E+02	-5.92	-6.22	-7.86	-0.88	0.64	0.0%	0.0%	1.1E-23
395	110-19-0	isobutyl acetate	116	-68	2.4E+03	1.1E+04	5.9E+01	14.0	3.5E-06	9.1E-07	1.1E-06	conf	conf	1.6E+03	2.2E+01	8.1E+02	-8.72	-8.47	-9.86	-0.68	0.49	0.0%	0.0%	1.3E-39
396	75-98-9	pivalic acid	102	10	2.1E+02	6.2E+04	2.8E+01	4.9	3.5E-06	2.2E-09	1.1E-06	conf	conf	1.0E+03	1.4E+01	4.9E+02	-6.27	-6.17	-7.11	-0.40	0.64	0.0%	0.0%	4.9E-22
397	75-10-5	difluoromethane	52	-160	1.0E+06	9.1E+03	5.1E+00	14.0	3.5E-06	3.5E-08	1.1E-08	conf	conf	1.0E+03	1.4E+01	4.9E+02	-9.22	-8.29	-10.79	-0.04	0.43	0.0%	0.0%	1.7E-53
398	120-12-7	anthracene	178	78	2.9E-04	6.6E-01	2.2E+04	14.0	3.5E-06	4.2E-09	3.5E-08	conf	conf	1.0E+03	1.4E+01	4.9E+02	-6.63	-6.40	-7.37	-4.73	0.81	0.3%	0.8%	8.0E-05
399	26761-45-5	2,3-epoxypropyl neodecanoate	228	49	6.8E-01	9.4E+00	5.4E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.6E+03	2.2E+01	8.2E+02	-9.02	-8.82	-10.03	-2.37	0.30	0.0%	0.0%	3.8E-28
400	80-43-3	bis(α,α-dimethylbenzyl) peroxide	270	104	1.0E-03	7.0E-01	7.6E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+03	1.7E+01	6.2E+02	-8.12	-8.14	-9.37	-2.57	0.78	0.0%	0.0%	1.3E-22
401	109-70-6	1-bromo-3-chloropropane	157	-46	7.3E+02	1.7E+03	2.6E+02	14.0	3.5E-06	8.9E-09	3.5E-08	conf	conf	1.0E+03	1.4E+01	4.9E+02	-8.33	-8.00	-9.85	-0.99	0.42	0.0%	0.0%	5.1E-37
402	693-23-2	dodecanedioic acid	230	143	2.6E-04	6.5E+01	1.5E+03	4.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.7E+03	2.3E+01	8.5E+02	-6.55	-7.22	-9.09	-0.46	1.02	0.0%	0.0%	3.0E-35
403	118-96-7	2,4,6-trinitrotoluene	227	124	2.3E-03	2.2E+02	9.8E+01	14.0	3.5E-06	2.2E-09	1.1E-07	conf	conf	9.9E+02	1.4E+01	4.8E+02	-6.11	-6.11	-7.05	-2.42	0.58	0.0%	0.0%	1.9E-11
404	611-06-3	1,3-dichloro-4-nitrobenzene	192	66	1.9E+00	7.5E+01	1.3E+03	14.0	3.5E-06	2.3E-09	3.5E-08	conf	conf	9.9E+02	1.4E+01	4.8E+02	-7.65	-7.37	-8.65	-2.46	0.70	0.0%	0.0%	4.5E-19
405	77881-13-1	(17α)-17-hydroxy-3-oxoandrost-4-ene-17-carbonitrile	313	183	4.6E-08	5.6E+01	9.1E+02	11.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.4E+03	2.0E+01	7.3E+02	-5.87	-6.76	-8.49	-2.99	0.17	0.0%	0.0%	2.1E-15
406	2243-62-1	1,5-naphthylenediamine	158	110	5.0E-04	1.2E+03	2.2E+01	14.0	3.5E-06	2.6E-09	1.1E-06	conf	conf	9.9E+02	1.4E+01	4.8E+02	-5.90	-6.16	-7.10	-1.96	0.82	0.0%	0.0%	1.0E-13
407	15763-76-5	sodium p-cumenesulphonate	222	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+03	1.8E+01	6.4E+02	-5.92	-6.23	-7.88	-0.50	0.70	0.0%	0.0%	3.0E-26
408	541-73-1	1,3-dichlorobenzene	147	-14	1.8E+02	1.2E+02	1.9E+03	14.0	3.5E-06	2.3E-09	3.5E-08	conf	conf	9.8E+02	1.4E+01	4.7E+02	-8.71	-8.39	-10.33	-1.76	0.54	0.0%	0.0%	8.5E-35
409	124-17-4	2-(2-butoxyethoxy)ethyl acetate	204	24	4.7E+00	7.5E+03	2.0E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.6E+03	2.3E+01	8.3E+02	-7.67	-7.45	-9.13	-0.46	0.57	0.0%	0.0%	1.6E-35
410	95-31-8	N-tert-butylbenzothiazole-2-sulphenamide	238	127	1.1E-03	5.8E+00	3.6E+02	10.6	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.4E+03	2.0E+01	7.3E+02	-7.02	-6.78	-8.53	-3.28	0.46	0.0%	0.0%	3.4E-14
411	5039-78-1	[2-(methacryloyloxy)ethyl]trimethylammonium chloride	208	87	9.9E-03	1.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+03	1.8E+01	6.3E+02	-5.93	-6.24	-7.89	-1.16	1.01	0.0%	0.0%	3.7E-22
412	2867-47-2	2-dimethylaminoethyl methacrylate	157	-20	9.6E+01	8.3E+04	9.3E+00	8.0	3.5E-06	5.5E-07	1.1E-06	conf	conf	1.5E+03	2.1E+01	7.7E+02	-7.39	-7.15	-8.77	-1.34	0.87	0.0%	0.0%	1.3E-26
413	141-10-6	6,10-dimethylundeca-3,5,9-trien-2-one	192	6	2.6E+00	1.8E+01	2.7E+04	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.4E+03	1.9E+01	6.9E+02	-8.88	-8.63	-9.87	-2.47	0.29	0.0%	0.0%	2.1E-26
414	78-96-6	1-aminopropan-2-ol	75	-29	1.0E+02	1.0E+06	6.5E-02	9.0	3.5E-06	4.1E-07	3.5E-06	conf	conf	1.5E+03	2.0E+01	7.4E+02	-6.92	-6.82	-8.58	-0.56	0.64	0.0%	0.0%	1.2E-30
415	616-45-5	2-pyrrolidone	85	46	4.7E+00	1.7E+06	4.8E-01	0	3.5E-06	1.8E-07	3.5E-06	conf	conf	1.3E+03	1.8E+01	6.6E+02	-5.88	-6.61	-8.22	0.07	1.17	0.0%	0.0%	1.2E-32
416	122-99-6	2-phenoxyethanol	138	22	6.0E-01	6.3E+03	1.3E+01	14.0	3.5E-06	6.9E-07	1.1E-06	conf	conf	1.5E+03	2.1E+01	7.8E+02	-7.24	-7.10	-8.87	-0.37	0.25	0.0%	0.0%	3.1E-34
417	2550-06-3	trichloro(3-chloropropyl)silane	212	-19	1.2E+02	3.8E+03	1.7E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	1.1E+03	1.6E+01	5.7E+02	-7.95	-7.69	-9.02	-0.07	0.39	0.0%	0.0%	1.0E-37
418	106-49-0	p-toluidine	107	12	1.9E-01	7.2E+03	4.2E+01	5.0	3.5E-06	4.3E-07	3.5E-07	conf	conf	1.4E+03	2.0E+01	7.2E+02	-6.01	-6.78	-8.61	-1.43	1.03	0.0%	0.0%	5.8E-25
419	462-06-6	fluorobenzene	96	-73	9.6E+03	9.0E+02	1.5E+02	14.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	9.2E+02	1.3E+01	4.4E+02	-9.17	-8.82	-11.06	-2.07	0.15	0.0%	0.0%	4.6E-38
420	101-84-8	diphenyl ether	170	35	2.3E+00	3.8E+01	1.1E+04	14.0	3.5E-06	5.0E-09	3.5E-07	conf	conf	9.3E+02	1.3E+01	4.5E+02	-8.00	-7.72	-9.03	-2.71	0.47	0.0%	0.0%	8.7E-20
421	110-15-6	succinic acid	118	83	1.4E-02	3.8E+05	1.8E-01	3.8	3.5E-06	9.4E-07	1.1E-06	conf	conf	1.5E+03	2.1E+01	7.6E+02	-5.99	-7.18	-9.02	-0.91	0.44	0.0%	0.0%	2.2E-31
422	99-54-7	1,2-dichloro-4-nitrobenzene	192	66	1.8E+00	7.7E+01	1.3E+03	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+02	1.3E+01	4.5E+02	-7.85	-7.56	-8.90	-2.44	0.70	0.0%	0.0%	1.3E-20
423	88-74-4	2-nitroaniline	138	72	2.2E-01	1.2E+03	1.0E+02	14.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	9.0E+02	1.3E+01	4.4E+02	-6.51	-6.25	-7.20	-1.37	0.70	0.0%	0.0%	4.4E-17
424	109-89-7	diethylamine	73	-80	3.1E+04	4.2E+05	6.5E+00	10.9	3.5E-06	5.0E-07	1.1E-06	conf	conf	1.4E+03	1.9E+01	7.0E+02	-8.36	-8.13	-9.29	-0.96	0.54	0.0%	0.0%	5.6E-33
425	124-07-2	octanoic acid	144	48	6.5E+00	1.3E+03	1.1E+03	4.9	3.5E-06	3.8E-06	1.1E-06	conf	conf	1.6E+03	2.2E+01	8.0E+02	-7.92	-8.13	-9.74	-1.19	0.45	0.0%	0.0%	1.4E-34
426	99-08-1	3-nitrotoluene	137	38	9.4E+00	2.8E+02	2.3E+02	14.0	3.5E-06	3.9E-09	1.1E-07	conf	conf	9.0E+02	1.3E+01	4.4E+02	-7.72	-7.45	-8.70	-1.64	0.70	0.0%	0.0%	3.5E-24
427	95-74-9	3-chloro-p-toluidine	142	42	5.0E+00	5.6E+02	1.9E+02	4.0	3.5E-06	6.9E-09	1.1E-06	conf	conf	9.0E+02	1.3E+01	4.4E+02	-6.24	-6.24	-7.26	-2.02	0.63	0.0%	0.0%	3.6E-14
428	112-61-8	methyl stearate	299	82	4.4E-03	9.1E-03	1.7E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+02	1.3E+01	4.5E+02	-8.44	-8.57	-9.63	-5.01	0.73	0.0%	0.0%	2.1E-11
429	7381-01-3	sodium 2-sulphonatoethyl laurate	330	87	9.9E-03	2.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+03	1.6E+01	5.7E+02	-5.96	-6.28	-7.93	-1.22	1.29	0.0%	0.0%	4.6E-22
430	140-31-8	2-piperazin-1-ylethylamine	129	54	8.8E+00	1.0E+06	2.7E-02	10.0	3.5E-06	9.3E-08	3.5E-06	conf	conf	1.1E+03	1.5E+01	5.4E+02	-6.25	-6.41	-7.90	-0.33	0.69	0.0%	0.0%	1.4E-27
431	615-60-1	4-chloro-o-xylene	141	-9	6.5E+01	2.5E+01	5.4E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.0E+03	1.4E+01	4.9E+02	-9.05	-8.76	-10.70	-2.66	0.16	0.0%	0.0%	7.8E-31
432	5124-30-1	4,4'-methylenedicyclohexyl diisocyanate	262	112	3.1E-03	1.8E+01	1.3E+06	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.9E+02	1.4E+01	4.9E+02	-7.59	-7.74	-8.90	-2.13	0.63	0.0%	0.0%	2.2E-22
433	109-86-4	2-methoxyethanol	76	-57	7.5E+02	8.8E+05	1.2E-01	14.0	3.5E-06	1.5E-06	1.1E-06	conf	conf	1.5E+03	2.1E+01	7.6E+02	-7.54	-7.39	-9.19	0.85	0.71	0.0%	0.0%	5.7E-47
434	556-88-7	1-nitroguanidine	104	60	4.6E-02	1.9E+05	1.9E-02	-1.0	3.5E-06	4.1E-07	3.5E-07	conf	conf	1.3E+03	1.8E+01	6.7E+02	-5.43	-6.63	-8.52	-0.08	0.87	0.0%	0.0%	9.8E-34
435	25586-42-9	tris(methylphenyl) phosphite	352	167	2.9E-06	3.4E-02	1.9E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.0E+02	1.3E+01	4.4E+02	-7.63	-8.22	-8.51	-4.05	0.27	0.0%	0.0%	9.3E-11
436	67-68-5	dimethyl sulfoxide	78	-56	2.6E+02	5.7E+05	1.5E+01	14.0	3.5E-06	2.2E-09	3.5E-06	conf	conf	8.7E+02	1.2E+01	4.2E+02	-6.62	-6.34	-7.30	1.53	0.52	0.0%	0.0%	2.8E-15
437	629-50-5	tridecane	184	-10	1.2E+01	1.2E-02	5.4E+06	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	8.8E+02	1.2E+01	4.3E+02	-9.47	-9.23	-11.91	-0.07	2.45	0.0%	0.0%	2.1E-64
438	4719-04-4	2,2',2''-(hexahydro-1,3,5-triazine-1,3,5-triyl)triethanol	219	155	5.5E-07	1.0E+06	2.1E-05	3.0	3.5E-06	7.1E-07	3.5E-06	conf	conf	1.4E+03	1.9E+01	7.1E+02	-5.87	-7.10	-8.88	-1.69	0.53	0.0%	0.0%	4.8E-25
439	5989-27-5	(R)-p-mentha-1,8-diene	136	-41	1.9E+02	7.7E+00	6.8E+04	14.0	3.5E-06	5.7E-07	3.5E-07	conf	conf	9.3E+02	1.3E+01	4.5E+02	-9.49	-9.21	-11.66	-2.27	0.75	0.0%	0.0%	2.6E-41
440	123-31-9	hydroquinone	110	46	2.2E-03	1.0E+05	1.1E+01	10.1	3.5E-06	1.9E-06	1.1E-06	conf	conf	1.5E+03	2.0E+01	7.5E+02	-6.55	-7.60	-9.36	-3.55	0.68	0.0%	0.0%	4.9E-17
441	96-22-0	pentan-3-one	86	-68	5.3E+03	1.1E+05	5.6E+00	14.0	3.5E-06	9.4E-07	1.1E-06	conf	conf	1.4E+03	1.9E+01	7.1E+02	-8.41	-8.21	-9.36	0.12	0.36	0.0%	0.0%	4.4E-42
442	109-60-4	propyl acetate	102	-69	4.7E+03	1.7E+04	2.3E+01	14.0	3.5E-06	9.1E-07	1.1E-06	conf	conf	1.3E+03	1.9E+01	6.8E+02	-8.79	-8.54	-9.97	-0.79	0.44	0.0%	0.0%	1.5E-39
443	60-00-4	edetic acid	292	315	5.0E-10	2.5E+02	1.4E-04	0.7	3.5E-06	5.1E-08	3.5E-07	conf	conf	9.8E+02	1.4E+01	4.8E+02	-5.25	-6.19	-7.55	-1.08	0.69	0.0%	0.0%	1.1E-20
444	142-82-5	heptane	100	-81	6.1E+03	2.4E+01	6.0E+03	14.0	3.5E-06	1.6E-06	1.1E-07	conf	conf	1.0E+03	1.4E+01	5.0E+02	-9.61	-9.20	-12.23	-1.42	0.70	0.0%	0.0%	4.2E-54
445	6358-85-6	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-N-phenylbutyramide]	630	350	2.9E-19	1.2E-04	1.1E+07	0.6	3.5E-06	3.5E-07	3.5E-08	conf	conf	1.2E+03	1.7E+01	6.3E+02	-6.92	-6.92	-8.44	-0.74	1.21	0.0%	0.0%	1.9E-28
446	756-80-9	O,O-dimethyl hydrogen dithiophosphate	158	-82	5.5E+01	2.7E+03	1.8E+01	-0.1	3.5E-06	2.7E-08	1.1E-06	conf	conf	9.1E+02	1.3E+01	4.4E+02	-5.94	-6.29	-7.49	-1.33	0.69	0.0%	0.0%	6.7E-19
447	127-91-3	pin-2(10)-ene	136	-15	3.3E+02	1.8E+01	2.2E+04	14.0	3.5E-06	1.1E-08	3.5E-08	conf	conf	8.3E+02	1.2E+01	4.0E+02	-9.33	-8.96	-11.34	-3.10	0.70	0.0%	0.0%	2.9E-32
448	21981-33-9	1,1,1,3,3-pentachlorobutane	230	-1	2.9E+02	3.6E+01	5.8E+04	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	8.5E+02	1.2E+01	4.1E+02	-9.28	-8.95	-11.26	-2.24	0.04	0.0%	0.0%	2.6E-38
449	111-71-7	heptanal	114	-43	4.7E+02	1.6E+03	1.9E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.2E+03	1.6E+01	5.8E+02	-8.60	-8.33	-9.82	-2.11	0.62	0.0%	0.0%	1.6E-28
450	110-42-9	methyl decanoate	186	2	1.4E+01	1.7E+01	2.0E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.8E+02	1.4E+01	4.9E+02	-8.92	-8.65	-10.37	-2.09	1.42	0.0%	0.0%	1.3E-32
451	29911-28-2	1-(2-butoxy-1-methylethoxy)propan-2-ol	190	18	4.8E-01	2.7E+05	1.3E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.4E+03	1.9E+01	7.0E+02	-6.39	-7.21	-9.15	-0.32	0.24	0.0%	0.0%	8.5E-37
452	108-21-4	isopropyl acetate	102	-81	8.1E+03	1.8E+04	1.9E+01	14.0	3.5E-06	5.2E-07	1.1E-06	conf	conf	1.2E+03	1.6E+01	5.9E+02	-8.76	-8.48	-10.09	-0.15	0.60	0.0%	0.0%	4.1E-46
453	5165-97-9	sodium 2-methyl-2-[(1-oxoallyl)amino]propanesulphonate	229	87	9.9E-03	1.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+03	1.5E+01	5.3E+02	-6.00	-6.31	-7.96	0.60	0.17	0.0%	0.0%	1.0E-34
454	13005-36-2	potassium phenylacetate	174	87	9.9E-03	1.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+03	1.5E+01	5.2E+02	-6.01	-6.31	-7.96	-1.84	0.64	0.0%	0.0%	1.0E-18
455	96-24-2	3-chloropropane-1,2-diol	111	-2	3.5E+00	1.1E+06	3.0E-01	13.7	3.5E-06	6.9E-07	1.1E-06	conf	conf	1.3E+03	1.8E+01	6.6E+02	-6.23	-6.96	-8.89	0.60	0.25	0.0%	0.0%	3.5E-42
456	79-22-1	methyl chloroformate	94	-82	1.7E+04	2.7E+04	1.4E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.3E+03	1.7E+01	6.4E+02	-8.90	-8.59	-10.35	-2.68	1.41	0.0%	0.0%	3.1E-28
457	56706-10-6	4,4,13,13-tetraethoxy-3,14-dioxa-8,9-dithia-4,13-disilahexadecane	475	171	2.6E-06	7.2E-02	6.0E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+03	1.7E+01	6.4E+02	-7.69	-7.65	-9.27	-0.58	1.31	0.0%	0.0%	1.2E-35
458	105-08-8	cyclohex-1,4-ylenedimethanol	144	38	1.9E-02	1.7E+05	3.1E+01	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.4E+03	1.9E+01	7.2E+02	-7.10	-8.18	-9.69	-0.45	0.68	0.0%	0.0%	4.5E-40
459	78-70-6	linalool	154	-11	1.1E+01	8.0E+02	2.4E+03	14.0	3.5E-06	3.2E-07	3.5E-07	conf	conf	1.1E+03	1.6E+01	5.7E+02	-7.95	-7.70	-8.91	-1.33	0.27	0.0%	0.0%	1.3E-27
460	999-97-3	1,1,1,3,3,3-hexamethyldisilazane	161	-58	1.7E+03	3.0E+01	4.2E+02	11.0	3.5E-06	8.4E-09	3.5E-09	conf	conf	7.9E+02	1.1E+01	3.8E+02	-9.22	-8.32	-11.01	-0.89	0.75	0.0%	0.0%	1.2E-47
461	111-90-0	2-(2-ethoxyethoxy)ethanol	134	-3	1.3E+01	1.8E+06	2.0E-01	14.0	3.5E-06	8.1E-07	3.5E-07	conf	conf	1.3E+03	1.8E+01	6.6E+02	-6.33	-6.87	-8.93	1.11	0.31	0.0%	0.0%	1.9E-24
462	107-46-0	hexamethyldisiloxane	162	-79	5.2E+03	1.5E+01	1.8E+05	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	7.8E+02	1.1E+01	3.8E+02	-9.50	-8.76	-11.47	-2.91	1.16	0.0%	0.0%	1.1E-34
463	111-14-8	heptanoic acid	130	37	1.6E+01	4.0E+03	3.5E+02	4.9	3.5E-06	3.9E-06	1.1E-06	conf	conf	1.4E+03	1.9E+01	7.0E+02	-7.87	-8.17	-9.80	-0.76	0.63	0.0%	0.0%	1.7E-38
464	526-95-4	D-gluconic acid	196	162	1.1E-07	7.2E+05	1.3E-02	3.4	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.3E+03	1.9E+01	6.9E+02	-6.27	-7.74	-9.65	1.96	1.57	0.0%	0.0%	3.2E-29
465	84-69-5	diisobutyl phthalate	278	18	3.2E-01	3.1E+01	2.9E+04	14.0	3.5E-06	8.8E-07	3.5E-07	conf	conf	1.1E+03	1.5E+01	5.5E+02	-8.34	-8.12	-9.39	-2.75	0.72	0.0%	0.0%	1.3E-21
466	111-64-8	octanoyl chloride	163	-7	8.5E+01	3.6E+01	3.0E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+03	1.4E+01	5.1E+02	-9.21	-8.90	-10.98	-2.01	1.10	0.0%	0.0%	7.3E-38
467	482-89-3	2-(1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one	262	191	3.1E-09	1.4E+02	1.3E+03	0	3.5E-06	3.3E-09	3.5E-07	conf	conf	7.6E+02	1.1E+01	3.7E+02	-5.97	-6.23	-7.18	0.41	0.85	0.0%	0.0%	1.2E-27
468	5873-54-1	o-(p-isocyanatobenzyl)phenyl isocyanate	250	99	6.3E-03	3.5E+01	1.7E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+03	1.4E+01	5.0E+02	-8.05	-8.00	-9.39	-0.89	0.64	0.0%	0.0%	3.2E-34
469	68-11-1	mercaptoacetic acid	92	19	5.5E+01	2.8E+05	1.1E+00	3.7	3.5E-06	4.5E-06	1.1E-06	conf	conf	1.3E+03	1.8E+01	6.8E+02	-6.70	-8.04	-9.81	-1.55	0.18	0.0%	0.0%	1.8E-32
470	4170-30-3	crotonaldehyde	70	-81	4.2E+03	1.5E+05	4.0E+00	14.0	3.5E-06	4.2E-06	3.5E-06	conf	conf	1.3E+03	1.8E+01	6.7E+02	-8.76	-8.63	-9.81	-1.99	0.96	0.0%	0.0%	2.9E-29
471	84852-53-9	1,1'-(ethane-1,2-diyl)bis[pentabromobenzene]	971	260	2.5E-11	2.6E-11	4.4E+13	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	7.4E+02	1.0E+01	3.6E+02	-13.59	-13.59	-13.59	-1.34	1.81	0.0%	0.0%	6.7E-69
472	142-84-7	dipropylamine	101	-54	3.3E+03	7.2E+04	6.2E+01	11.0	3.5E-06	4.9E-07	3.5E-07	conf	conf	1.1E+03	1.6E+01	5.8E+02	-8.33	-8.10	-9.28	-1.61	0.70	0.0%	0.0%	3.2E-28
473	78-90-0	propylenediamine	74	-23	2.1E+03	1.0E+06	6.3E-02	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	1.0E+03	1.5E+01	5.3E+02	-6.97	-6.67	-8.13	-0.69	0.66	0.0%	0.0%	1.2E-26
474	7398-69-8	diallyldimethylammonium chloride	162	87	9.9E-03	1.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.6E+02	1.3E+01	4.8E+02	-6.05	-6.36	-8.00	-1.69	0.75	0.0%	0.0%	9.2E-20
475	119851-28-4	601-639-3	281	124	7.5E-04	4.0E+00	1.0E+05	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	1.0E+03	1.4E+01	5.1E+02	-8.01	-7.88	-9.38	-3.36	0.50	0.0%	0.0%	3.8E-18
476	5089-70-3	(3-chloropropyl)triethoxysilane	241	29	2.3E+00	1.8E+02	1.1E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.1E+03	1.5E+01	5.5E+02	-7.97	-7.72	-9.01	-0.69	0.86	0.0%	0.0%	7.0E-33
477	107-41-5	2-methylpentane-2,4-diol	118	-7	7.8E+00	5.3E+05	3.8E+00	14.0	3.5E-06	4.1E-07	1.1E-06	conf	conf	1.1E+03	1.6E+01	5.7E+02	-6.70	-6.92	-8.70	0.91	0.22	0.0%	0.0%	3.6E-43
478	10175-31-2	688-329-1	170	18	1.6E+01	1.3E+03	2.5E+02	8.2	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.1E+03	1.5E+01	5.5E+02	-7.86	-7.63	-8.87	-2.57	0.59	0.0%	0.0%	1.2E-19
479	2768-02-7	trimethoxyvinylsilane	148	-49	2.1E+03	1.4E+04	4.8E-01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.2E+03	1.7E+01	6.4E+02	-8.89	-8.64	-10.31	-0.70	0.09	0.0%	0.0%	3.7E-43
480	58-86-6	xylose	150	96	1.0E-04	1.0E+06	1.0E-02	12.5	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.3E+03	1.8E+01	6.5E+02	-6.52	-7.74	-9.67	-0.33	1.57	0.0%	0.0%	6.2E-41
481	142-91-6	isopropyl palmitate	299	72	2.7E-02	1.1E-02	1.4E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.5E+02	1.1E+01	3.7E+02	-8.67	-8.76	-10.25	-0.09	1.93	0.0%	0.0%	5.1E-48
482	110-27-0	isopropyl myristate	270	44	1.1E-01	6.2E-02	1.5E+07	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.8E+02	1.1E+01	3.8E+02	-9.26	-9.16	-10.78	-4.18	0.39	0.0%	0.0%	2.1E-21
483	818-61-1	2-hydroxyethyl acrylate	116	-16	1.7E+01	2.3E+05	5.6E-01	14.0	3.5E-06	4.4E-07	1.1E-06	conf	conf	1.1E+03	1.5E+01	5.6E+02	-6.96	-6.88	-8.71	-2.27	0.34	0.0%	0.0%	1.9E-20
484	97-86-9	isobutyl methacrylate	142	-54	4.2E+02	1.4E+03	4.7E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.2E+03	1.7E+01	6.1E+02	-9.33	-9.10	-10.53	-1.19	0.87	0.0%	0.0%	6.5E-41
485	929-06-6	2-(2-aminoethoxy)ethanol	105	14	3.3E+00	1.0E+06	1.3E-02	9.4	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.2E+03	1.7E+01	6.1E+02	-6.33	-7.13	-9.16	-0.57	0.16	0.0%	0.0%	6.4E-35
486	3048-64-4	5-vinylnorborn-2-ene	120	-41	1.0E+03	2.7E+02	4.2E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+02	1.3E+01	4.6E+02	-9.37	-9.09	-11.16	-2.20	0.22	0.0%	0.0%	7.9E-38
487	37439-34-2	sodium 3,5,6-trichloropyridin-2-olate	220	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+02	1.3E+01	4.6E+02	-6.07	-6.37	-8.03	-1.82	0.64	0.0%	0.0%	3.7E-19
488	541-41-3	ethyl chloroformate	109	-69	6.2E+03	1.4E+04	4.3E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.2E+03	1.6E+01	6.1E+02	-9.17	-8.92	-10.61	-1.06	1.87	0.0%	0.0%	1.1E-42
489	85-42-7	cyclohexane-1,2-dicarboxylic anhydride	154	-2	7.1E+00	3.7E+03	1.5E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.2E+03	1.6E+01	5.9E+02	-7.97	-7.75	-9.30	-0.10	0.49	0.0%	0.0%	1.0E-39
490	110-62-3	valeraldehyde	86	-68	4.4E+03	2.5E+04	2.0E+01	14.0	3.5E-06	4.1E-06	3.5E-06	conf	conf	1.2E+03	1.7E+01	6.2E+02	-9.24	-9.05	-10.26	-1.59	0.37	0.0%	0.0%	1.7E-35
491	112-69-6	hexadecyldimethylamine	270	63	3.8E-02	1.3E-02	2.6E+07	10.1	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.3E+02	1.0E+01	3.6E+02	-9.19	-9.13	-10.83	-3.88	0.66	0.0%	0.0%	1.7E-23
492	101-02-0	triphenyl phosphite	310	144	1.0E-02	9.8E-01	4.2E+06	14.0	3.5E-06	8.4E-08	1.1E-07	conf	conf	7.1E+02	1.0E+01	3.5E+02	-8.25	-8.20	-9.07	-3.25	0.27	0.0%	0.0%	4.5E-17
493	609-15-4	ethyl 2-chloroacetoacetate	165	-3	4.7E+01	2.6E+03	9.5E-01	7.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.2E+03	1.7E+01	6.2E+02	-8.39	-8.30	-9.76	-1.70	1.28	0.0%	0.0%	5.4E-31
494	75-18-3	dimethyl sulphide	62	-108	6.4E+04	1.5E+04	8.3E+00	14.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	6.8E+02	9.6E+00	3.3E+02	-9.01	-8.64	-10.73	-1.34	0.50	0.0%	0.0%	2.5E-41
495	106-95-6	3-bromopropene	121	-81	1.9E+04	3.5E+03	1.0E+02	14.0	3.5E-06	1.6E-06	1.1E-06	conf	conf	9.1E+02	1.3E+01	4.6E+02	-9.45	-9.14	-11.46	-3.29	0.41	0.0%	0.0%	9.6E-32
496	32360-05-7	octadecyl methacrylate	339	100	6.4E-04	1.3E-04	4.2E+09	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	6.8E+02	9.5E+00	3.3E+02	-8.20	-8.23	-9.24	-5.43	1.27	0.0%	0.0%	2.8E-08
497	89-78-1	menthol	156	-6	1.0E+00	9.4E+02	2.4E+03	14.0	3.5E-06	3.2E-07	3.5E-07	conf	conf	9.7E+02	1.3E+01	4.9E+02	-7.42	-7.18	-8.75	-1.25	0.56	0.0%	0.0%	4.3E-27
498	109-69-3	1-chlorobutane	93	-85	1.2E+04	6.9E+02	3.6E+02	14.0	3.5E-06	2.3E-08	1.1E-07	conf	conf	6.8E+02	9.5E+00	3.3E+02	-9.37	-8.94	-11.34	-0.12	0.59	0.0%	0.0%	3.7E-58
499	90-04-0	o-anisidine	123	29	1.4E+01	1.1E+04	1.4E+01	5.0	3.5E-06	6.0E-07	1.1E-06	conf	conf	1.1E+03	1.5E+01	5.4E+02	-6.75	-7.20	-8.98	-1.67	0.51	0.0%	0.0%	7.9E-26
500	75-94-5	trichloro(vinyl)silane	161	-66	7.2E+03	1.6E+03	2.3E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	8.4E+02	1.2E+01	4.2E+02	-9.37	-9.03	-11.40	-0.56	0.19	0.0%	0.0%	2.3E-54
501	13466-78-9	3,7,7-trimethylbicyclo[4.1.0]hept-3-ene	136	-14	2.8E+02	2.8E+01	4.1E+04	14.0	3.5E-06	3.2E-07	1.1E-07	conf	conf	7.0E+02	9.8E+00	3.4E+02	-9.46	-9.17	-11.38	-2.07	0.15	0.0%	0.0%	1.1E-40
502	5333-42-6	2-octyldodecan-1-ol	299	95	3.6E-05	7.5E-04	4.3E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	6.8E+02	9.5E+00	3.3E+02	-8.06	-8.37	-8.77	-1.91	1.73	0.0%	0.0%	6.2E-23
503	104-88-1	4-chlorobenzaldehyde	141	9	1.4E+01	9.5E+02	2.2E+02	14.0	3.5E-06	5.8E-07	3.5E-07	conf	conf	1.0E+03	1.4E+01	5.2E+02	-8.12	-7.90	-9.13	-2.04	0.47	0.0%	0.0%	1.9E-24
504	108-44-1	m-toluidine	107	12	4.1E+01	7.3E+03	4.2E+01	5.0	3.5E-06	5.0E-07	3.5E-07	conf	conf	1.0E+03	1.4E+01	5.1E+02	-6.97	-7.06	-8.86	-1.97	0.84	0.0%	0.0%	3.8E-23
505	56-84-8	aspartic acid	133	218	3.5E-05	1.9E+05	4.8E-05	1.7	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.1E+03	1.6E+01	5.8E+02	-6.32	-7.72	-9.72	-0.63	0.97	0.0%	0.0%	7.5E-39
506	78-40-0	triethyl phosphate	182	4	2.2E+01	3.1E+05	7.4E+00	14.0	3.5E-06	2.6E-08	3.5E-07	conf	conf	7.0E+02	9.8E+00	3.4E+02	-6.61	-6.37	-7.56	-0.42	0.56	0.0%	0.0%	8.8E-25
507	61260-55-7	N,N'-bis(2,2,6,6-tetramethylpiperidin-4-yl)hexane-1,6-diamine	395	193	1.9E-05	2.8E+01	2.7E+04	10.5	3.5E-06	3.5E-07	1.1E-07	conf	conf	8.6E+02	1.2E+01	4.3E+02	-6.61	-7.23	-8.83	-1.10	0.49	0.0%	0.0%	1.2E-28
508	98-94-2	cyclohexyldimethylamine	127	-39	3.3E+02	2.1E+03	2.0E+02	10.0	3.5E-06	3.8E-08	1.1E-06	conf	conf	7.0E+02	9.8E+00	3.4E+02	-8.37	-8.08	-9.59	-1.76	0.70	0.0%	0.0%	2.2E-29
509	2524-04-1	O,O-diethyl phosphorochloridothioate	189	-74	5.3E+01	5.6E+02	2.3E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.1E+02	1.3E+01	4.6E+02	-8.53	-8.27	-9.65	-2.22	0.13	0.0%	0.0%	1.2E-26
510	27394-99-6	N-(1-cyanoethyl)formamide	98	70	3.9E-01	1.0E+06	6.3E-02	12.2	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.6E+02	1.3E+01	4.9E+02	-5.77	-6.67	-8.57	-1.42	1.37	0.0%	0.0%	8.4E-25
511	75-75-2	methanesulphonic acid	96	26	3.6E+00	4.8E+05	4.2E-03	1.7	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.1E+03	1.5E+01	5.7E+02	-6.74	-8.12	-9.77	-1.29	0.52	0.0%	0.0%	4.2E-34
512	372-09-8	cyanoacetic acid	85	38	4.7E+00	1.2E+06	1.7E-01	2.4	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.1E+03	1.5E+01	5.7E+02	-6.61	-7.95	-9.77	-1.43	0.61	0.0%	0.0%	5.7E-33
513	91-76-9	6-phenyl-1,3,5-triazine-2,4-diyldiamine	187	159	1.7E-05	7.0E+03	2.8E+01	4.4	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.1E+03	1.5E+01	5.7E+02	-6.94	-8.03	-9.77	-1.20	0.22	0.0%	0.0%	8.6E-35
514	25899-50-7	(Z)-pent-2-enenitrile	81	-47	5.4E+02	3.0E+03	1.3E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.1E+02	1.3E+01	4.6E+02	-8.54	-8.27	-9.62	-0.92	0.37	0.0%	0.0%	9.8E-36
515	2100-42-7	1-chloro-2,5-dimethoxybenzene	173	25	1.4E+01	5.0E+02	6.3E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+03	1.4E+01	5.2E+02	-8.57	-8.36	-9.55	-1.99	0.63	0.0%	0.0%	1.9E-27
516	37971-36-1	2-phosphonobutane-1,2,4-tricarboxylic acid	270	90	8.1E-09	1.6E+04	2.2E-02	1.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+03	1.5E+01	5.4E+02	-5.83	-7.13	-9.18	0.06	0.89	0.0%	0.0%	4.1E-40
517	110-01-0	tetrahydrothiophene	88	-49	2.0E+03	8.4E+03	6.2E+01	14.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	6.3E+02	8.7E+00	3.0E+02	-8.36	-8.07	-9.63	-0.99	0.45	0.0%	0.0%	2.5E-35
518	96-29-7	butanone oxime	87	-58	1.6E+02	2.2E+04	4.9E+01	12.5	3.5E-06	2.7E-07	3.5E-07	conf	conf	9.0E+02	1.3E+01	4.5E+02	-7.66	-7.42	-8.72	-0.61	0.87	0.0%	0.0%	2.5E-31
519	865-33-8	potassium methanolate	70	87	9.9E-03	4.8E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.1E+02	1.1E+01	4.0E+02	-6.15	-6.43	-8.07	0.82	0.70	0.0%	0.0%	3.1E-37
520	165184-98-5	639-566-4	216	44	7.1E-02	1.1E+00	6.6E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	8.6E+02	1.2E+01	4.3E+02	-8.92	-8.70	-9.81	-2.91	0.68	0.0%	0.0%	3.2E-23
521	6940-53-0	1-chloro-2,5-dimethoxy-4-nitrobenzene	218	95	4.5E-02	9.6E+01	4.2E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+03	1.4E+01	5.2E+02	-7.89	-7.66	-9.35	-1.52	0.44	0.0%	0.0%	2.4E-29
522	1193-21-1	4,6-dichloropyrimidine	149	26	5.8E+01	2.6E+03	1.7E+01	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+02	1.3E+01	4.6E+02	-8.04	-7.79	-9.11	-1.39	0.69	0.0%	0.0%	1.4E-28
523	1073-69-4	(4-chlorophenyl)hydrazine	143	44	5.9E+00	9.9E+04	2.8E+01	5.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+02	1.3E+01	4.7E+02	-6.14	-6.87	-8.68	-2.97	0.74	0.0%	0.0%	1.7E-16
524	4553-62-2	2-methylglutaronitrile	108	11	1.8E+00	2.0E+05	1.9E+00	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+02	1.3E+01	4.7E+02	-6.31	-6.77	-8.63	-0.09	0.64	0.0%	0.0%	1.6E-34

525	108-32-7	propylene carbonate	102	20	5.6E+00	9.6E+02	1.2E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.1E+03	1.5E+01	5.5E+02	-8.31	-8.19	-9.75	-1.41	1.08	0.0%	0.0%	5.2E-33
526	6358-64-1	4-chloro-2,5-dimethoxyaniline	188	79	1.6E-01	1.7E+03	7.6E+01	3.3	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.0E+03	1.4E+01	5.2E+02	-6.69	-7.54	-9.32	-1.80	0.74	0.0%	0.0%	3.6E-27
527	2893-78-9	troclosene sodium	220	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.8E+02	1.1E+01	3.9E+02	-6.13	-6.44	-8.09	-2.56	1.42	0.0%	0.0%	1.4E-15
528	109-61-5	propyl chloroformate	123	-57	2.6E+03	6.5E+03	1.3E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.0E+03	1.4E+01	5.2E+02	-9.29	-9.06	-10.68	-1.86	1.69	0.0%	0.0%	1.0E-36
529	288-13-1	pyrazole	68	0	3.3E+01	4.2E+05	1.1E+00	2.5	3.5E-06	4.0E-07	1.1E-07	conf	conf	9.2E+02	1.3E+01	4.7E+02	-5.77	-6.77	-8.68	0.27	0.68	0.0%	0.0%	1.0E-37
530	142-16-5	bis(2-ethylhexyl) maleate	341	29	2.6E-01	9.8E-03	8.7E+07	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	6.1E+02	8.5E+00	2.9E+02	-8.90	-8.85	-10.80	-1.53	1.18	0.0%	0.0%	2.9E-40
531	506-93-4	guanidinium nitrate	122	87	9.9E-03	8.4E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.8E+02	1.1E+01	3.9E+02	-6.15	-6.45	-8.09	-0.88	0.97	0.0%	0.0%	3.5E-25
532	14433-76-2	N,N-dimethyldecan-1-amide	199	61	2.1E-01	1.3E-01	2.8E+03	0	3.5E-06	4.0E-07	1.1E-07	conf	conf	7.1E+02	9.9E+00	3.6E+02	-6.26	-7.00	-8.90	-1.97	0.26	0.0%	0.0%	2.1E-23
533	103-50-4	dibenzyl ether	198	56	2.9E-01	1.7E+01	3.0E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.3E+02	1.3E+01	4.8E+02	-8.49	-8.27	-9.50	-2.56	0.50	0.0%	0.0%	1.6E-23
534	77-90-7	tributyl O-acetylcitrate	402	94	6.1E-04	3.9E+00	1.9E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	8.0E+02	1.1E+01	4.0E+02	-7.47	-7.27	-8.90	-2.12	0.62	0.0%	0.0%	1.9E-22
535	83261-15-8	isobutyl (S)-2-chloropropionate	165	-39	2.2E+02	1.2E+03	2.8E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.8E+02	1.4E+01	5.0E+02	-9.33	-9.12	-10.49	-1.28	0.36	0.0%	0.0%	8.9E-40
536	14806-72-5	tris(2-hydroxyethyl)ammonium acetate	209	87	9.9E-03	1.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.6E+02	1.1E+01	3.8E+02	-6.15	-6.45	-8.10	-0.60	0.27	0.0%	0.0%	4.4E-27
537	1477-55-0	m-phenylenebis(methylamine)	136	60	1.9E+00	2.6E+03	1.4E+00	9.4	3.5E-06	3.5E-07	1.1E-07	conf	conf	8.8E+02	1.2E+01	4.5E+02	-7.15	-6.88	-8.65	-1.48	0.29	0.0%	0.0%	6.4E-25
538	106-93-4	1,2-dibromoethane	188	-39	1.5E+03	3.7E+03	1.0E+02	14.0	3.5E-06	1.4E-08	1.1E-07	conf	conf	6.0E+02	8.4E+00	2.9E+02	-8.61	-8.30	-10.17	-1.72	0.70	0.0%	0.0%	6.8E-34
539	110-97-4	1,1'-iminodipropan-2-ol	133	26	1.7E-01	1.0E+06	1.3E-01	9.0	3.5E-06	3.4E-07	3.5E-06	conf	conf	8.7E+02	1.2E+01	4.4E+02	-6.17	-6.95	-8.71	-0.31	0.47	0.0%	0.0%	1.8E-33
540	85-41-6	phthalimide	147	177	1.4E-06	3.4E+03	2.0E+01	9.3	3.5E-06	3.5E-07	1.1E-06	conf	conf	8.7E+02	1.2E+01	4.4E+02	-6.17	-7.01	-8.72	-1.64	0.45	0.0%	0.0%	2.2E-24
541	611-20-1	salicylonitrile	119	54	3.2E-01	1.5E+04	4.1E+01	6.9	3.5E-06	1.1E-05	3.5E-06	conf	conf	1.0E+03	1.4E+01	5.3E+02	-8.22	-8.94	-10.34	-1.49	0.32	0.0%	0.0%	6.5E-37
542	149-73-5	trimethyl orthoformate	106	-76	4.9E+03	6.0E+04	9.3E-01	14.0	3.5E-06	1.2E-06	3.5E-07	conf	conf	9.5E+02	1.3E+01	4.9E+02	-8.58	-8.30	-9.76	-0.27	0.75	0.0%	0.0%	3.2E-42
543	98-56-6	4-chloro-α,α,α-trifluorotoluene	181	-30	9.1E+02	4.1E+01	4.0E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	5.9E+02	8.2E+00	2.8E+02	-9.46	-9.00	-11.55	-2.47	0.39	0.0%	0.0%	9.8E-39
544	2524-03-0	O,O-dimethyl phosphorochloridothioate	161	-98	4.0E+02	3.2E+03	2.5E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+02	1.3E+01	4.7E+02	-8.90	-8.67	-10.03	-1.33	0.39	0.0%	0.0%	1.0E-35
545	141-79-7	4-methylpent-3-en-2-one	98	-64	1.6E+03	7.4E+03	2.3E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.1E+02	1.3E+01	4.7E+02	-8.98	-8.74	-10.07	-0.69	0.20	0.0%	0.0%	2.9E-41
546	4454-05-1	3,4-dihydro-2-methoxy-2H-pyran	114	-45	2.8E+03	1.9E+04	7.6E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+02	1.3E+01	4.7E+02	-8.78	-8.52	-9.99	-1.54	1.09	0.0%	0.0%	8.0E-34
547	2436-90-0	3,7-dimethylocta-1,6-diene	138	-66	6.7E+02	2.5E+00	7.6E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	6.3E+02	8.8E+00	3.1E+02	-9.79	-9.49	-12.43	-2.80	0.06	0.0%	0.0%	2.5E-43
548	128-39-2	2,6-di-tert-butylphenol	206	77	9.4E-01	1.3E+01	3.0E+04	11.3	3.5E-06	3.5E-06	1.1E-06	conf	conf	8.4E+02	1.2E+01	4.3E+02	-9.33	-9.14	-10.31	-2.73	0.52	0.0%	0.0%	1.2E-27
549	24800-44-0	[(methylethylene)bis(oxy)]dipropanol	192	46	6.4E-02	2.2E+04	3.2E-01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	8.4E+02	1.2E+01	4.3E+02	-6.09	-6.75	-8.65	0.74	0.60	0.0%	0.0%	2.7E-41
550	526-98-7	L-xylo-hex-2-ulosonic acid	194	158	8.1E-08	2.0E+05	8.9E-04	1.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.7E+02	1.4E+01	5.0E+02	-6.39	-7.83	-9.78	1.51	1.42	0.0%	0.0%	3.6E-30
551	80-09-1	4,4'-sulphonyldiphenol	250	176	6.3E-08	2.0E+03	4.5E+01	7.7	3.5E-06	7.4E-09	3.5E-07	conf	conf	5.7E+02	8.0E+00	2.8E+02	-5.83	-6.39	-7.39	-1.78	0.87	0.0%	0.0%	5.6E-16
552	52829-07-9	bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate	481	211	5.0E-08	3.3E-01	3.2E+06	9.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	6.5E+02	9.0E+00	3.2E+02	-7.85	-8.50	-9.44	-2.31	0.43	0.0%	0.0%	1.2E-24
553	56966-52-0	5-chloro-2-(2,4-dichlorophenoxy)aniline	289	137	2.3E-04	1.4E+00	1.7E+04	2.8	3.5E-06	1.1E-06	3.5E-08	conf	conf	9.2E+02	1.3E+01	4.7E+02	-6.60	-7.14	-9.28	-3.41	0.19	0.0%	0.0%	2.5E-17
554	99-88-7	4-isopropylaniline	135	23	1.3E+01	2.5E+02	3.4E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+02	1.3E+01	4.7E+02	-8.70	-8.49	-9.65	-2.04	0.58	0.0%	0.0%	7.1E-28
555	24549-06-2	6-ethyl-2-toluidine	135	40	9.9E+00	1.3E+03	4.6E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+02	1.3E+01	4.7E+02	-8.24	-8.03	-9.39	-1.51	0.28	0.0%	0.0%	1.2E-29
556	4193-55-9	disodium 4,4'-bis[6-anilino-[4-[bis(2-hydroxyethyl)amino]-1,3,5-triazin-2-yl]amino]stilbene-2,2'-disulphonate	961	87	9.9E-03	6.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.2E+02	1.0E+01	3.6E+02	-6.15	-6.47	-8.14	-0.61	0.64	0.0%	0.0%	2.8E-27
557	6172-80-1	612-366-4	136	-33	1.7E+02	3.2E+04	2.3E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+02	1.3E+01	4.7E+02	-8.07	-7.90	-9.35	-2.54	0.38	0.0%	0.0%	1.1E-22
558	93-84-5	1,3-dihydro-5-nitro-2H-benzimidazol-2-one	179	148	5.0E-04	4.2E+03	1.0E+01	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.2E+02	1.3E+01	4.7E+02	-6.14	-7.18	-9.28	-1.76	1.14	0.0%	0.0%	3.4E-27
559	1003-52-7	4-methyloxazole-5-carbonitrile	108	16	9.6E+01	5.3E+03	2.0E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+02	1.3E+01	4.7E+02	-8.20	-7.99	-9.41	-0.34	0.30	0.0%	0.0%	1.1E-38
560	78-97-7	lactonitrile	71	-29	2.7E+01	1.5E+06	6.5E-02	11.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+02	1.3E+01	4.7E+02	-6.84	-7.28	-9.27	-3.20	0.92	0.0%	0.0%	2.2E-18
561	13043-55-5	7-methylenepentadecane	224	13	1.9E+00	1.4E-03	1.3E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.6E+02	7.9E+00	2.7E+02	-8.92	-8.98	-11.07	-4.95	0.41	0.0%	0.0%	1.2E-18
562	97-65-4	itaconic acid	130	87	1.2E-02	4.5E+04	4.6E-01	3.9	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.4E+02	1.3E+01	4.8E+02	-6.72	-8.04	-9.85	-1.04	0.73	0.0%	0.0%	1.2E-36
563	109-52-4	valeric acid	102	15	9.6E+01	3.5E+04	3.6E+01	4.9	3.5E-06	4.1E-06	1.1E-06	conf	conf	9.4E+02	1.3E+01	4.8E+02	-7.76	-8.29	-9.95	-1.18	0.35	0.0%	0.0%	2.6E-36
564	79-94-7	2,2',6,6'-tetrabromo-4,4'-isopropylidenediphenol	544	206	4.6E-09	1.9E-03	1.6E+07	7.7	3.5E-06	4.1E-08	1.1E-06	conf	conf	5.4E+02	7.6E+00	2.6E+02	-7.52	-8.43	-8.52	-3.43	0.73	0.0%	0.0%	1.8E-13
565	37640-57-6	1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triazine-2,4,6-triamine (1:1)	255	87	9.9E-03	1.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.0E+02	9.7E+00	3.5E+02	-6.18	-6.49	-8.14	0.19	0.64	0.0%	0.0%	5.4E-33
566	6485-55-8	cis-2,6-dimethylmorpholine	115	1	6.3E+02	5.0E+03	1.9E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.2E+02	1.3E+01	4.7E+02	-9.03	-8.84	-10.27	-0.73	0.21	0.0%	0.0%	1.2E-42
567	15667-63-7	1-cyanoallyl acetate	125	-158	1.6E+03	1.4E+04	1.5E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.2E+02	1.3E+01	4.7E+02	-9.01	-8.82	-10.29	-3.62	0.63	0.0%	0.0%	8.5E-22
568	2549-53-3	tetradecyl methacrylate	282	55	2.4E-02	1.8E-02	4.6E+07	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.7E+02	7.9E+00	2.8E+02	-9.09	-9.09	-10.54	-4.82	0.71	0.0%	0.0%	1.5E-16
569	35453-19-1	5-amino-2,4,6-triiodoisophthalic acid	559	232	2.0E-09	1.7E+00	1.4E+02	1.3	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.3E+02	1.3E+01	4.8E+02	-7.05	-8.10	-9.82	-2.08	0.39	0.0%	0.0%	1.0E-28
570	75-08-1	ethanethiol	62	-102	6.9E+04	9.1E+03	1.9E+01	10.7	3.5E-06	2.8E-09	1.1E-06	conf	conf	5.3E+02	7.4E+00	2.6E+02	-9.30	-8.98	-11.09	-2.95	0.93	0.0%	0.0%	1.5E-31
571	3238-40-2	furan-2,5-dicarboxylic acid	156	118	1.3E-05	8.8E+04	7.6E+00	2.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.2E+02	1.3E+01	4.7E+02	-6.79	-8.04	-9.82	-0.37	0.56	0.0%	0.0%	8.6E-42
572	167004-78-6	605-460-1	261	-45	1.0E-01	2.4E+03	7.1E-01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.2E+02	1.3E+01	4.7E+02	-7.85	-7.89	-9.86	-2.42	0.39	0.0%	0.0%	1.1E-26
573	939-97-9	4-tert-butylbenzaldehyde	162	25	6.1E+00	5.5E+01	4.2E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	8.0E+02	1.1E+01	4.1E+02	-8.99	-8.75	-9.95	-2.47	0.85	0.0%	0.0%	5.3E-27
574	18479-58-8	2,6-dimethyloct-7-en-2-ol	156	-13	1.7E+01	7.4E+02	3.0E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	8.2E+02	1.1E+01	4.2E+02	-8.62	-8.41	-9.58	-1.36	0.19	0.0%	0.0%	3.8E-32
575	121-03-9	4-nitrotoluene-2-sulphonic acid	217	151	2.9E-06	7.9E+02	1.6E-01	0.2	3.5E-06	3.5E-06	1.1E-07	conf	conf	9.1E+02	1.3E+01	4.7E+02	-6.26	-7.53	-9.78	-0.28	1.28	0.0%	0.0%	2.7E-42
576	590-86-3	isovaleraldehyde	86	-79	6.9E+03	1.9E+04	1.7E+01	14.0	3.5E-06	3.8E-07	3.5E-06	conf	conf	7.4E+02	1.0E+01	3.7E+02	-8.87	-8.60	-10.09	-1.52	0.72	0.0%	0.0%	9.7E-35
577	100-54-9	nicotinonitrile	104	25	1.8E+01	1.8E+04	2.2E+00	1.0	3.5E-06	5.5E-09	1.1E-07	conf	conf	5.3E+02	7.4E+00	2.6E+02	-5.65	-6.33	-7.32	-0.37	0.23	0.0%	0.0%	1.5E-23
578	393-75-9	4-chloro-3,5-dinitro-α,α,α-trifluorotoluene	271	102	5.1E-02	6.0E-01	1.7E+03	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	8.1E+02	1.1E+01	4.1E+02	-8.85	-8.64	-9.98	-2.54	1.12	0.0%	0.0%	1.1E-26
579	112-91-4	oleonitrile	263	88	9.5E-03	9.3E-04	3.2E+07	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.4E+02	7.6E+00	2.6E+02	-9.32	-9.27	-11.28	-4.77	0.37	0.0%	0.0%	7.0E-21
580	106-94-5	1-bromopropane	123	-79	1.8E+04	2.2E+03	1.4E+02	14.0	3.5E-06	2.1E-08	1.1E-06	conf	conf	5.2E+02	7.2E+00	2.5E+02	-9.41	-9.11	-11.34	-1.27	0.70	0.0%	0.0%	3.2E-47
581	45021-77-0	trimethyl-3-[(1-oxoallyl)amino]propylammonium chloride	207	87	9.9E-03	1.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.7E+02	9.3E+00	3.3E+02	-6.20	-6.51	-8.16	-0.71	0.34	0.0%	0.0%	9.3E-27
582	106-92-3	allyl 2,3-epoxypropyl ether	114	-45	5.7E+02	6.2E+04	2.8E+00	14.0	3.5E-06	4.9E-08	3.5E-07	conf	conf	5.9E+02	8.2E+00	2.9E+02	-7.64	-7.37	-8.56	-1.11	0.48	0.0%	0.0%	8.6E-27
583	924-42-5	N-(hydroxymethyl)acrylamide	101	69	2.7E-02	2.3E+05	1.5E-02	-1.3	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.0E+02	1.2E+01	4.6E+02	-6.45	-7.92	-9.82	-2.12	1.00	0.0%	0.0%	1.8E-28
584	96-49-1	ethylene carbonate	88	13	2.9E+00	1.0E+05	4.6E-01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	8.5E+02	1.2E+01	4.4E+02	-6.91	-7.22	-9.28	1.27	0.42	0.0%	0.0%	9.8E-27
585	540-84-1	2,2,4-trimethylpentane	114	-86	5.9E+03	2.0E+00	1.2E+04	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	5.8E+02	8.1E+00	2.9E+02	-9.81	-9.51	-12.53	-2.75	0.62	0.0%	0.0%	1.3E-44
586	84-66-2	diethyl phthalate	222	-2	3.4E-01	5.3E+02	4.5E+02	14.0	3.5E-06	8.3E-07	3.5E-07	conf	conf	8.1E+02	1.1E+01	4.1E+02	-7.85	-7.62	-9.30	-1.49	0.36	0.0%	0.0%	3.5E-29
587	105-45-3	methyl acetoacetate	116	-31	1.7E+02	3.4E+04	2.0E-01	10.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	8.8E+02	1.2E+01	4.5E+02	-8.34	-8.21	-9.85	-0.61	0.71	0.0%	0.0%	5.1E-40
588	110-05-4	di-tert-butyl peroxide	146	-43	3.7E+03	1.8E+02	2.8E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	5.9E+02	8.2E+00	2.9E+02	-9.70	-9.40	-11.99	-1.63	0.64	0.0%	0.0%	7.1E-50
589	119-61-9	benzophenone	182	64	1.2E-01	4.8E+01	1.4E+03	14.0	3.5E-06	2.5E-09	3.5E-07	conf	conf	5.0E+02	6.9E+00	2.4E+02	-7.21	-6.94	-8.04	-2.45	0.70	0.0%	0.0%	6.9E-16
590	92-52-4	biphenyl	154	25	1.0E+00	5.0E+00	5.8E+03	14.0	3.5E-06	9.1E-07	3.5E-08	conf	conf	7.2E+02	1.0E+01	3.7E+02	-8.91	-8.69	-10.04	-2.61	0.70	0.0%	0.0%	1.3E-26
591	79-77-6	(E)-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	192	52	3.0E+00	3.2E+02	2.6E+04	14.0	3.5E-06	6.3E-08	1.1E-06	conf	conf	5.4E+02	7.6E+00	2.7E+02	-7.92	-7.69	-8.90	-2.15	0.32	0.0%	0.0%	2.9E-22
592	2495-27-4	hexadecyl methacrylate	311	82	3.5E-03	4.5E-03	4.4E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.0E+02	6.9E+00	2.4E+02	-8.53	-8.68	-9.74	-5.02	0.95	0.0%	0.0%	8.1E-12
593	15214-89-8	2-acrylamido-2-methylpropanesulphonic acid	207	161	9.0E-07	4.1E+04	6.5E-03	-1.9	3.5E-06	3.5E-06	3.5E-06	conf	conf	8.4E+02	1.2E+01	4.3E+02	-6.68	-8.18	-9.86	-0.06	0.76	0.0%	0.0%	8.3E-45
594	107-88-0	butane-1,3-diol	90	-21	4.3E+00	1.0E+06	5.1E-01	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	8.4E+02	1.2E+01	4.3E+02	-7.31	-8.14	-9.89	0.41	0.26	0.0%	0.0%	2.7E-49
595	15625-89-5	2-ethyl-2-[[(1-oxoallyl)oxy]methyl]-1,3-propanediyl diacrylate	296	27	7.5E-02	7.1E+01	7.2E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	8.1E+02	1.1E+01	4.2E+02	-8.73	-8.55	-10.04	-2.29	0.54	0.0%	0.0%	8.6E-29
596	5102-83-0	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxobutyramide]	686	350	6.2E-21	1.5E-06	1.3E+08	0.6	3.5E-06	3.5E-07	3.5E-08	conf	conf	7.0E+02	9.8E+00	3.6E+02	-8.82	-8.82	-8.82	-0.74	1.21	0.0%	0.0%	4.1E-31
597	106-88-7	1,2-epoxybutane	72	-87	2.5E+04	2.9E+04	7.2E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	7.4E+02	1.0E+01	3.7E+02	-9.22	-8.93	-10.59	-0.74	0.32	0.0%	0.0%	2.9E-45
598	69416-61-1	potassium (R)-(4-hydroxyphenyl)[(3-methoxy-1-methyl-3-oxoprop-1-enyl)amino]acetate	303	87	9.9E-03	2.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.9E+02	8.2E+00	3.0E+02	-6.25	-6.56	-8.22	-1.84	0.64	0.0%	0.0%	4.0E-20
599	108-11-2	4-methylpentan-2-ol	102	-63	5.0E+02	1.6E+04	4.8E+01	14.0	3.5E-06	4.0E-07	3.5E-06	conf	conf	6.8E+02	9.5E+00	3.5E+02	-8.45	-8.20	-9.34	-0.39	0.34	0.0%	0.0%	9.7E-38
600	26399-02-0	2-ethylhexyl oleate	395	134	2.0E-05	6.0E-06	2.4E+11	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.5E+02	6.3E+00	2.2E+02	-8.22	-8.22	-8.22	0.35	1.10	0.0%	0.0%	9.5E-35
601	760-67-8	2-ethylhexanoyl chloride	163	-18	5.8E+01	2.0E+01	2.5E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	5.1E+02	7.2E+00	2.5E+02	-9.34	-9.03	-11.07	-2.04	0.92	0.0%	0.0%	2.3E-38
602	2530-87-2	3-chloropropyltrimethoxysilane	199	-4	4.5E+01	2.2E+03	3.6E+00	14.0	3.5E-06	1.1E-07	1.1E-07	conf	conf	5.7E+02	7.9E+00	2.8E+02	-8.04	-7.75	-9.10	-0.07	0.39	0.0%	0.0%	2.1E-38
603	551-16-6	6-aminopenicillanic acid	216	296	2.4E-07	5.8E+03	4.0E+00	4.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	6.7E+02	9.4E+00	3.4E+02	-5.87	-6.93	-8.75	-0.91	0.99	0.0%	0.0%	1.9E-29
604	15708-41-5	sodium feredetate	367	87	9.9E-03	2.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.8E+02	8.1E+00	2.9E+02	-6.25	-6.57	-8.22	-1.07	0.48	0.0%	0.0%	8.5E-25
605	120-92-3	cyclopentanone	84	-41	1.6E+03	4.4E+04	4.3E+00	14.0	3.5E-06	9.4E-07	1.1E-06	conf	conf	7.3E+02	1.0E+01	3.7E+02	-8.58	-8.39	-9.54	0.59	0.60	0.0%	0.0%	8.3E-48
606	143-22-6	2-(2-(2-butoxyethoxy)ethoxy)ethanol	206	56	6.9E-02	1.2E+06	1.0E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.4E+02	1.0E+01	3.8E+02	-6.25	-7.29	-9.38	0.24	0.32	0.0%	0.0%	2.7E-43
607	24634-61-5	potassium (E,E)-hexa-2,4-dienoate	150	87	9.9E-03	1.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.7E+02	8.0E+00	2.9E+02	-6.28	-6.58	-8.22	-0.18	0.54	0.0%	0.0%	7.5E-31
608	111-30-8	glutaral	100	-30	2.5E+02	6.1E+05	6.6E-01	14.0	3.5E-06	4.4E-06	1.1E-06	conf	conf	7.7E+02	1.1E+01	4.0E+02	-8.31	-8.16	-9.99	-2.28	0.65	0.0%	0.0%	1.5E-28
609	118-79-6	2,4,6-tribromophenol	331	107	4.0E-02	1.6E+01	1.5E+04	6.2	3.5E-06	2.3E-08	3.5E-07	conf	conf	4.6E+02	6.5E+00	2.3E+02	-7.06	-6.80	-7.92	-2.70	0.84	0.0%	0.0%	4.5E-14
610	84-65-1	anthraquinone	208	128	5.1E-06	1.6E+01	2.2E+03	14.0	3.5E-06	3.6E-09	3.5E-07	conf	conf	4.3E+02	6.0E+00	2.1E+02	-6.39	-6.64	-7.62	-1.62	0.44	0.0%	0.0%	4.9E-18
611	931-87-3	(Z)-cyclooctene	110	-59	1.2E+03	2.4E+01	8.7E+03	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	4.5E+02	6.3E+00	2.2E+02	-9.75	-9.44	-12.01	-2.21	0.88	0.0%	0.0%	7.7E-45
612	1663-39-4	tert-butyl acrylate	128	-51	1.7E+03	2.6E+03	1.2E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	6.4E+02	8.9E+00	3.3E+02	-9.31	-9.04	-10.73	-2.28	0.52	0.0%	0.0%	8.3E-34
613	3009-97-0	anilinoacetonitrile	132	45	1.2E+00	6.5E+04	1.4E+01	-0.6	3.5E-06	3.5E-07	3.5E-07	conf	conf	6.3E+02	8.8E+00	3.2E+02	-6.15	-7.01	-8.83	-1.11	0.64	0.0%	0.0%	1.5E-28
614	646-06-0	1,3-dioxolane	74	-75	1.4E+04	9.0E+05	4.9E-01	14.0	3.5E-06	4.1E-06	3.5E-07	conf	conf	7.4E+02	1.0E+01	3.8E+02	-8.54	-8.32	-10.00	-0.40	1.27	0.0%	0.0%	4.4E-43
615	89-83-8	thymol	150	38	2.2E+00	5.6E+02	3.3E+03	14.0	3.5E-06	2.6E-08	1.1E-06	conf	conf	4.5E+02	6.3E+00	2.2E+02	-7.50	-7.25	-8.44	-2.06	0.42	0.0%	0.0%	4.0E-20
616	119-47-1	6,6'-di-tert-butyl-2,2'-methylenedi-p-cresol	341	187	3.3E-07	1.9E-02	9.3E+07	10.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.5E+02	6.2E+00	2.2E+02	-7.98	-8.61	-8.99	-4.30	1.14	0.0%	0.0%	1.1E-11
617	123-54-6	pentane-2,4-dione	100	-29	1.2E+03	4.6E+05	1.1E+00	8.9	3.5E-06	4.8E-06	1.1E-06	conf	conf	7.4E+02	1.0E+01	3.8E+02	-8.55	-8.43	-10.05	-1.01	0.26	0.0%	0.0%	2.1E-38
618	123-30-8	4-aminophenol	109	54	4.4E-03	2.2E+04	1.7E+00	5.0	3.5E-06	5.2E-07	1.1E-06	conf	conf	6.5E+02	9.1E+00	3.3E+02	-6.32	-7.27	-9.07	-3.58	0.84	0.0%	0.0%	2.3E-15
619	16066-35-6	p-cumenesulphonic acid	200	111	1.1E-04	2.5E+03	1.9E+00	0.7	3.5E-06	3.5E-07	1.1E-07	conf	conf	6.2E+02	8.6E+00	3.1E+02	-5.75	-6.84	-8.74	-0.90	0.64	0.0%	0.0%	2.2E-29
620	105-76-0	dibutyl maleate	228	-28	7.1E-01	1.3E+02	1.4E+04	14.0	3.5E-06	1.2E-06	1.1E-06	conf	conf	6.2E+02	8.6E+00	3.1E+02	-8.53	-8.33	-9.71	-2.31	0.59	0.0%	0.0%	2.1E-26
621	137-26-8	thiram (reach)	240	107	1.5E-03	3.9E+02	5.0E+01	-2.0	3.5E-06	2.4E-08	3.5E-07	conf	conf	4.4E+02	6.2E+00	2.2E+02	-5.99	-6.53	-7.71	-3.82	1.10	0.1%	0.0%	1.5E-08
622	126-73-8	tributyl phosphate	266	65	4.7E-01	1.0E+03	6.6E+03	14.0	3.5E-06	2.6E-08	3.5E-07	conf	conf	4.4E+02	6.1E+00	2.1E+02	-7.15	-6.94	-8.13	-1.90	0.49	0.0%	0.0%	2.7E-19
623	98-13-5	trichloro(phenyl)silane	212	6	4.6E+01	1.4E+03	4.0E+03	14.0	3.5E-06	2.9E-08	1.1E-07	conf	conf	4.4E+02	6.1E+00	2.1E+02	-8.26	-7.98	-9.30	0.13	0.90	0.0%	0.0%	1.2E-41
624	513-35-9	2-methylbut-2-ene	70	-116	6.2E+04	3.1E+02	4.4E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.8E+02	6.7E+00	2.4E+02	-9.89	-9.57	-12.47	-2.22	0.22	0.0%	0.0%	7.1E-49
625	101-39-3	α-methylcinnamaldehyde	146	3	3.3E+00	2.8E+02	2.3E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	6.7E+02	9.3E+00	3.4E+02	-8.44	-8.25	-9.55	-2.23	0.54	0.0%	0.0%	6.3E-26
626	38103-06-9	4,4'-[(isopropylidene)bis(p-phenyleneoxy)]diphthalic dianhydride	520	285	4.4E-13	3.7E-04	7.4E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.1E+02	5.8E+00	2.0E+02	-7.92	-8.36	-8.53	-4.02	0.71	0.0%	0.0%	5.7E-11
627	79-46-9	2-nitropropane	89	-38	2.1E+03	1.6E+04	7.4E+00	8.2	3.5E-06	2.2E-09	1.1E-06	conf	conf	4.0E+02	5.6E+00	2.0E+02	-8.41	-8.13	-9.49	-0.55	0.61	0.0%	0.0%	1.1E-37
628	5466-77-3	2-ethylhexyl 4-methoxycinnamate	290	100	1.8E-03	1.8E-01	6.3E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.9E+02	6.9E+00	2.5E+02	-8.83	-8.74	-9.87	-1.60	1.73	0.0%	0.0%	1.7E-32
629	91507-67-4	O-(1-chloroethyl) S-methyl carbonothioate	155	-28	1.4E+02	2.1E+03	2.5E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	6.4E+02	8.9E+00	3.3E+02	-8.93	-8.72	-9.95	-1.99	0.85	0.0%	0.0%	2.8E-30
630	107-25-5	methyl vinyl ether	58	-116	2.0E+05	4.5E+04	2.6E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.5E+02	7.6E+00	2.8E+02	-9.44	-8.91	-10.99	-1.37	0.12	0.0%	0.0%	2.9E-43
631	4316-73-8	sodium sarcosinate	111	87	9.9E-03	7.7E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.1E+02	7.1E+00	2.5E+02	-6.34	-6.63	-8.27	0.25	1.09	0.0%	0.0%	2.0E-34
632	100-46-9	benzylamine	107	-1	1.0E+02	7.1E+03	1.2E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	5.7E+02	8.0E+00	2.9E+02	-7.84	-7.56	-8.83	-1.21	0.29	0.0%	0.0%	6.6E-28
633	693-36-7	dioctadecyl 3,3'-thiodipropionate	683	272	5.3E-13	2.4E-12	4.8E+17	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.8E+02	5.4E+00	1.9E+02	-14.63	-14.63	-14.63	-0.81	0.73	0.0%	0.0%	5.5E-87
634	102-06-7	1,3-diphenylguanidine	211	120	5.3E-04	1.0E+02	7.8E+02	10.1	3.5E-06	3.5E-06	3.5E-07	conf	conf	6.5E+02	9.1E+00	3.4E+02	-7.73	-8.44	-10.03	-2.02	0.49	0.0%	0.0%	1.1E-30
635	107-92-6	butyric acid	88	3	2.8E+02	1.1E+05	1.2E+01	4.9	3.5E-06	4.1E-06	1.1E-06	conf	conf	6.7E+02	9.4E+00	3.5E+02	-7.76	-8.41	-10.08	-0.56	0.63	0.0%	0.0%	1.9E-42
636	3033-77-0	2,3-epoxypropyltrimethylammonium chloride	152	87	9.9E-03	1.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.0E+02	6.9E+00	2.5E+02	-6.34	-6.64	-8.28	-0.60	1.03	0.0%	0.0%	2.5E-28
637	94-36-0	dibenzoyl peroxide	242	-2	9.3E-03	1.4E+02	2.7E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	6.1E+02	8.4E+00	3.1E+02	-8.02	-7.93	-9.56	-3.52	0.63	0.0%	0.0%	3.2E-18
638	110-16-7	maleic acid	116	84	1.3E-09	5.5E+04	1.1E+00	3.0	3.5E-06	4.7E-06	1.1E-06	conf	conf	6.7E+02	9.3E+00	3.4E+02	-6.87	-8.28	-10.09	-1.17	0.75	0.0%	0.0%	1.6E-37
639	106-65-0	dimethyl succinate	146	-95	5.8E+01	1.9E+05	2.5E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	6.6E+02	9.2E+00	3.4E+02	-8.38	-8.21	-9.99	-0.55	0.34	0.0%	0.0%	9.0E-42
640	106-24-1	geraniol	154	-11	2.1E+00	3.4E+02	3.0E+03	14.0	3.5E-06	5.8E-07	1.1E-06	conf	conf	5.7E+02	7.9E+00	2.9E+02	-8.24	-8.00	-9.38	-1.70	0.23	0.0%	0.0%	2.5E-28
641	60-24-2	2-mercaptoethanol	78	-46	1.1E+02	1.0E+05	6.3E-01	9.7	3.5E-06	4.2E-06	3.5E-06	conf	conf	6.6E+02	9.2E+00	3.4E+02	-8.61	-8.46	-10.06	-1.78	1.12	0.0%	0.0%	1.4E-32
642	111-85-3	1-chlorooctane	149	-36	1.2E+02	2.5E+00	3.3E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.2E+02	5.9E+00	2.1E+02	-9.91	-9.61	-12.32	-2.44	0.74	0.0%	0.0%	1.5E-45
643	3425-89-6	1,2,3,6-tetrahydro-4-methylphthalic anhydride	166	16	3.2E+00	8.1E+03	3.2E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	6.3E+02	8.8E+00	3.3E+02	-8.74	-8.57	-10.07	-0.59	0.41	0.0%	0.0%	4.2E-42
644	29806-73-3	2-ethylhexyl palmitate	369	117	1.4E-04	3.9E-05	4.1E+10	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.7E+02	5.2E+00	1.8E+02	-8.31	-8.21	-8.70	0.29	0.94	0.0%	0.0%	4.9E-38
645	121-57-3	sulphanilic acid	173	128	3.5E-07	3.9E+04	8.3E-03	0.3	3.5E-06	5.7E-09	1.1E-06	conf	conf	3.7E+02	5.2E+00	1.8E+02	-5.74	-6.54	-7.52	-1.31	0.29	0.0%	0.0%	3.6E-19
646	91-15-6	phthalonitrile	128	59	1.1E-01	2.4E+03	1.2E+01	14.0	3.5E-06	3.7E-08	1.1E-07	conf	conf	4.1E+02	5.7E+00	2.0E+02	-6.67	-6.57	-7.85	-1.17	0.46	0.0%	0.0%	7.1E-22
647	6358-31-2	2-[(2-methoxy-4-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxobutyramide	386	242	4.3E-10	8.0E+00	9.8E+02	-0.1	3.5E-06	3.5E-07	1.1E-07	conf	conf	5.3E+02	7.4E+00	2.7E+02	-6.30	-6.96	-8.82	-3.51	1.73	0.0%	0.0%	1.7E-14
648	112-16-3	lauroyl chloride	219	37	2.3E+00	2.7E-01	2.8E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	3.8E+02	5.4E+00	1.9E+02	-9.69	-9.39	-11.64	-2.36	0.82	0.0%	0.0%	2.1E-40
649	13674-87-8	tris[2-chloro-1-(chloromethyl)ethyl] phosphate	431	88	3.8E-05	1.9E+00	4.5E+03	14.0	3.5E-06	1.2E-08	3.5E-08	conf	conf	3.7E+02	5.2E+00	1.8E+02	-6.82	-6.68	-7.74	-2.35	0.44	0.0%	0.0%	7.1E-15
650	143230-42-6	604-340-6	353	170	1.3E-05	4.1E+01	1.6E+01	1.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	6.0E+02	8.3E+00	3.1E+02	-6.51	-7.53	-9.51	-2.42	1.28	0.0%	0.0%	2.0E-24
651	95-54-5	o-phenylenediamine	108	53	7.1E-03	3.4E+04	1.4E+00	5.0	3.5E-06	3.5E-09	1.1E-06	conf	conf	3.6E+02	5.0E+00	1.7E+02	-6.11	-6.58	-7.53	-2.16	0.90	0.0%	0.0%	8.4E-15
652	111-11-5	methyl octanoate	158	-21	6.8E+01	1.2E+02	2.1E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.2E+02	7.2E+00	2.6E+02	-9.39	-9.13	-10.76	-1.62	1.03	0.0%	0.0%	3.0E-39
653	7336-20-1	disodium 4,4'-diaminostilbene-2,2'-disulphonate	414	87	9.9E-03	2.9E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.5E+02	6.3E+00	2.3E+02	-6.36	-6.68	-8.33	-0.53	0.64	0.0%	0.0%	3.9E-29
654	112-76-5	stearoyl chloride	303	95	3.4E-02	4.8E-04	2.5E+07	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.6E+02	5.0E+00	1.8E+02	-9.59	-9.51	-11.97	-2.36	1.09	0.0%	0.0%	3.6E-43
655	87-62-7	2,6-xylidine	121	29	2.3E+01	1.7E+03	1.5E+02	4.0	3.5E-06	4.4E-08	1.1E-07	conf	conf	3.9E+02	5.5E+00	1.9E+02	-6.47	-6.66	-7.98	-1.10	0.31	0.0%	0.0%	4.6E-23
656	612-83-9	3,3'-dichlorobenzidine dihydrochloride	326	87	9.9E-03	2.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.4E+02	6.2E+00	2.2E+02	-6.37	-6.69	-8.34	-2.47	0.31	0.0%	0.0%	2.4E-17
657	687-47-8	ethyl (S)-2-hydroxypropionate	118	-28	1.4E+02	3.7E+04	6.6E-01	12.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	6.0E+02	8.3E+00	3.1E+02	-8.53	-8.40	-10.01	-0.04	0.41	0.0%	0.0%	2.2E-46
658	79-21-0	peracetic acid	76	-42	3.2E+03	3.8E+05	8.5E-02	8.2	3.5E-06	4.5E-06	1.1E-06	conf	conf	6.0E+02	8.3E+00	3.1E+02	-8.61	-8.48	-10.09	-3.06	0.67	0.0%	0.0%	4.9E-24
659	26760-64-5	2-methylbutene	70	-117	8.1E+04	6.0E+02	5.2E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	3.6E+02	5.1E+00	1.8E+02	-9.88	-9.52	-12.26	-2.22	0.22	0.0%	0.0%	5.9E-47
660	498-66-8	Norbornylene	94	-61	4.3E+03	2.1E+02	7.1E+02	14.0	3.5E-06	2.6E-08	3.5E-07	conf	conf	3.4E+02	4.8E+00	1.6E+02	-9.71	-9.39	-11.72	-1.99	0.19	0.0%	0.0%	3.2E-44
661	86-74-8	carbazole	167	100	5.4E-05	8.4E+00	1.7E+03	14.0	3.5E-06	2.2E-09	1.1E-07	conf	conf	3.4E+02	4.8E+00	1.7E+02	-6.59	-6.67	-7.61	-2.22	0.70	0.0%	0.0%	6.6E-15
662	15827-60-8	[[(phosphonomethyl)imino]bis[ethane-2,1-diylnitrilobis(methylene)]]tetrakisphosphonic acid	573	90	2.7E-09	1.0E+06	1.9E-10	0.4	3.5E-06	3.5E-07	3.5E-07	conf	conf	5.1E+02	7.1E+00	2.6E+02	-5.79	-6.88	-8.80	-1.04	1.40	0.0%	0.0%	7.2E-29
663	151-56-4	aziridine	43	-60	3.1E+04	1.0E+06	5.2E-01	8.0	3.5E-06	5.0E-07	1.1E-06	conf	conf	5.2E+02	7.3E+00	2.7E+02	-8.37	-8.16	-9.23	-2.03	0.68	0.0%	0.0%	4.4E-25
664	115-86-6	triphenyl phosphate	326	87	6.3E-05	2.3E+00	5.0E+04	14.0	3.5E-06	6.1E-07	1.1E-07	conf	conf	4.6E+02	6.4E+00	2.3E+02	-7.78	-7.83	-9.40	-2.83	0.84	0.0%	0.0%	3.2E-21
665	131860-97-4	603-525-9	321	161	2.7E-05	6.3E+01	2.9E+01	1.1	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.5E+02	7.7E+00	2.8E+02	-6.62	-7.58	-9.55	-3.00	1.31	0.0%	0.0%	4.0E-21
666	55934-93-5	[(butoxymethylethoxy)methylethoxy]propan-1-ol	248	55	7.7E-03	6.2E+02	1.9E+01	13.5	3.5E-06	1.1E-06	1.1E-06	conf	conf	5.5E+02	7.6E+00	2.8E+02	-7.52	-7.81	-9.58	-0.31	0.62	0.0%	0.0%	2.5E-40
667	108-99-6	3-methylpyridine	93	-26	7.0E+02	5.4E+05	2.2E+01	5.0	3.5E-06	1.2E-08	1.1E-07	conf	conf	3.4E+02	4.8E+00	1.7E+02	-6.36	-6.59	-7.65	-0.42	0.30	0.0%	0.0%	2.5E-25
668	603-35-0	triphenylphosphine	262	109	1.4E-03	4.9E+00	1.0E+05	14.0	3.5E-06	2.6E-08	1.1E-08	conf	conf	3.4E+02	4.7E+00	1.6E+02	-7.27	-7.06	-8.18	-1.69	0.75	0.0%	0.0%	9.3E-21
669	51981-21-6	tetrasodium N,N-bis(carboxylatomethyl)-L-glutamate	351	87	9.9E-03	2.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.2E+02	5.9E+00	2.1E+02	-6.39	-6.71	-8.36	0.10	0.38	0.0%	0.0%	5.5E-34
670	6197-30-4	octocrilene	361	181	4.2E-07	3.5E-02	7.6E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.7E+02	5.1E+00	1.8E+02	-8.25	-8.81	-9.61	-1.60	2.11	0.0%	0.0%	1.2E-30
671	75-66-1	2-methylpropane-2-thiol	90	-82	2.2E+04	4.4E+03	1.4E+02	11.3	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.3E+02	6.0E+00	2.1E+02	-9.71	-9.41	-11.56	-1.69	0.29	0.0%	0.0%	1.9E-45
672	78-63-7	di-tert-butyl 1,1,4,4-tetramethyltetramethylene diperoxide	290	65	1.3E+00	1.4E-01	3.5E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.5E+02	4.9E+00	1.7E+02	-9.92	-9.72	-12.01	-3.11	0.67	0.0%	0.0%	2.4E-37
673	3047-33-4	1,3,5-triazine-2,4,6(1H,3H,5H)-trione, trisodium salt	195	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.2E+02	5.9E+00	2.1E+02	-6.41	-6.71	-8.36	0.61	0.46	0.0%	0.0%	6.7E-38
674	110-60-1	tetramethylenediamine	88	1	3.1E+02	1.0E+06	2.3E-01	10.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	5.6E+02	7.8E+00	2.9E+02	-8.24	-8.11	-10.01	-1.19	0.68	0.0%	0.0%	9.5E-37
675	98-09-9	benzenesulphonyl chloride	177	61	3.3E+00	8.9E+02	8.7E+02	14.0	3.5E-06	8.6E-07	1.1E-07	conf	conf	5.1E+02	7.1E+00	2.6E+02	-8.22	-8.02	-9.49	-1.69	0.51	0.0%	0.0%	3.4E-29
676	78-42-2	tris(2-ethylhexyl) phosphate	435	87	8.1E-05	1.9E-04	3.1E+09	14.0	3.5E-06	1.6E-08	3.5E-07	conf	conf	3.2E+02	4.4E+00	1.5E+02	-8.41	-8.50	-9.08	-1.66	0.69	0.0%	0.0%	1.5E-26
677	2425-77-6	2-hexyldecan-1-ol	242	51	2.4E-03	2.6E-02	4.6E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.6E+02	5.0E+00	1.8E+02	-9.38	-9.29	-10.25	-1.91	1.73	0.0%	0.0%	5.1E-33
678	541-05-9	hexamethylcyclotrisiloxane	222	1	4.4E+02	3.4E+01	4.4E+05	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	3.1E+02	4.4E+00	1.5E+02	-9.70	-9.19	-11.65	-0.26	0.60	0.0%	0.0%	6.9E-60
679	108-22-5	isopropenyl acetate	100	-80	5.7E+03	3.7E+04	1.9E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	5.3E+02	7.4E+00	2.7E+02	-9.44	-9.26	-10.57	-1.68	0.22	0.0%	0.0%	3.0E-37
680	13463-41-7	pyrithione zinc	318	87	9.9E-03	2.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.0E+02	5.6E+00	2.0E+02	-6.42	-6.73	-8.38	-4.51	1.53	0.3%	0.1%	1.6E-08
681	79-92-5	camphene	136	-15	2.4E+02	1.8E+01	2.2E+04	14.0	3.5E-06	2.1E-08	3.5E-08	conf	conf	3.1E+02	4.3E+00	1.5E+02	-9.73	-9.37	-11.67	-1.84	1.01	0.0%	0.0%	4.9E-45
682	149-44-0	sodium hydroxymethanesulphinate	118	87	9.9E-03	8.2E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.0E+02	5.6E+00	2.0E+02	-6.44	-6.74	-8.38	-0.91	0.36	0.0%	0.0%	6.9E-27
683	112-55-0	dodecane-1-thiol	202	16	9.9E-01	2.5E-02	1.5E+06	10.7	3.5E-06	3.5E-07	1.1E-07	conf	conf	3.2E+02	4.4E+00	1.5E+02	-9.95	-9.70	-12.16	-2.59	1.33	0.0%	0.0%	7.3E-43
684	4979-32-2	N,N-dicyclohexylbenzothiazole-2-sulphenamide	347	192	8.2E+00	3.4E-02	8.9E+05	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	3.1E+02	4.4E+00	1.5E+02	-9.94	-9.66	-12.39	-2.61	0.65	0.0%	0.0%	1.3E-44
685	151-21-3	sodium dodecyl sulphate	288	87	9.9E-03	2.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.9E+02	5.5E+00	2.0E+02	-6.43	-6.74	-8.39	-2.26	0.60	0.0%	0.0%	1.0E-18
686	106-23-0	citronellal	154	-28	3.4E+01	2.9E+02	3.4E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.7E+02	6.5E+00	2.4E+02	-9.27	-9.02	-10.24	-1.91	0.23	0.0%	0.0%	6.8E-33
687	1185-55-3	trimethoxy(methyl)silane	136	-60	4.5E+03	1.9E+04	2.1E-01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.8E+02	6.7E+00	2.5E+02	-9.13	-8.83	-10.51	-0.49	0.67	0.0%	0.0%	1.0E-46
688	24280-93-1	mycophenolic acid	320	216	2.1E-08	2.7E+02	1.7E+04	4.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.0E+02	6.9E+00	2.5E+02	-7.01	-7.82	-9.56	-2.37	0.38	0.0%	0.0%	4.4E-25
689	60-29-7	diethyl ether	74	-101	7.2E+04	4.8E+04	1.1E+01	14.0	3.5E-06	3.0E-08	3.5E-07	conf	conf	3.1E+02	4.3E+00	1.5E+02	-9.12	-8.79	-10.74	0.24	0.70	0.0%	0.0%	8.1E-56
690	123-99-9	azelaic acid	188	127	3.1E-03	3.8E+03	5.0E+01	4.6	3.5E-06	1.1E-06	1.1E-06	conf	conf	5.0E+02	6.9E+00	2.6E+02	-6.99	-7.84	-9.62	-1.95	0.68	0.0%	0.0%	3.2E-28
691	919-30-2	3-aminopropyltriethoxysilane	221	56	9.8E+00	2.8E+04	2.0E+00	9.9	3.5E-06	1.1E-06	1.1E-06	conf	conf	5.0E+02	6.9E+00	2.6E+02	-8.02	-7.82	-9.61	-0.42	0.96	0.0%	0.0%	1.3E-39
692	2935-90-2	methyl 3-mercaptopropionate	120	-40	2.5E+02	5.0E+04	6.5E+00	9.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	5.2E+02	7.2E+00	2.7E+02	-8.76	-8.63	-10.09	-2.86	0.71	0.0%	0.0%	2.8E-25
693	142-47-2	sodium hydrogen glutamate	169	87	9.9E-03	1.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.9E+02	5.4E+00	1.9E+02	-6.45	-6.75	-8.40	-1.31	1.35	0.0%	0.0%	2.1E-24
694	10326-41-7	(R)-lactic acid	90	23	3.8E+00	7.7E+05	2.2E-01	14.0	3.5E-06	4.7E-07	3.5E-07	conf	conf	4.6E+02	6.4E+00	2.3E+02	-6.44	-7.12	-9.07	-0.25	0.50	0.0%	0.0%	1.0E-36
695	15022-08-9	diallyl carbonate	142	-74	7.7E+02	1.5E+04	8.5E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.8E+02	6.7E+00	2.5E+02	-8.98	-8.77	-10.01	-2.21	0.92	0.0%	0.0%	3.9E-29
696	1071-22-3	3-(trichlorosilyl)propiononitrile	189	7	6.0E+01	1.1E+04	3.3E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	4.4E+02	6.1E+00	2.2E+02	-8.09	-7.85	-9.22	-0.81	0.85	0.0%	0.0%	1.7E-33
697	111-92-2	dibutylamine	129	-30	3.4E+02	2.0E+03	5.9E+02	11.0	3.5E-06	5.0E-07	3.5E-07	conf	conf	4.3E+02	6.0E+00	2.2E+02	-9.07	-8.81	-10.17	-1.56	0.70	0.0%	0.0%	4.1E-35
698	126-71-6	triisobutyl phosphate	266	16	1.7E+00	3.1E+02	4.0E+03	14.0	3.5E-06	2.6E-08	3.5E-07	conf	conf	3.1E+02	4.4E+00	1.5E+02	-7.86	-7.59	-8.81	-1.49	1.01	0.0%	0.0%	7.4E-26
699	674-82-8	but-3-en-3-olide	84	-36	1.6E+03	9.3E+04	4.1E-01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	5.1E+02	7.0E+00	2.6E+02	-8.79	-8.65	-10.11	-0.54	0.24	0.0%	0.0%	7.1E-43
700	3622-84-2	N-butylbenzenesulphonamide	213	108	1.9E-02	1.1E+03	2.0E+02	10.1	3.5E-06	3.5E-07	1.1E-07	conf	conf	4.3E+02	6.0E+00	2.2E+02	-7.15	-7.23	-9.03	-1.29	0.13	0.0%	0.0%	1.0E-28
701	6358-30-1	8,18-dichloro-5,15-diethyl-5,15-dihydrodiindolo[3,2-b:3',2'-m]triphenodioxazine	589	339	7.1E-17	1.6E-05	2.1E+09	14.0	3.5E-06	3.5E-07	3.5E-08	conf	conf	2.9E+02	4.0E+00	1.4E+02	-8.05	-8.11	-8.32	-0.68	0.49	0.0%	0.0%	5.4E-28
702	90-72-2	2,4,6-tris(dimethylaminomethyl)phenol	265	134	2.1E-04	5.8E+04	5.9E+00	8.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	5.0E+02	7.0E+00	2.6E+02	-7.17	-8.31	-10.14	-0.63	0.43	0.0%	0.0%	2.8E-42
703	98-59-9	tosyl chloride	191	75	1.6E-01	2.1E+02	3.1E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	4.1E+02	5.7E+00	2.1E+02	-7.77	-7.53	-9.14	-1.43	0.43	0.0%	0.0%	1.6E-28
704	24468-13-1	2-ethylhexyl chloroformate	193	-8	3.4E+01	3.2E+01	3.2E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.3E+02	6.0E+00	2.2E+02	-9.92	-9.66	-11.50	-2.44	0.67	0.0%	0.0%	1.3E-38
705	2008-39-1	dimethylammonium 2,4-dichlorophenoxyacetate	266	87	9.9E-03	1.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.7E+02	5.1E+00	1.8E+02	-6.46	-6.77	-8.42	-0.82	0.50	0.0%	0.0%	9.1E-28
706	288-88-0	1,2,4-triazole	69	22	8.0E+01	1.6E+05	1.7E-01	2.0	3.5E-06	8.1E-07	1.1E-07	conf	conf	4.6E+02	6.4E+00	2.4E+02	-6.22	-7.31	-9.36	-0.61	0.70	0.0%	0.0%	3.9E-36
707	3794-83-0	tetrasodium (1-hydroxyethylidene)bisphosphonate	294	87	9.9E-03	2.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.7E+02	5.1E+00	1.8E+02	-6.46	-6.77	-8.42	-0.74	1.48	0.0%	0.0%	2.4E-28

708	122-52-1	triethyl phosphite	166	-21	3.7E+02	1.7E+09	5.5E+00	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	4.2E+02	5.8E+00	2.1E+02	-6.31	-7.16	-9.00	-0.07	0.54	0.0%	0.0%	1.5E-37
709	7173-62-8	(Z)-N-9-octadecenylpropane-1,3-diamine	325	142	6.5E-05	1.7E-04	3.0E+07	10.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.0E+02	4.2E+00	1.5E+02	-9.37	-9.36	-10.51	-3.98	0.50	0.0%	0.0%	4.8E-21
710	98-67-9	4-hydroxybenzenesulphonic acid	174	129	4.4E-05	2.5E+04	2.2E-02	1.0	3.5E-06	1.1E-05	3.5E-06	conf	conf	4.9E+02	6.9E+00	2.5E+02	-7.42	-9.00	-10.61	-0.82	0.67	0.0%	0.0%	9.5E-45
711	121-43-7	trimethyl borate	104	-83	2.0E+04	1.5E+08	1.3E-02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.6E+02	6.5E+00	2.4E+02	-7.73	-7.61	-9.55	-0.78	0.63	0.0%	0.0%	2.2E-36
712	1241-94-7	2-ethylhexyl diphenyl phosphate	362	87	4.5E-03	9.0E-02	2.0E+06	14.0	3.5E-06	1.3E-08	3.5E-07	conf	conf	2.8E+02	3.9E+00	1.3E+02	-8.96	-8.81	-9.90	-3.16	0.87	0.0%	0.0%	3.1E-22
713	2409-55-4	2-tert-butyl-p-cresol	164	52	1.7E+00	5.3E+02	9.3E+03	10.8	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.4E+02	6.1E+00	2.2E+02	-9.08	-8.92	-10.28	-2.67	0.05	0.0%	0.0%	7.6E-28
714	92-70-6	3-hydroxy-2-naphthoic acid	188	141	8.3E-06	4.8E+02	2.6E+03	3.0	3.5E-06	3.5E-06	3.5E-07	conf	conf	4.8E+02	6.6E+00	2.5E+02	-7.42	-8.22	-10.11	-1.26	0.25	0.0%	0.0%	5.9E-37
715	106-22-9	citronellol	156	-12	2.3E+00	3.5E+02	3.6E+03	14.0	3.5E-06	4.1E-07	1.1E-06	conf	conf	4.0E+02	5.5E+00	2.0E+02	-8.29	-8.05	-9.40	-2.07	0.48	0.0%	0.0%	5.7E-26
716	2420-17-9	5-(4-hydroxyphenyl)imidazolidine-2,4-dione	192	198	5.1E-08	5.6E+03	1.0E+00	14.0	3.5E-06	1.1E-05	3.5E-06	conf	conf	4.8E+02	6.7E+00	2.5E+02	-7.62	-8.91	-10.62	-2.00	0.62	0.0%	0.0%	3.9E-35
717	95-75-0	3,4-dichlorotoluene	161	4	3.1E+01	3.6E+01	6.8E+03	14.0	3.5E-06	2.7E-09	3.5E-08	conf	conf	2.7E+02	3.8E+00	1.3E+02	-9.16	-8.86	-10.66	-2.57	0.26	0.0%	0.0%	3.5E-31
718	78-67-1	2,2'-dimethyl-2,2'-azodipropiononitrile	164	44	1.9E-01	7.2E+02	7.4E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	4.0E+02	5.5E+00	2.0E+02	-7.70	-7.47	-9.13	-1.58	0.55	0.0%	0.0%	1.8E-27
719	15307-79-6	sodium [2-[(2,6-dichlorophenyl)amino]phenyl]acetate	318	269	4.2E-12	4.6E+05	3.7E+00	4.4	3.5E-06	2.2E-09	3.5E-08	conf	conf	2.7E+02	3.8E+00	1.3E+02	-5.71	-6.54	-7.48	-1.47	0.64	0.0%	0.0%	4.3E-18
720	591-27-5	3-aminophenol	109	54	2.5E-01	9.3E+04	1.7E+00	4.0	3.5E-06	3.9E-09	1.1E-06	conf	conf	2.7E+02	3.8E+00	1.3E+02	-6.24	-6.71	-7.66	-1.91	0.84	0.0%	0.0%	1.1E-16
721	121-45-9	trimethyl phosphite	124	-58	3.0E+03	8.7E+04	1.9E-01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.4E+02	6.2E+00	2.3E+02	-8.80	-8.58	-9.92	0.08	0.39	0.0%	0.0%	1.4E-46
722	106-48-9	4-chlorophenol	129	29	5.3E+00	1.1E+04	1.4E+02	9.6	3.5E-06	2.2E-09	3.5E-07	conf	conf	2.7E+02	3.8E+00	1.3E+02	-7.12	-6.85	-7.82	-2.02	0.53	0.0%	0.0%	6.1E-17
723	123-35-3	7-Methyl-3-methylene-1,6-octadiene	136	-65	3.2E+02	1.1E+01	7.6E+04	14.0	3.5E-06	4.4E-07	3.5E-07	conf	conf	2.8E+02	4.0E+00	1.4E+02	-10.00	-9.71	-12.18	-1.11	0.70	0.0%	0.0%	1.0E-56
724	420-04-2	cyanamide (reach)	42	-36	1.9E+03	2.5E+05	1.5E-01	1.0	3.5E-06	7.5E-09	3.5E-07	conf	conf	2.7E+02	3.8E+00	1.3E+02	-5.98	-6.67	-7.67	-2.04	0.73	0.0%	0.0%	4.3E-16
725	108-74-7	hexahydro-1,3,5-trimethyl-1,3,5-triazine	129	17	3.1E+02	8.1E+05	7.1E-03	5.1	3.5E-06	3.5E-06	3.5E-07	conf	conf	4.7E+02	6.5E+00	2.4E+02	-7.02	-8.09	-10.13	-2.16	0.86	0.0%	0.0%	2.3E-30
726	116-37-0	1,1'-isopropylidenebis(p-phenyleneoxy)dipropan-2-ol	344	175	6.8E-09	2.0E+03	1.1E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	3.7E+02	5.1E+00	1.9E+02	-6.70	-7.52	-9.13	-1.98	0.31	0.0%	0.0%	8.8E-25
727	109-73-9	butylamine	73	-59	1.3E+04	4.9E+05	6.8E+00	10.0	3.5E-06	4.1E-07	1.1E-06	conf	conf	4.0E+02	5.6E+00	2.0E+02	-8.56	-8.33	-9.46	-1.27	0.70	0.0%	0.0%	6.2E-32
728	95-16-9	benzothiazole	135	57	9.9E+00	1.1E+03	1.5E+02	2.4	3.5E-06	4.8E-09	3.5E-07	conf	conf	2.7E+02	3.8E+00	1.3E+02	-6.25	-6.71	-7.70	-1.42	0.58	0.0%	0.0%	1.6E-19
729	4511-42-6	(3S-cis)-3,6-dimethyl-1,4-dioxane-2,5-dione	144	26	2.1E-02	1.5E+07	4.5E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.6E+02	6.4E+00	2.4E+02	-7.33	-8.52	-10.14	-0.25	0.50	0.0%	0.0%	1.1E-45
730	112-11-8	isopropyl oleate	325	89	1.5E-03	2.3E-03	8.3E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.7E+02	3.8E+00	1.3E+02	-8.67	-8.83	-9.73	-4.91	0.78	0.0%	0.0%	2.9E-12
731	54839-24-6	2-ethoxy-1-methylethyl acetate	146	-38	3.7E+02	1.6E+04	1.0E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.4E+02	6.1E+00	2.2E+02	-8.84	-8.65	-9.87	-0.62	0.24	0.0%	0.0%	3.9E-40
732	126-58-9	2,2,2',2'-tetrakis(hydroxymethyl)-3,3'-oxydipropan-1-ol	254	192	2.3E-10	1.0E+06	2.5E-03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.4E+02	6.1E+00	2.2E+02	-6.32	-7.47	-9.55	2.55	0.80	0.0%	0.0%	1.6E-28
733	22818-40-2	D-N-(4-hydroxyphenyl)glycine	167	239	5.9E-06	4.8E+03	5.6E-03	2.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.6E+02	6.4E+00	2.4E+02	-6.74	-8.20	-10.12	-1.83	0.72	0.0%	0.0%	1.2E-32
734	10595-60-5	N,N'-bis(1,3-dimethylbutylidene)-2,2'-iminobis(ethylamine)	267	1	8.3E-02	1.9E+01	4.3E+07	10.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.9E+02	4.1E+00	1.4E+02	-8.83	-9.21	-9.92	-2.95	0.27	0.0%	0.0%	1.2E-23
735	36177-92-1	N-butyl-2,2,6,6-tetramethylpiperidin-4-amine	212	80	2.0E-01	3.6E+03	7.6E+02	10.3	3.5E-06	3.5E-07	3.5E-07	conf	conf	3.8E+02	5.3E+00	1.9E+02	-7.63	-7.46	-9.15	-1.52	0.74	0.0%	0.0%	5.8E-28
736	74-95-3	dibromomethane	174	-52	6.5E+03	1.1E+04	3.3E+01	14.0	3.5E-06	2.0E-08	1.1E-07	conf	conf	2.6E+02	3.7E+00	1.3E+02	-9.02	-8.69	-10.66	-1.13	0.22	0.0%	0.0%	1.9E-42
737	751-83-7	[3-methyl-5-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4-pentadienyl]triphenylphosphonium sulphate	1027	87	9.9E-03	7.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.3E+02	4.6E+00	1.7E+02	-6.48	-6.81	-8.47	-4.22	0.64	0.1%	0.0%	6.3E-10
738	103-09-3	2-ethylhexyl acetate	172	-20	5.1E+01	1.8E+02	5.5E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.0E+02	5.6E+00	2.1E+02	-9.84	-9.61	-11.00	-1.63	0.42	0.0%	0.0%	3.7E-41
739	21542-96-1	N,N-dimethyldocosylamine	354	117	2.1E-04	5.0E-06	2.2E+10	10.1	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.5E+02	3.5E+00	1.2E+02	-8.61	-8.51	-9.50	-3.83	2.15	0.0%	0.0%	3.0E-16
740	17796-82-6	N-(cyclohexylthio)phthalimide	261	198	3.5E-07	1.0E+02	5.8E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.9E+02	5.5E+00	2.0E+02	-7.09	-8.13	-9.69	-2.27	0.51	0.0%	0.0%	1.4E-26
741	78-51-3	tris(2-butoxyethyl) phosphate	398	86	1.6E-04	2.4E+00	1.0E+03	14.0	3.5E-06	3.0E-08	3.5E-07	conf	conf	2.8E+02	3.8E+00	1.3E+02	-7.16	-6.93	-8.14	-1.50	0.33	0.0%	0.0%	1.2E-21
742	111-86-4	octylamine	129	-10	1.3E+02	3.2E+02	6.3E+02	10.0	3.5E-06	5.0E-07	3.5E-07	conf	conf	3.6E+02	5.0E+00	1.8E+02	-9.27	-9.00	-10.54	-2.65	0.70	0.0%	0.0%	8.3E-30
743	112-67-4	palmitoyl chloride	275	77	1.2E-01	1.3E-02	2.5E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.7E+02	3.8E+00	1.3E+02	-10.05	-9.84	-12.07	-2.36	1.10	0.0%	0.0%	4.1E-44
744	5460-09-3	sodium hydrogen 4-amino-5-hydroxynaphthalene-2,7-disulphonate	341	87	9.9E-03	2.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.3E+02	4.5E+00	1.6E+02	-6.51	-6.82	-8.47	-0.06	0.64	0.0%	0.0%	1.3E-33
745	97-36-9	2',4'-dimethylacetoacetanilide	205	138	1.1E-03	7.5E+02	3.5E+01	0.6	3.5E-06	3.5E-07	1.1E-07	conf	conf	3.8E+02	5.2E+00	1.9E+02	-6.24	-7.12	-9.01	-2.28	0.91	0.0%	0.0%	3.7E-22
746	36727-29-4	3,5,5-trimethylhexanoyl chloride	177	-11	1.6E+02	3.0E+00	6.0E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	3.0E+02	4.1E+00	1.5E+02	-10.00	-9.68	-12.48	-1.73	0.95	0.0%	0.0%	1.6E-53
747	108-87-2	methylcyclohexane	98	-74	5.5E+03	2.7E+01	3.9E+03	14.0	3.5E-06	2.1E-08	3.5E-07	conf	conf	2.5E+02	3.5E+00	1.2E+02	-9.98	-9.66	-12.35	-1.81	0.70	0.0%	0.0%	1.6E-51
748	99-96-7	4-hydroxybenzoic acid	138	94	9.4E-04	1.2E+04	2.5E+01	4.6	3.5E-06	1.4E-06	1.1E-06	conf	conf	4.2E+02	5.9E+00	2.2E+02	-7.06	-8.00	-9.77	-1.04	0.52	0.0%	0.0%	5.4E-36
749	108-45-2	m-phenylenediamine	108	53	2.5E-01	2.0E+04	4.1E-01	5.1	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.2E+02	5.8E+00	2.1E+02	-6.66	-7.82	-9.66	-1.58	0.98	0.0%	0.0%	3.6E-31
750	105-56-6	ethyl cyanoacetate	113	-11	2.9E+01	2.3E+04	1.0E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.4E+02	6.1E+00	2.2E+02	-8.58	-8.43	-10.14	-0.83	0.40	0.0%	0.0%	1.0E-40
751	3173-72-6	1,5-naphthylene diisocyanate	210	77	4.6E-03	4.2E+02	2.3E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.7E+02	5.1E+00	1.9E+02	-7.89	-8.26	-9.78	-1.56	1.45	0.0%	0.0%	4.2E-32
752	770-35-4	1-phenoxypropan-2-ol	152	21	6.9E-01	2.9E+03	3.3E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.1E+02	5.7E+00	2.1E+02	-8.20	-8.00	-9.70	-0.57	0.52	0.0%	0.0%	3.4E-39
753	95-73-8	2,4-dichlorotoluene	161	4	4.6E+01	6.1E+01	6.8E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	2.7E+02	3.8E+00	1.3E+02	-9.22	-8.93	-10.71	-2.57	0.26	0.0%	0.0%	1.5E-31
754	92-84-2	phenothiazine	199	122	1.1E-04	3.3E+01	6.6E+03	0.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.1E+02	5.7E+00	2.1E+02	-7.27	-7.98	-9.71	-0.99	0.51	0.0%	0.0%	7.1E-36
755	85-40-5	1,2,3,6-tetrahydrophthalimide	151	172	1.6E-05	5.8E+04	2.0E+00	9.3	3.5E-06	3.5E-06	3.5E-07	conf	conf	4.3E+02	6.0E+00	2.2E+02	-6.79	-7.99	-10.13	-1.32	1.44	0.0%	0.0%	1.2E-36
756	10233-13-3	isopropyl laurate	242	23	5.1E-01	9.0E-02	1.5E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.7E+02	3.7E+00	1.3E+02	-10.06	-9.83	-11.90	-2.12	1.89	0.0%	0.0%	1.3E-44
757	90-05-1	guaiacol	124	25	1.5E+01	3.9E+04	2.2E+01	10.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.1E+02	5.7E+00	2.1E+02	-8.22	-8.01	-9.70	-0.88	0.47	0.0%	0.0%	9.7E-37
758	598-78-7	2-chloropropionic acid	109	8	1.0E+02	1.6E+05	5.8E+00	2.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.1E+02	5.7E+00	2.1E+02	-6.53	-7.72	-9.67	-0.90	0.65	0.0%	0.0%	2.4E-36
759	111-29-5	pentane-1,5-diol	104	3	5.6E-01	5.9E+05	1.9E+00	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	4.2E+02	5.9E+00	2.2E+02	-7.50	-8.53	-10.20	-0.13	0.62	0.0%	0.0%	3.4E-47
760	99-63-8	isophthaloyl dichloride	203	68	6.3E-01	6.9E+02	7.6E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.2E+02	5.9E+00	2.2E+02	-8.74	-8.57	-10.22	0.03	0.79	0.0%	0.0%	6.5E-49
761	52722-86-8	4-hydroxy-2,2,6,6-tetramethylpiperidine-1-ethanol	201	96	1.1E-03	8.6E+04	3.9E+00	8.5	3.5E-06	3.5E-06	3.5E-06	conf	conf	4.2E+02	5.8E+00	2.2E+02	-7.46	-8.58	-10.22	-0.83	0.50	0.0%	0.0%	2.8E-41
762	98-73-7	4-tert-butylbenzoic acid	178	81	1.1E-02	2.6E+00	6.0E+03	4.1	3.5E-06	1.5E-08	1.1E-06	conf	conf	2.5E+02	3.5E+00	1.2E+02	-6.78	-6.85	-7.96	-1.57	0.69	0.0%	0.0%	3.3E-20
763	112-25-4	2-hexyloxyethanol	146	3	6.1E+00	8.5E+03	3.5E+01	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	4.1E+02	5.8E+00	2.1E+02	-8.95	-8.77	-10.26	-0.82	0.18	0.0%	0.0%	9.4E-42
764	100-66-3	anisole	108	-41	4.5E+02	3.3E+03	1.2E+02	14.0	3.5E-06	5.9E-07	1.1E-06	conf	conf	3.6E+02	5.1E+00	1.9E+02	-9.14	-8.89	-10.14	-1.73	0.75	0.0%	0.0%	1.3E-33
765	25498-49-1	[2-(2-methoxymethylethoxy)methylethoxy]propanol	206	25	7.1E-01	2.0E+04	6.3E-01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	3.6E+02	5.0E+00	1.8E+02	-7.16	-7.16	-9.03	0.99	0.25	0.0%	0.0%	8.6E-47
766	139-33-3	disodium dihydrogen ethylenediaminetetraacetate	336	87	9.9E-03	2.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.1E+02	4.3E+00	1.5E+02	-6.53	-6.84	-8.50	-1.16	0.78	0.0%	0.0%	4.8E-26
767	13048-33-4	hexamethylene diacrylate	226	-30	2.2E+00	2.1E+02	1.2E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.8E+02	5.3E+00	1.9E+02	-8.78	-8.57	-9.87	-2.47	0.31	0.0%	0.0%	1.9E-26
768	111-88-6	octane-1-thiol	146	-28	5.0E+01	2.6E+01	1.6E+04	10.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.1E+02	4.3E+00	1.5E+02	-9.81	-9.53	-11.38	-3.98	0.64	0.0%	0.0%	2.0E-26
769	431-89-0	1,1,1,2,3,3,3-heptafluoropropane	170	-153	4.1E+05	4.5E+00	3.2E+02	14.0	3.5E-06	3.5E-08	3.5E-08	conf	conf	2.4E+02	3.3E+00	1.1E+02	-9.95	-9.61	-12.34	-0.88	0.59	0.0%	0.0%	1.3E-60
770	79-31-2	isobutyric acid	88	-8	4.4E+02	1.1E+05	1.0E+01	4.9	3.5E-06	4.7E-06	1.1E-06	conf	conf	4.1E+02	5.7E+00	2.1E+02	-8.15	-8.70	-10.35	-0.62	0.52	0.0%	0.0%	3.7E-44
771	109-53-5	isobutyl vinyl ether	100	-88	1.1E+04	4.4E+03	6.6E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	3.3E+02	4.5E+00	1.6E+02	-9.74	-9.44	-11.47	-1.37	0.12	0.0%	0.0%	1.8E-47
772	122-62-3	bis(2-ethylhexyl) sebacate	427	51	2.6E-04	4.9E-04	1.2E+10	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.3E+02	3.3E+00	1.1E+02	-8.46	-8.46	-8.86	-2.11	2.88	0.0%	0.0%	2.9E-22
773	688-84-6	2-ethylhexyl methacrylate	198	-8	1.0E+01	2.8E+01	4.4E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	3.3E+02	4.7E+00	1.7E+02	-9.99	-9.75	-11.19	-1.98	1.12	0.0%	0.0%	7.4E-40
774	16652-76-9	O-benzyl-L-valine toluene-p-sulphonate	379	87	9.9E-03	2.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.0E+02	4.2E+00	1.5E+02	-6.54	-6.85	-8.51	-1.14	0.64	0.0%	0.0%	3.1E-26
775	1120-21-4	undecane	156	-32	8.4E+01	1.1E-01	5.5E+05	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.4E+02	3.3E+00	1.2E+02	-10.14	-9.85	-12.64	-0.07	2.41	0.0%	0.0%	2.1E-72
776	598-56-1	ethyldimethylamine	73	-97	6.6E+04	1.1E+05	3.4E+00	10.0	3.5E-06	5.1E-08	3.5E-06	conf	conf	2.5E+02	3.5E+00	1.2E+02	-9.05	-8.76	-10.49	-1.46	0.70	0.0%	0.0%	2.3E-38
777	25013-15-4	vinyltoluene	118	-30	2.8E+02	1.2E+02	2.8E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.7E+02	3.7E+00	1.3E+02	-9.58	-9.28	-11.21	-2.56	0.27	0.0%	0.0%	2.3E-35
778	127-95-7	potassium hydrogen oxalate	128	87	9.9E-03	8.8E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.0E+02	4.1E+00	1.5E+02	-6.57	-6.86	-8.51	-0.20	0.68	0.0%	0.0%	8.5E-33
779	140-11-4	benzyl acetate	150	-1	2.5E+01	2.9E+03	1.2E+02	14.0	3.5E-06	6.7E-07	3.5E-07	conf	conf	3.6E+02	5.0E+00	1.8E+02	-8.47	-8.26	-9.58	-1.87	0.63	0.0%	0.0%	1.5E-28
780	280-57-9	1,4-diazabicyclooctane	112	21	6.6E+00	1.0E+06	3.2E-01	9.0	3.5E-06	3.7E-09	3.5E-06	conf	conf	2.3E+02	3.2E+00	1.1E+02	-6.72	-6.79	-7.74	-0.30	0.61	0.0%	0.0%	1.0E-26
781	16090-02-1	disodium 4,4'-bis[(4-anilino-6-morpholino-1,3,5-triazin-2-yl)amino]stilbene-2,2'-disulphonate	925	87	9.9E-03	6.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.9E+02	4.1E+00	1.5E+02	-6.54	-6.86	-8.53	-0.59	0.82	0.0%	0.0%	4.1E-30
782	19372-44-2	bis(pentane-2,4-dionato)calcium	238	87	9.9E-03	1.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.9E+02	4.1E+00	1.5E+02	-6.56	-6.87	-8.52	-1.29	0.48	0.0%	0.0%	2.6E-25
783	3164-85-0	potassium 2-ethylhexanoate	182	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.9E+02	4.1E+00	1.5E+02	-6.56	-6.87	-8.52	-0.86	0.45	0.0%	0.0%	3.6E-28
784	1003-14-1	propyloxirane	86	-74	1.2E+04	1.9E+04	2.2E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.5E+02	4.9E+00	1.8E+02	-9.45	-9.15	-10.84	-0.59	0.39	0.0%	0.0%	6.7E-49
785	1120-49-6	didecylamine	298	94	2.7E-03	2.1E-03	4.7E+08	10.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.3E+02	3.2E+00	1.1E+02	-8.87	-9.02	-10.16	-5.30	0.61	0.0%	0.0%	1.8E-12
786	98-51-1	4-tert-butyltoluene	148	-10	7.9E+01	9.3E+00	2.8E+04	14.0	3.5E-06	4.5E-08	1.1E-07	conf	conf	2.3E+02	3.2E+00	1.1E+02	-9.85	-9.56	-11.69	-2.50	0.70	0.0%	0.0%	1.3E-39
787	107-43-7	betaine	117	160	7.1E-05	1.0E+06	1.2E-03	1.9	3.5E-06	3.5E-06	1.1E-06	conf	conf	3.9E+02	5.4E+00	2.0E+02	-6.79	-8.24	-10.18	0.03	0.86	0.0%	0.0%	1.7E-48
788	100-61-8	N-methylaniline	107	-21	5.8E+01	2.6E+03	4.2E+01	5.0	3.5E-06	5.8E-09	3.5E-07	conf	conf	2.3E+02	3.2E+00	1.1E+02	-7.10	-6.86	-7.81	-1.75	1.17	0.0%	0.0%	2.5E-18
789	763-69-9	ethyl 3-ethoxypropionate	146	-27	2.0E+02	1.8E+04	1.2E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	3.8E+02	5.3E+00	2.0E+02	-9.06	-8.93	-10.28	-0.38	0.62	0.0%	0.0%	1.1E-45
790	176969-34-9	3-(difluoromethyl)-1-methyl-1H-pyrazole-4-carboxylic acid	176	83	3.3E-01	7.7E+03	6.9E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.7E+02	5.1E+00	1.9E+02	-7.72	-7.73	-9.70	-0.58	0.32	0.0%	0.0%	4.1E-39
791	99-66-1	2-propylvaleric acid	144	38	1.1E+01	5.1E+03	9.1E+02	4.9	3.5E-06	1.6E-06	3.5E-07	conf	conf	3.7E+02	5.2E+00	1.9E+02	-7.85	-8.11	-9.95	-1.34	0.70	0.0%	0.0%	4.4E-35
792	25307-17-9	2,2'-(octadec-9-enylimino)bisethanol	356	174	4.3E-09	8.5E-04	4.3E+06	9.3	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.5E+02	3.5E+00	1.3E+02	-8.29	-9.02	-9.84	-4.10	0.73	0.0%	0.0%	1.3E-16
793	142-22-3	diallyl 2,2'-oxydiethyl dicarbonate	274	43	8.6E-03	5.5E+02	3.5E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.6E+02	5.0E+00	1.9E+02	-7.64	-7.86	-9.75	-1.84	0.82	0.0%	0.0%	7.1E-30
794	124-68-5	2-amino-2-methylpropanol	89	-9	6.6E+01	9.2E+05	1.8E-01	9.5	3.5E-06	3.5E-06	3.5E-06	conf	conf	3.8E+02	5.3E+00	2.0E+02	-8.37	-8.44	-10.22	-0.58	0.22	0.0%	0.0%	1.7E-43
795	97-00-7	1-chloro-2,4-dinitrobenzene	203	93	6.5E-02	5.9E+01	1.9E+02	14.0	3.5E-06	3.2E-08	1.1E-07	conf	conf	2.4E+02	3.4E+00	1.2E+02	-7.39	-7.12	-8.32	-3.11	0.65	0.0%	0.0%	4.6E-14
796	112-85-6	docosanoic acid	341	159	6.5E-05	2.0E-04	8.1E+09	4.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.4E+02	3.4E+00	1.2E+02	-8.36	-8.42	-9.28	-2.17	0.22	0.0%	0.0%	1.6E-24
797	109-01-3	1-methylpiperazine	100	19	9.3E+02	1.0E+06	2.6E-01	9.0	3.5E-06	2.2E-09	3.5E-06	conf	conf	2.2E+02	3.1E+00	1.1E+02	-7.31	-7.04	-8.03	0.01	0.32	0.0%	0.0%	7.3E-31
798	91161-71-6	Terbinafin	291	147	7.8E-05	2.0E+00	6.5E+05	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	2.7E+02	3.8E+00	1.4E+02	-8.43	-8.60	-9.91	-4.22	0.64	0.0%	0.0%	2.1E-16
799	95-96-5	dilactide	144	26	2.1E-02	1.5E+07	4.5E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	3.8E+02	5.2E+00	1.9E+02	-7.42	-8.60	-10.23	-0.25	0.50	0.0%	0.0%	1.8E-46
800	108-30-5	succinic anhydride	100	-53	2.4E-01	7.3E+03	6.5E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	3.8E+02	5.2E+00	1.9E+02	-8.13	-8.46	-10.24	-0.71	0.34	0.0%	0.0%	1.6E-42
801	553-86-6	(3H)-benzofuran-2-one	134	31	2.2E+00	2.6E+03	3.0E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.6E+02	5.0E+00	1.8E+02	-8.06	-7.86	-9.69	-1.69	1.04	0.0%	0.0%	1.4E-30
802	90-43-7	biphenyl-2-ol	170	87	9.4E-02	2.5E+02	1.9E+03	10.0	3.5E-06	5.7E-07	3.5E-08	conf	conf	3.2E+02	4.5E+00	1.6E+02	-7.88	-7.65	-9.42	-2.55	0.80	0.0%	0.0%	4.7E-23
803	109-09-1	2-chloropyridine	114	-13	2.1E+02	1.0E+03	2.8E+01	1.0	3.5E-06	2.2E-09	1.1E-07	conf	conf	2.1E+02	3.0E+00	1.0E+02	-5.97	-6.75	-7.69	-1.47	1.69	0.0%	0.0%	3.1E-19
804	593-56-6	methoxyammonium chloride	84	87	9.9E-03	5.8E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E+02	3.8E+00	1.4E+02	-6.61	-6.90	-8.54	-3.20	0.25	0.0%	0.0%	1.2E-14
805	124-64-1	tetrakis(hydroxymethyl)phosphonium chloride	191	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E+02	3.8E+00	1.4E+02	-6.59	-6.90	-8.55	-2.97	2.08	0.0%	0.0%	8.2E-16
806	92-15-9	2'-methoxyacetoacetanilide	207	138	1.2E-03	5.7E+03	3.4E+00	0.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.5E+02	4.9E+00	1.8E+02	-6.52	-7.71	-9.70	-1.72	1.17	0.0%	0.0%	2.3E-30
807	126-81-8	5,5-dimethylcyclohexane-1,3-dione	140	41	6.3E-01	5.8E+04	2.0E+01	5.4	3.5E-06	1.4E-07	1.1E-06	conf	conf	2.8E+02	3.9E+00	1.4E+02	-6.66	-7.15	-8.73	-0.59	0.87	0.0%	0.0%	1.5E-31
808	18423-20-6	3,5,7-triaza-1-azoniatricyclo[3.3.1.13,7]decane nitrate	203	87	9.9E-03	1.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E+02	3.8E+00	1.4E+02	-6.60	-6.90	-8.55	-1.36	0.64	0.0%	0.0%	4.8E-25
809	629-82-3	dioctyl ether	242	29	1.1E+00	7.2E-02	8.7E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.2E+02	3.1E+00	1.1E+02	-10.03	-9.87	-12.18	-0.47	0.75	0.0%	0.0%	4.1E-63
810	124-13-0	octanal	128	-31	2.0E+02	5.0E+02	6.0E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.2E+02	4.4E+00	1.6E+02	-9.54	-9.29	-10.79	-2.19	0.41	0.0%	0.0%	5.6E-35
811	5343-92-0	pentane-1,2-diol	104	-10	7.1E-01	5.4E+04	1.6E+00	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	3.6E+02	5.0E+00	1.9E+02	-8.02	-8.59	-10.26	0.66	0.53	0.0%	0.0%	3.5E-55
812	1120-24-7	decyldimethylamine	185	1	1.4E+01	1.7E+00	2.9E+04	10.1	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.2E+02	3.1E+00	1.1E+02	-9.93	-9.63	-11.85	-3.78	0.78	0.0%	0.0%	4.7E-31
813	13361-34-7	2-ethylhexyl cyanoacetate	197	44	3.4E-01	6.0E+01	7.8E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	3.3E+02	4.6E+00	1.7E+02	-8.71	-8.49	-9.90	-1.91	0.40	0.0%	0.0%	1.9E-30
814	79-39-0	methacrylamide	85	33	3.9E+00	2.8E+05	5.5E-01	-0.4	3.5E-06	3.5E-06	1.1E-06	conf	conf	3.6E+02	5.0E+00	1.8E+02	-7.13	-8.45	-10.25	-1.28	0.06	0.0%	0.0%	6.8E-38
815	19438-60-9	hexahydro-4-methylphthalic anhydride	168	5	4.4E+00	1.5E+01	3.9E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	3.4E+02	4.7E+00	1.7E+02	-9.84	-9.62	-11.02	-0.67	0.29	0.0%	0.0%	7.5E-50
816	137862-53-4	N-Pentanoyl-N-{[2'-(1H-tetrazol-5-yl)biphenyl-4-yl]methyl}-L-valine	436	294	1.1E-13	1.3E-02	4.5E+03	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	2.7E+02	3.8E+00	1.4E+02	-5.85	-6.82	-8.47	-0.85	0.55	0.0%	0.0%	6.5E-28
817	109-87-5	dimethoxymethane	76	-95	5.5E+04	2.4E+05	6.5E-01	14.0	3.5E-06	9.8E-07	3.5E-07	conf	conf	3.3E+02	4.6E+00	1.7E+02	-9.19	-8.85	-10.44	0.33	0.70	0.0%	0.0%	9.2E-54
818	626-43-7	3,5-dichloroaniline	162	46	1.1E+00	1.8E+02	2.3E+02	2.0	3.5E-06	2.2E-09	3.5E-08	conf	conf	2.0E+02	2.8E+00	9.8E+01	-6.00	-6.73	-7.68	-2.38	0.84	0.0%	0.0%	1.8E-14
819	5567-15-7	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-chloro-2,5-dimethoxyphenyl)-3-oxobutyramide]	819	350	2.4E-23	1.9E-06	3.5E+07	-1.0	3.5E-06	1.2E-07	1.1E-08	conf	conf	2.6E+02	3.6E+00	1.3E+02	-8.73	-8.73	-8.73	-1.44	0.35	0.0%	0.0%	1.1E-25
820	866-84-2	tripotassium citrate	306	87	9.9E-03	2.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+02	3.6E+00	1.3E+02	-6.61	-6.92	-8.57	0.34	0.43	0.0%	0.0%	2.1E-37
821	99-76-3	methyl 4-hydroxybenzoate	152	51	1.1E-01	5.6E+03	1.0E+02	8.5	3.5E-06	1.1E-05	3.5E-06	conf	conf	3.5E+02	4.9E+00	1.8E+02	-8.99	-9.46	-10.81	-1.27	0.28	0.0%	0.0%	1.4E-42
822	75-37-6	1,1-difluoroethane	66	-158	5.1E+05	8.0E+03	1.3E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.4E+02	3.3E+00	1.2E+02	-10.15	-9.71	-12.06	-0.85	0.36	0.0%	0.0%	4.6E-58
823	75-26-3	2-bromopropane	123	-91	2.9E+04	2.7E+03	1.2E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.4E+02	3.4E+00	1.2E+02	-10.01	-9.69	-12.16	-1.26	0.20	0.0%	0.0%	5.4E-55
824	112-40-3	dodecane	170	-21	3.1E+01	3.5E-02	1.7E+06	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.0E+02	2.8E+00	9.8E+01	-10.20	-9.93	-12.69	-0.07	2.47	0.0%	0.0%	6.4E-73
825	15375-84-5	disodium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4-)-N,N',O,O',ON,ON']manganate(2-)	389	87	9.9E-03	2.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.5E+02	3.5E+00	1.3E+02	-6.61	-6.93	-8.59	-0.47	0.73	0.0%	0.0%	2.2E-31
826	106-79-6	dimethyl sebacate	230	-27	1.5E+00	9.7E+01	2.2E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.8E+02	3.9E+00	1.4E+02	-8.61	-8.37	-9.61	-2.25	0.34	0.0%	0.0%	3.6E-26
827	2186-92-7	p-(dimethoxymethyl)anisole	182	23	6.5E+00	1.9E+03	3.3E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.2E+02	4.5E+00	1.7E+02	-8.45	-8.27	-9.81	-0.78	0.28	0.0%	0.0%	2.2E-38
828	115-19-5	2-methylbut-3-yn-2-ol	84	-35	2.2E+03	2.5E+05	2.8E+00	13.6	3.5E-06	1.1E-08	3.5E-06	conf	conf	2.0E+02	2.8E+00	9.8E+01	-8.00	-7.72	-8.84	0.03	0.43	0.0%	0.0%	4.7E-37
829	102-82-9	tributylamine	185	1	2.1E+01	3.3E+01	2.9E+04	11.0	3.5E-06	9.8E-09	1.1E-07	conf	conf	2.0E+02	2.7E+00	9.4E+01	-9.33	-9.05	-10.76	-1.58	0.70	0.0%	0.0%	1.4E-39
830	55-63-0	glycerol trinitrate	227	50	3.6E+00	2.6E+04	3.2E+01	14.0	3.5E-06	1.5E-06	1.1E-07	conf	conf	3.3E+02	4.5E+00	1.7E+02	-8.10	-7.89	-9.87	-2.17	0.90	0.0%	0.0%	2.0E-28
831	17095-24-8	tetrasodium 4-amino-5-hydroxy-3,6-bis[[4-[[2-(sulphonatooxy)ethyl]sulphonyl]phenyl]azo]naphthalene-2,7-disulph	992	87	9.9E-03	6.9E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.5E+02	3.5E+00	1.3E+02	-6.61	-6.93	-8.60	-1.05	0.68	0.0%	0.0%	2.2E-27
832	108-59-8	dimethyl malonate	132	-108	1.2E+02	1.2E+05	8.1E-01	13.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	3.4E+02	4.7E+00	1.7E+02	-8.68	-8.54	-10.26	-0.74	0.64	0.0%	0.0%	2.0E-42
833	23783-42-8	3,6,9,12-tetraoxotridecanol	208	62	1.4E-02	2.0E+05	1.9E-02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.2E+02	4.5E+00	1.6E+02	-6.52	-7.57	-9.72	1.45	0.61	0.0%	0.0%	1.1E-29
834	126-33-0	tetrahydrothiophene 1,1-dioxide	120	16	5.5E-01	3.4E+04	5.8E-01	14.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	1.9E+02	2.7E+00	9.3E+01	-6.67	-6.76	-7.71	-0.21	0.56	0.0%	0.0%	4.2E-27
835	123-91-1	1,4-dioxane	88	-64	5.4E+03	4.4E+04	4.8E-01	14.0	3.5E-06	3.7E-09	3.5E-07	conf	conf	1.9E+02	2.7E+00	9.4E+01	-8.70	-8.40	-9.88	0.85	0.70	0.0%	0.0%	2.1E-53
836	15307-93-4	2,6-dichloro-N-phenylaniline	238	100	1.0E-02	2.9E+00	3.8E+04	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	2.7E+02	3.8E+00	1.4E+02	-8.75	-8.55	-9.97	-3.05	0.13	0.0%	0.0%	2.3E-23
837	1193-24-4	6-hydroxy-1H-pyrimidin-4-one	112	83	2.3E-01	6.7E+04	3.0E+00	5.4	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.8E+02	4.0E+00	1.4E+02	-6.40	-7.34	-9.16	-1.26	1.47	0.0%	0.0%	7.1E-30
838	821-06-7	(E)-1,4-dibromobut-2-ene	214	-16	3.0E+01	8.9E+02	6.0E+02	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.7E+02	3.8E+00	1.4E+02	-8.82	-8.58	-9.86	-1.24	0.82	0.0%	0.0%	3.8E-35
839	778-94-9	2-nitro-4-(trifluoromethyl)benzonitrile	216	81	1.8E-01	1.6E+02	2.1E+02	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	3.1E+02	4.3E+00	1.6E+02	-8.30	-8.10	-9.81	-2.70	0.50	0.0%	0.0%	1.5E-24
840	119-64-2	1,2,3,4-tetrahydronaphthalene	132	-4	3.3E+01	2.4E+01	9.1E+03	14.0	3.5E-06	2.4E-08	1.1E-07	conf	conf	1.9E+02	2.7E+00	9.3E+01	-9.47	-9.18	-10.96	-2.25	0.70	0.0%	0.0%	8.0E-36
841	145783-14-8	4,6-dichloro-5-nitro-2-(propylthio)pyrimidine	268	145	6.8E-04	2.0E+01	1.5E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.7E+02	3.8E+00	1.4E+02	-7.64	-7.54	-9.27	-4.31	0.36	0.0%	0.0%	6.7E-13
842	118-58-1	benzyl salicylate	228	115	2.4E-03	1.1E+02	2.0E+04	9.8	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.8E+02	3.9E+00	1.4E+02	-8.20	-8.37	-9.90	-2.86	0.24	0.0%	0.0%	4.3E-24
843	4813-57-4	octadecyl acrylate	325	99	1.1E-03	2.0E-04	1.2E+09	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.9E+02	2.6E+00	9.1E+01	-8.86	-8.98	-10.23	-0.85	0.26	0.0%	0.0%	3.2E-41
844	103-74-2	2-(2-pyridyl)ethanol	123	38	1.2E+00	7.0E+03	2.4E+00	5.0	3.5E-06	2.7E-08	3.5E-07	conf	conf	2.0E+02	2.8E+00	9.9E+01	-6.31	-6.89	-8.09	-0.62	1.11	0.0%	0.0%	7.7E-27
845	81-84-5	naphthalene-1,8-dicarboxylic anhydride	198	93	5.5E-05	1.1E+02	1.7E+03	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	3.0E+02	4.1E+00	1.5E+02	-7.16	-8.08	-9.84	-1.63	0.29	0.0%	0.0%	4.4E-32
846	109-54-6	3-chloropropyl(dimethyl)amine	122	-50	1.1E+03	8.6E+04	1.9E+01	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.7E+02	3.8E+00	1.4E+02	-8.42	-8.17	-9.49	-2.10	0.76	0.0%	0.0%	2.6E-26
847	256-96-2	5H-dibenz[b,f]azepine	193	104	7.7E-04	1.7E+01	1.1E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.7E+02	3.8E+00	1.4E+02	-7.74	-7.67	-9.31	-2.42	0.25	0.0%	0.0%	3.9E-23
848	56-81-5	glycerol	92	19	1.1E-02	1.0E+06	2.2E-02	14.0	3.5E-06	1.2E-06	3.5E-06	conf	conf	3.1E+02	4.3E+00	1.6E+02	-6.91	-7.94	-9.82	0.94	0.39	0.0%	0.0%	1.3E-53
849	95-82-9	2,5-dichloroaniline	162	46	2.0E+00	1.8E+02	2.3E+02	2.0	3.5E-06	2.3E-09	3.5E-08	conf	conf	1.8E+02	2.6E+00	8.9E+01	-6.01	-6.77	-7.73	-2.44	0.73	0.0%	0.0%	2.2E-14
850	115-95-7	linalyl acetate	196	-2	1.7E+01	3.6E+02	2.5E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.8E+02	3.8E+00	1.4E+02	-9.76	-9.57	-10.73	-1.57	0.40	0.0%	0.0%	2.2E-39
851	81-13-0	dexpanthenol	205	161	2.0E-06	1.3E+05	1.2E-02	-1.5	3.5E-06	1.1E-06	1.1E-06	conf	conf	3.0E+02	4.2E+00	1.6E+02	-6.49	-7.87	-9.76	0.17	1.15	0.0%	0.0%	6.5E-46
852	7695-91-2	3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-benzopyran-6-yl acetate	473	203	5.4E-06	1.8E-06	1.8E+12	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+02	2.5E+00	8.8E+01	-8.74	-8.74	-8.74	-0.34	1.01	0.0%	0.0%	1.8E-33
853	95-80-7	4-methyl-m-phenylenediamine	122	67	7.6E-02	3.5E+04	1.4E+00	5.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	1.8E+02	2.5E+00	8.8E+01	-6.20	-6.83	-7.77	-1.05	1.44	0.0%	0.0%	4.3E-22
854	14025-21-9	disodium [[N,N'-ethylenediylbis[N-(carboxylatomethyl)glycinato]](4-)-N,N',O,O',ON,ON']zincate(2-)	400	87	9.9E-03	2.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+02	3.3E+00	1.2E+02	-6.64	-6.96	-8.62	-0.48	0.71	0.0%	0.0%	1.5E-31
855	530-48-3	1,1-diphenylethylene	180	21	8.4E-01	1.0E+01	7.2E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.7E+02	3.8E+00	1.4E+02	-9.39	-9.17	-10.32	-2.70	0.18	0.0%	0.0%	6.3E-28
856	136-30-1	sodium dibutyldithiocarbamate	227	87	9.9E-03	1.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+02	3.3E+00	1.2E+02	-6.66	-6.96	-8.61	-2.19	1.31	0.0%	0.0%	2.2E-20
857	112-50-5	2-(2-(2-ethoxyethoxy)ethoxy)ethanol	178	36	3.0E-01	3.8E+06	1.1E-01	14.0	3.5E-06	7.0E-07	3.5E-07	conf	conf	2.9E+02	4.1E+00	1.5E+02	-6.43	-7.44	-9.49	1.21	0.89	0.0%	0.0%	3.8E-28
858	111-36-4	butyl isocyanate	99	-39	2.6E+03	7.7E+03	1.8E+02	14.0	3.5E-06	2.4E-07	3.5E-06	conf	conf	2.4E+02	3.3E+00	1.2E+02	-9.25	-8.97	-10.50	-1.38	0.48	0.0%	0.0%	4.1E-39
859	15307-86-5	diclofenac	296	175	8.2E-06	1.6E+01	1.0E+04	4.4	3.5E-06	2.2E-09	1.1E-07	conf	conf	1.8E+02	2.5E+00	8.8E+01	-6.69	-6.84	-7.79	-1.69	0.63	0.0%	0.0%	1.6E-18
860	101-72-4	N-isopropyl-N'-phenyl-p-phenylenediamine	226	104	9.5E-03	1.3E+01	1.9E+03	4.6	3.5E-06	3.5E-06	3.5E-07	conf	conf	3.1E+02	4.4E+00	1.6E+02	-7.82	-8.55	-10.41	-2.31	1.01	0.0%	0.0%	2.8E-31
861	103-83-3	benzyldimethylamine	135	-13	1.2E+02	1.7E+03	5.6E+01	9.0	3.5E-06	1.7E-07	1.1E-07	conf	conf	2.4E+02	3.3E+00	1.2E+02	-8.80	-8.53	-9.88	-1.99	0.85	0.0%	0.0%	8.9E-30
862	2312-35-8	propargite	350	169	5.3E-08	8.7E-02	5.2E+04	14.0	3.5E-06	6.2E-09	3.5E-07	conf	conf	1.8E+02	2.5E+00	8.8E+01	-6.91	-7.41	-8.39	-2.36	1.44	0.0%	0.0%	3.4E-18
863	78-69-3	3,7-dimethyloctan-3-ol	158	-12	9.5E+00	4.6E+01	4.0E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.7E+02	3.8E+00	1.4E+02	-9.56	-9.31	-10.62	-1.78	0.18	0.0%	0.0%	7.2E-37
864	2528-61-2	heptanoyl chloride	149	-18	8.5E+02	1.5E+02	9.5E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.0E+02	2.8E+00	9.8E+01	-9.84	-9.48	-11.75	-1.68	1.04	0.0%	0.0%	3.6E-47
865	756-79-6	dimethyl methylphosphonate	124	-48	1.2E+02	7.1E+04	2.6E-01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	3.0E+02	4.1E+00	1.5E+02	-8.27	-8.09	-9.78	-1.54	1.62	0.0%	0.0%	2.3E-32
866	105-74-8	dilauroyl peroxide	399	56	2.7E-04	1.3E-04	2.2E+10	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+02	2.5E+00	8.6E+01	-8.64	-8.58	-9.10	-6.45	1.13	0.0%	0.0%	1.6E-25
867	149-30-4	benzothiazole-2-thiol	167	86	5.6E-03	1.4E+02	7.2E+02	6.9	3.5E-06	5.4E-09	3.5E-07	conf	conf	1.8E+02	2.5E+00	8.8E+01	-7.09	-6.96	-7.93	-2.45	0.76	0.0%	0.0%	2.5E-15
868	100-63-0	phenylhydrazine	108	25	5.1E+00	3.7E+05	6.2E+00	9.0	3.5E-06	4.6E-08	3.5E-07	conf	conf	2.0E+02	2.8E+00	1.0E+02	-6.83	-6.94	-8.27	-2.52	0.48	0.0%	0.0%	1.1E-16
869	304-59-6	potassium sodium tartrate	210	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+02	3.2E+00	1.2E+02	-6.67	-6.97	-8.62	-0.41	0.48	0.0%	0.0%	4.7E-32
870	661-95-0	1,2-dibromo-1,1,2,3,3,3-hexafluoropropane	310	-38	6.3E+03	5.1E+01	8.5E+03	14.0	3.5E-06	1.1E-07	1.1E-07	conf	conf	1.8E+02	2.5E+00	8.8E+01	-10.03	-9.67	-12.34	-2.03	0.11	0.0%	0.0%	1.9E-49
871	328-84-7	3,4-dichloro-α,α,α-trifluorotoluene	215	1	1.8E+02	8.3E+00	1.7E+04	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	1.8E+02	2.5E+00	8.8E+01	-10.00	-9.60	-12.12	-2.69	0.35	0.0%	0.0%	1.3E-41
872	2043-57-4	1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-8-iodooctane	474	-16	3.9E+02	6.2E-04	4.3E+06	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.8E+02	2.5E+00	8.8E+01	-10.09	-9.91	-12.57	-3.23	0.32	0.0%	0.0%	7.2E-41
873	366-18-7	2,2'-bipyridyl	156	78	3.8E-01	3.9E+03	2.4E+01	4.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.9E+02	4.1E+00	1.5E+02	-6.90	-7.87	-9.82	-1.64	1.03	0.0%	0.0%	8.2E-32
874	80-53-5	p-menthane-1,8-diol	172	49	2.8E-02	1.4E+05	2.1E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.9E+02	4.0E+00	1.5E+02	-7.16	-8.10	-9.85	-1.08	0.96	0.0%	0.0%	2.8E-36
875	137-16-6	sodium N-lauroylsarcosinate	293	87	9.9E-03	2.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+02	3.2E+00	1.1E+02	-6.66	-6.97	-8.63	-1.25	0.26	0.0%	0.0%	2.9E-26
876	110-03-2	2,5-dimethylhexane-2,5-diol	146	19	5.8E-01	1.5E+05	3.3E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.9E+02	4.1E+00	1.5E+02	-7.50	-8.12	-9.85	-0.69	0.38	0.0%	0.0%	2.1E-39
877	134-32-7	1-naphthylamine	143	71	1.5E-01	8.1E+01	1.8E+02	14.0	3.5E-06	8.3E-09	3.5E-07	conf	conf	1.8E+02	2.5E+00	8.8E+01	-7.53	-7.25	-8.32	-2.41	0.56	0.0%	0.0%	1.5E-17
878	34090-76-1	tetrahydro-4-methylphthalic anhydride	166	25	2.6E+00	5.3E+03	4.6E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.9E+02	4.0E+00	1.5E+02	-9.17	-9.01	-10.43	-1.00	0.17	0.0%	0.0%	1.0E-41
879	100-37-8	2-diethylaminoethanol	117	-16	8.6E+01	4.0E+05	1.1E+00	10.0	3.5E-06	7.8E-08	3.5E-06	conf	conf	2.1E+02	3.0E+00	1.1E+02	-7.42	-7.17	-8.58	-0.54	0.70	0.0%	0.0%	6.9E-31
880	1709-70-2	3,3',3'',5,5',5''-hexa-tert-butyl-α,α',α''-(mesitylene-2,4,6-triyl)tri-p-cresol	775	350	4.2E-20	3.7E-14	1.5E+17	10.8	3.5E-06	1.1E-06	1.1E-07	conf	conf	1.7E+02	2.4E+00	8.4E+01	-16.43	-16.43	-16.43	-0.97	1.28	0.0%	0.0%	2.2E-108
881	75-36-5	acetyl chloride	78	-81	4.0E+04	5.6E+04	3.4E-01	14.0	3.5E-06	4.5E-06	3.5E-07	conf	conf	2.9E+02	4.1E+00	1.5E+02	-9.64	-9.15	-11.37	-1.70	0.97	0.0%	0.0%	1.1E-43
882	6271-80-3	4'-chloro-2-nitrobiphenyl	234	123	1.1E-03	2.1E+00	1.7E+04	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	2.1E+02	2.9E+00	1.0E+02	-7.67	-7.45	-8.89	-5.31	4.62	0.0%	0.1%	1.6E-07
883	3039-83-6	sodium ethylenesulphonate	130	87	9.9E-03	9.0E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+02	3.1E+00	1.1E+02	-6.69	-6.99	-8.63	-0.56	1.59	0.0%	0.0%	4.6E-31
884	15834-04-5	2,2-bis[[(1-oxopentyl)oxy]methyl]propane-1,3-diyl divalerate	473	150	1.2E-06	3.4E-02	5.5E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.0E+02	2.7E+00	9.7E+01	-8.61	-9.08	-9.95	-0.87	0.96	0.0%	0.0%	9.1E-39
885	110964-79-9	4-(methylsulfonyl)-2-nitrobenzoic acid	245	174	1.1E-05	2.9E+02	8.3E-01	1.6	3.5E-06	3.5E-06	3.5E-07	conf	conf	3.0E+02	4.2E+00	1.5E+02	-6.98	-8.27	-10.33	-0.29	0.41	0.0%	0.0%	6.2E-47
886	15687-27-1	ibuprofen	206	94	2.5E-02	2.8E+01	6.2E+03	4.3	3.5E-06	1.7E-08	3.5E-07	conf	conf	1.8E+02	2.5E+00	8.8E+01	-6.81	-6.96	-8.09	-1.69	0.73	0.0%	0.0%	3.3E-20
887	20298-69-5	cis-2-tert-butylcyclohexyl acetate	198	11	7.1E+00	4.3E-01	2.6E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.2E+02	3.1E+00	1.1E+02	-10.38	-10.10	-12.76	-2.13	0.32	0.0%	0.0%	2.3E-52
888	60142-95-2	1-(aminomethyl)cyclohexaneacetic acid hydrochloride	208	87	9.9E-03	1.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+02	3.1E+00	1.1E+02	-6.69	-6.99	-8.64	-1.84	0.64	0.0%	0.0%	1.2E-22
889	29964-84-9	isodecyl methacrylate	226	14	1.6E+00	1.5E+00	4.2E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.0E+02	2.8E+00	9.9E+01	-10.04	-9.79	-11.42	-2.54	1.77	0.0%	0.0%	3.6E-37
890	6535-46-2	3-hydroxy-N-(o-tolyl)-4-[(2,4,5-trichlorophenyl)azo]naphthalene-2-carboxamide	485	290	1.1E-14	1.7E-04	1.6E+09	9.2	3.5E-06	3.5E-08	3.5E-08	conf	conf	1.7E+02	2.4E+00	8.1E+01	-8.27	-8.34	-8.54	-5.33	0.67	0.0%	0.0%	2.3E-06

891	109-83-1	2-methylaminoethanol	75	-36	1.1E+02	1.0E+06	7.1E-02	9.9	3.5E-06	3.5E-06	3.5E-06	conf	conf	3.0E+02	4.1E+00	1.5E+02	-8.52	-8.51	-10.32	-1.28	0.33	0.0%	0.0%	1.9E-38
892	18379-25-4	trichloro(2,4,4-trimethylpentyl)silane	248	-8	1.1E+02	1.8E+02	1.8E+05	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.1E+02	2.9E+00	1.0E+02	-9.96	-9.71	-11.38	-1.17	1.10	0.0%	0.0%	1.5E-48
893	186817-80-1	606-097-1	202	28	1.2E-01	8.0E+02	4.9E+02	12.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.9E+02	4.0E+00	1.5E+02	-9.04	-8.92	-10.41	-1.24	0.59	0.0%	0.0%	1.7E-39
894	67786-25-8	tetrasodium 4,4'-bis[[4-[bis(2-hydroxypropyl)amino]-6-[(4-sulphonatophenyl)amino]-1,3,5-triazin-2-yl]amino]-stilbe	1221	87	9.9E-03	8.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+02	3.0E+00	1.1E+02	-6.66	-6.99	-8.66	-0.63	0.58	0.0%	0.0%	9.2E-31
895	873-94-9	3,3,5-trimethylcyclohexan-1-one	140	7	1.2E+02	1.8E+03	2.6E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.7E+02	3.8E+00	1.4E+02	-9.35	-9.12	-10.28	-1.20	0.29	0.0%	0.0%	8.7E-39
896	1758-73-2	aminoiminomethanesulphinic acid	108	87	9.9E-03	7.5E+02	3.0E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.2E+02	3.0E+00	1.1E+02	-8.41	-8.99	-10.49	-0.89	0.42	0.0%	0.0%	4.8E-43
897	85-68-7	benzyl butyl phthalate	312	61	5.9E-03	2.3E+00	6.9E+04	14.0	3.5E-06	7.5E-07	3.5E-07	conf	conf	2.3E+02	3.2E+00	1.1E+02	-8.68	-8.52	-9.94	-3.05	0.51	0.0%	0.0%	3.5E-23
898	16111-62-9	bis(2-ethylhexyl) peroxydicarbonate	346	64	3.0E-04	1.2E+00	9.3E+06	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.8E+02	2.5E+00	8.7E+01	-8.37	-8.78	-9.57	-1.45	0.38	0.0%	0.0%	1.9E-31
899	894-86-0	disodium [2,2'-bi-1H-indole]-3,3'-diolate	308	87	9.9E-03	2.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+02	3.0E+00	1.1E+02	-6.68	-7.00	-8.65	-6.00	0.64	0.0%	0.0%	1.1E-22
900	599-64-4	4-(α,α-dimethylbenzyl)phenol	212	103	3.9E-03	1.3E+01	1.3E+04	10.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.3E+02	3.2E+00	1.2E+02	-8.03	-7.85	-9.44	-2.96	0.10	0.0%	0.0%	1.1E-20
901	55589-62-3	6-methyl-1,2,3-oxathiazin-4(3H)-one 2,2-dioxide, potassium salt	201	225	5.8E-09	8.8E+08	5.0E-03	8.2	3.5E-06	8.2E-07	3.5E-06	conf	conf	2.7E+02	3.8E+00	1.4E+02	-6.64	-7.75	-9.63	0.36	0.64	0.0%	0.0%	1.4E-46
902	4767-03-7	2,2-bis(hydroxymethyl)propionic acid	134	86	1.7E-04	8.8E+05	8.5E-02	4.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.9E+02	4.0E+00	1.5E+02	-6.99	-8.44	-10.32	0.36	1.17	0.0%	0.0%	7.7E-53
903	6259-76-3	hexyl salicylate	222	100	3.3E-03	2.5E+01	1.1E+05	9.8	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.2E+02	3.1E+00	1.1E+02	-8.65	-8.61	-10.02	-3.20	0.26	0.0%	0.0%	1.1E-22
904	4698-11-7	10-methoxy-5H-dibenz[b,f]azepine	223	126	1.4E-03	2.1E+01	2.2E+03	0.8	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.8E+02	3.8E+00	1.4E+02	-7.35	-7.96	-9.86	-2.70	0.80	0.0%	0.0%	7.4E-25
905	18282-59-2	4-bromo-1,2-dichlorobenzene	226	37	7.2E+00	1.3E+01	1.5E+04	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	1.8E+02	2.5E+00	8.9E+01	-9.39	-9.11	-10.85	-2.63	0.19	0.0%	0.0%	3.6E-32
906	212322-56-0	Ethyl N-[3-amino-4-(methylamino)benzoyl]-N-pyridin-2-yl-β-alaninate	342	206	1.1E-07	9.4E+02	8.7E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.8E+02	3.8E+00	1.4E+02	-6.67	-7.80	-9.79	-1.40	0.76	0.0%	0.0%	2.3E-33
907	29518-11-4	4-phenylmorpholin-3-one	177	102	1.1E-02	3.6E+02	3.5E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.8E+02	3.8E+00	1.4E+02	-7.64	-7.80	-9.81	-1.67	1.25	0.0%	0.0%	1.3E-31
908	7534-94-3	exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl methacrylate	222	54	1.4E+00	5.6E+01	5.8E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.4E+02	3.3E+00	1.2E+02	-9.72	-9.55	-10.72	-2.82	0.20	0.0%	0.0%	7.5E-30
909	682-09-7	2,2-bis(allyloxymethyl)butan-1-ol	214	55	2.1E-02	3.0E+02	7.4E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.7E+02	3.8E+00	1.4E+02	-8.16	-8.06	-9.87	-0.26	0.38	0.0%	0.0%	3.1E-43
910	112-02-7	cetrimonium chloride	320	213	3.7E-08	5.9E-03	1.5E+03	14.0	3.5E-06	4.6E-07	3.5E-07	conf	conf	2.5E+02	3.4E+00	1.2E+02	-7.46	-7.80	-9.50	-3.48	0.83	0.0%	0.0%	4.3E-18
911	2942-59-8	2-chloronicotinic acid	158	85	1.6E-01	2.0E+03	9.8E+00	-1.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.7E+02	3.8E+00	1.4E+02	-6.77	-7.85	-9.82	-1.27	0.78	0.0%	0.0%	1.3E-34
912	17689-77-9	triacetoxyethylsilane	234	-34	1.0E+01	3.7E+03	5.5E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.9E+02	4.0E+00	1.5E+02	-8.98	-8.85	-10.40	-0.37	0.92	0.0%	0.0%	6.4E-47
913	1719-58-0	chlorodimethylvinylsilane	121	-92	1.0E+04	3.0E+02	6.9E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.9E+02	2.7E+00	9.6E+01	-10.18	-9.83	-12.54	-0.48	0.26	0.0%	0.0%	6.7E-67
914	1333-07-9	toluenesulphonamide	171	91	8.1E-03	2.3E+03	8.3E+00	10.1	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.4E+02	3.4E+00	1.2E+02	-6.65	-7.30	-9.19	-0.78	0.28	0.0%	0.0%	1.4E-33
915	24605-36-5	sodium hydrogen 2-aminobenzene-1,4-disulphonate	297	87	9.9E-03	2.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+02	2.9E+00	1.0E+02	-6.70	-7.01	-8.67	-1.84	0.64	0.0%	0.0%	8.7E-23
916	107-19-7	prop-2-yn-1-ol	56	-49	1.3E+03	3.7E+05	3.8E-01	13.6	3.5E-06	2.9E-06	3.5E-06	conf	conf	2.8E+02	3.9E+00	1.4E+02	-8.85	-8.72	-10.22	-2.43	0.41	0.0%	0.0%	5.0E-29
917	2702-72-9	sodium 2,4-dichlorophenoxyacetate	243	87	9.9E-03	1.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+02	2.9E+00	1.0E+02	-6.70	-7.01	-8.67	-0.76	1.00	0.0%	0.0%	7.5E-30
918	2136-89-2	α,α,α,2-tetrachlorotoluene	230	40	1.5E+00	7.7E+00	3.5E+04	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	1.8E+02	2.5E+00	8.9E+01	-9.22	-8.95	-10.45	-0.33	0.64	0.0%	0.0%	1.2E-47
919	75-29-6	2-chloropropane	79	-114	6.8E+04	4.3E+03	1.0E+02	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.8E+02	2.5E+00	8.6E+01	-9.99	-9.48	-11.98	-0.69	0.25	0.0%	0.0%	8.4E-59
920	79-14-1	glycollic acid	76	23	2.3E+00	3.9E+05	8.5E-02	3.8	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.8E+02	3.9E+00	1.4E+02	-7.19	-8.53	-10.36	-0.95	0.43	0.0%	0.0%	1.9E-41
921	32539-83-6	3,4,5,6,7,8,9,10,11,12,13,14-dodecahydro-2H-cyclododeca[b]pyran	222	57	1.6E-01	1.0E+00	6.0E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.0E+02	2.7E+00	9.8E+01	-9.81	-9.61	-10.74	-3.80	0.71	0.0%	0.0%	2.0E-23
922	520-26-3	hesperidin	611	350	1.6E-24	1.7E+03	1.9E-01	9.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.7E+02	3.7E+00	1.4E+02	-6.45	-7.61	-9.74	-0.20	1.88	0.0%	0.0%	1.2E-42
923	101-14-4	4,4'-methylenebis[2-chloroaniline]	267	157	5.2E-04	7.7E+00	3.0E+03	3.3	3.5E-06	3.5E-07	3.5E-08	conf	conf	2.4E+02	3.3E+00	1.2E+02	-6.67	-7.27	-9.19	-2.80	0.26	0.0%	0.0%	3.5E-20
924	67-52-7	barbituric acid	128	199	7.5E-08	1.4E+04	5.6E-02	4.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.8E+02	3.9E+00	1.4E+02	-6.98	-8.45	-10.33	-0.62	1.80	0.0%	0.0%	5.0E-44
925	96-31-1	1,3-dimethylurea	88	20	2.0E-01	1.7E+05	2.4E-01	0	3.5E-06	7.2E-09	3.5E-07	conf	conf	1.6E+02	2.3E+00	7.9E+01	-6.10	-6.88	-7.89	0.61	0.66	0.0%	0.0%	3.2E-34
926	122-60-1	2,3-epoxypropyl phenyl ether	150	13	4.7E+00	1.1E+03	4.1E+01	14.0	3.5E-06	1.6E-07	3.5E-07	conf	conf	2.1E+02	3.0E+00	1.1E+02	-8.05	-7.80	-9.13	-1.42	0.31	0.0%	0.0%	1.7E-28
927	108-18-9	diisopropylamine	101	-78	8.8E+01	6.0E+04	4.4E+01	14.0	3.5E-06	5.0E-07	3.5E-07	conf	conf	2.5E+02	3.4E+00	1.3E+02	-8.10	-7.87	-9.48	-0.86	0.59	0.0%	0.0%	3.8E-35
928	110-44-1	hexa-2,4-dienoic acid	112	25	1.3E+00	2.2E+03	4.2E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.8E+02	3.8E+00	1.4E+02	-8.99	-8.82	-10.39	-1.08	0.36	0.0%	0.0%	1.1E-40
929	84-74-2	dibutyl phthalate	278	6	3.0E-02	1.5E+01	4.1E+04	14.0	3.5E-06	8.9E-07	3.5E-07	conf	conf	2.2E+02	3.1E+00	1.1E+02	-8.71	-8.53	-10.00	-2.83	0.50	0.0%	0.0%	6.8E-25
930	110-64-5	but-2-ene-1,4-diol	88	-9	7.3E-01	2.5E+05	3.7E-01	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	2.8E+02	3.8E+00	1.4E+02	-7.68	-8.61	-10.37	-0.70	0.43	0.0%	0.0%	9.8E-44
931	7785-26-4	(-)-pin-2(3)-ene	136	-14	5.4E+02	2.8E+01	1.9E+04	14.0	3.5E-06	9.7E-08	1.1E-07	conf	conf	1.6E+02	2.2E+00	7.8E+01	-10.09	-9.77	-12.13	-2.61	0.97	0.0%	0.0%	1.8E-42
932	627-93-0	dimethyl adipate	174	-72	9.2E+01	1.3E+04	2.5E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.7E+02	3.8E+00	1.4E+02	-9.19	-9.06	-10.43	-2.03	1.22	0.0%	0.0%	1.8E-33
933	118-69-4	2,6-dichlorotoluene	161	4	4.8E+01	6.1E+01	6.8E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	1.7E+02	2.4E+00	8.5E+01	-9.43	-9.14	-10.92	-2.20	0.36	0.0%	0.0%	6.1E-36
934	324763-46-4	608-748-5	462	306	1.7E-14	9.7E-03	4.1E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+02	2.5E+00	9.0E+01	-8.22	-9.08	-9.97	-3.30	1.02	0.0%	0.0%	8.3E-22
935	104-75-6	2-ethylhexylamine	129	-21	2.2E+02	3.6E+02	5.4E+02	10.0	3.5E-06	2.2E-07	1.1E-07	conf	conf	1.9E+02	2.7E+00	9.6E+01	-9.37	-9.08	-10.81	-1.98	0.59	0.0%	0.0%	8.0E-37
936	1975-78-6	decanenitrile	153	11	5.3E+00	1.1E+02	6.0E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.2E+02	3.0E+00	1.1E+02	-9.01	-8.76	-9.93	-2.79	0.72	0.0%	0.0%	9.9E-25
937	5593-70-4	titanium tetrabutanolate	388	87	9.9E-03	2.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+02	2.8E+00	1.0E+02	-6.71	-7.03	-8.68	0.00	0.33	0.0%	0.0%	1.3E-35
938	28178-42-9	2,6-diisopropylphenyl isocyanate	203	21	3.3E+00	1.6E+01	3.2E+05	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.8E+02	2.5E+00	9.0E+01	-9.57	-9.32	-10.59	-2.01	0.64	0.0%	0.0%	8.0E-35
939	141-57-1	trichloro(propyl)silane	178	-51	1.8E+03	8.9E+03	9.8E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.4E+02	3.3E+00	1.2E+02	-9.65	-9.39	-10.85	0.31	0.30	0.0%	0.0%	1.5E-57
940	102-60-3	1,1',1'',1'''-ethylenedinitrilotetrapropan-2-ol	292	154	1.2E-06	3.1E+05	8.3E-03	7.2	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.6E+02	3.6E+00	1.3E+02	-6.56	-7.76	-9.80	-0.45	1.18	0.0%	0.0%	5.4E-41
941	638-29-9	valeryl chloride	121	-42	4.0E+03	2.6E+03	1.0E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.2E+02	3.1E+00	1.1E+02	-9.81	-9.49	-11.48	-1.30	0.81	0.0%	0.0%	3.4E-48
942	34893-92-0	1,3-dichloro-5-isocyanatobenzene	188	24	1.5E+01	1.6E+02	7.6E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	1.8E+02	2.5E+00	9.0E+01	-9.00	-8.74	-10.13	-2.35	0.45	0.0%	0.0%	5.0E-29
943	53928-30-6	3,5,6-tri-O-.benzyl-1,2-O-isopropylidene-α-D-glucofuranose	491	240	5.3E-10	1.7E-01	3.7E+05	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.8E+02	2.5E+00	9.0E+01	-7.44	-8.23	-9.53	-2.48	0.06	0.0%	0.0%	3.9E-24
944	274-09-9	1,3-benzodioxolane	122	4	1.9E+02	3.7E+02	1.1E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.3E+02	3.3E+00	1.2E+02	-9.71	-9.45	-10.99	-1.37	0.82	0.0%	0.0%	2.9E-43
945	980-26-7	5,12-dihydro-2,9-dimethylquino[2,3-b]acridine-7,14-dione	340	247	1.9E-12	3.3E-02	6.0E+04	0	3.5E-06	3.5E-07	3.5E-08	conf	conf	2.0E+02	2.7E+00	1.0E+02	-6.91	-7.31	-9.21	-0.82	0.72	0.0%	0.0%	2.0E-33
946	2687-91-4	1-ethylpyrrolidin-2-one	113	30	1.4E+01	4.8E+04	2.4E+00	-0.3	3.5E-06	3.5E-06	3.5E-06	conf	conf	2.6E+02	3.7E+00	1.4E+02	-7.65	-8.83	-10.41	-0.33	0.31	0.0%	0.0%	2.6E-47
947	60207-89-8	2-(bromomethyl)-2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxolane	354	130	6.2E-04	3.8E-01	3.3E+05	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.8E+02	2.5E+00	9.0E+01	-8.48	-8.38	-9.72	-3.06	0.52	0.0%	0.0%	9.1E-22
948	93-68-5	2'-methylacetoacetanilide	191	135	1.4E-03	7.9E+02	9.8E+00	0.6	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.5E+02	3.5E+00	1.3E+02	-7.11	-8.11	-9.91	-2.04	1.04	0.0%	0.0%	1.3E-29
949	156-43-4	p-phenetidine	137	40	2.9E+00	4.7E+03	4.5E+01	5.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.5E+02	3.5E+00	1.3E+02	-7.58	-8.01	-9.90	-2.16	0.65	0.0%	0.0%	1.0E-28
950	88-85-7	dinoseb	240	138	9.9E-03	2.7E+02	4.7E+03	4.2	3.5E-06	8.3E-09	1.1E-07	conf	conf	1.5E+02	2.2E+00	7.5E+01	-6.75	-6.92	-7.95	-3.45	0.64	0.0%	0.0%	6.1E-11
951	126-92-1	sodium etasulfate	232	87	9.9E-03	1.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.9E+02	2.7E+00	9.7E+01	-6.74	-7.05	-8.70	-1.02	0.68	0.0%	0.0%	2.7E-28
952	125-12-2	exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acetate	196	34	1.4E+01	3.8E+02	7.2E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.4E+02	3.3E+00	1.2E+02	-9.74	-9.55	-10.73	-2.39	0.45	0.0%	0.0%	5.7E-33
953	95-92-1	diethyl oxalate	146	-95	9.7E+01	1.8E+04	2.5E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.5E+02	3.4E+00	1.3E+02	-8.64	-8.47	-9.91	-1.73	0.70	0.0%	0.0%	7.6E-32
954	17832-28-9	4-(vinyloxy)butan-1-ol	116	-22	3.3E+01	1.0E+05	2.7E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.5E+02	3.5E+00	1.3E+02	-8.29	-8.09	-9.88	-1.31	0.21	0.0%	0.0%	9.8E-35
955	105-34-0	methyl cyanoacetate	99	-23	4.7E+01	1.2E+05	3.4E-01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.6E+02	3.6E+00	1.3E+02	-8.63	-8.49	-10.36	-1.22	1.15	0.0%	0.0%	2.9E-39
956	10540-29-1	tamoxifen	372	181	4.6E-06	8.6E-03	2.0E+06	8.0	3.5E-06	1.6E-08	1.1E-07	conf	conf	1.5E+02	2.1E+00	7.2E+01	-8.05	-8.31	-9.02	-4.24	0.13	0.0%	0.0%	4.5E-12
957	108-23-6	isopropyl chloroformate	123	-68	4.0E+03	4.4E+03	1.1E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.2E+02	3.1E+00	1.1E+02	-9.75	-9.46	-11.31	-1.36	0.51	0.0%	0.0%	3.8E-46
958	106-91-2	2,3-epoxypropyl methacrylate	142	-23	8.3E+01	2.6E+04	6.5E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.6E+02	3.6E+00	1.3E+02	-9.03	-8.89	-10.41	-1.90	0.40	0.0%	0.0%	2.8E-34
959	78-11-5	pentaerithrityl tetranitrate	316	119	5.6E-04	6.3E+03	2.4E+02	14.0	3.5E-06	1.7E-07	1.1E-07	conf	conf	2.0E+02	2.7E+00	9.9E+01	-6.60	-7.31	-8.97	-0.63	0.64	0.0%	0.0%	4.6E-33
960	636-30-6	2,4,5-trichloroaniline	196	71	2.6E-01	2.7E+01	1.0E+03	1.0	3.5E-06	2.2E-09	3.5E-08	conf	conf	1.5E+02	2.0E+00	7.1E+01	-6.39	-6.86	-7.81	-2.54	0.84	0.0%	0.0%	2.5E-14
961	63-05-8	androst-4-ene-3,17-dione	286	145	2.4E-04	2.2E+01	5.8E+02	14.0	3.5E-06	3.3E-07	1.1E-07	conf	conf	2.1E+02	3.0E+00	1.1E+02	-7.42	-7.57	-9.33	-1.86	0.26	0.0%	0.0%	7.1E-27
962	124-63-0	methanesulphonyl chloride	115	-8	3.1E+02	7.1E+04	1.9E+01	14.0	3.5E-06	7.8E-07	3.5E-06	conf	conf	2.3E+02	3.3E+00	1.2E+02	-8.62	-8.39	-9.81	-1.73	0.23	0.0%	0.0%	4.4E-31
963	79-30-1	isobutyryl chloride	107	-67	8.0E+03	6.6E+03	2.8E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.1E+02	3.0E+00	1.1E+02	-9.76	-9.43	-11.38	-1.88	1.03	0.0%	0.0%	3.3E-42
964	4488-57-7	3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-indene	134	-18	2.3E+02	8.8E+02	2.4E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.2E+02	3.1E+00	1.1E+02	-9.69	-9.44	-10.82	-1.96	0.47	0.0%	0.0%	5.0E-37
965	135-19-3	2-naphthol	144	68	2.2E-02	2.5E+02	4.9E+02	9.6	3.5E-06	6.7E-07	3.5E-07	conf	conf	2.3E+02	3.1E+00	1.2E+02	-8.11	-7.98	-9.70	-2.40	0.43	0.0%	0.0%	9.2E-26
966	211915-06-9	Dabigatran etexilate	628	350	4.2E-18	4.8E-03	3.8E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+02	2.5E+00	9.1E+01	-7.62	-8.80	-10.04	-3.53	0.20	0.0%	0.0%	6.9E-21
967	29761-21-5	isodecyl diphenyl phosphate	390	89	6.3E-06	9.1E-03	1.9E+07	14.0	3.5E-06	1.6E-08	3.5E-07	conf	conf	1.4E+02	2.0E+00	6.9E+01	-8.30	-8.98	-9.41	-0.96	1.19	0.0%	0.0%	6.8E-34
968	98-92-0	nicotinamide	122	99	2.6E-02	1.8E+05	3.5E-01	3.0	3.5E-06	2.3E-07	3.5E-07	conf	conf	2.0E+02	2.8E+00	1.0E+02	-6.35	-7.32	-9.07	0.50	0.31	0.0%	0.0%	6.8E-43
969	56-41-7	L-alanine	89	244	3.6E-06	5.6E+05	1.0E-03	2.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.4E+02	3.3E+00	1.2E+02	-6.46	-7.74	-9.82	-1.64	1.07	0.0%	0.0%	8.1E-32
970	624-48-6	dimethyl maleate	144	-96	1.1E+01	1.8E+04	1.6E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.5E+02	3.4E+00	1.3E+02	-9.00	-8.82	-10.44	-2.05	0.38	0.0%	0.0%	1.9E-33
971	128-04-1	sodium dimethyldithiocarbamate	143	87	9.9E-03	9.9E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.6E+00	9.2E+01	-6.77	-7.07	-8.72	-2.95	0.94	0.0%	0.0%	8.2E-17
972	504-60-9	penta-1,3-diene	68	-109	5.5E+04	4.6E+02	2.8E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.7E+02	2.3E+00	8.3E+01	-10.32	-9.92	-12.78	-1.76	0.25	0.0%	0.0%	3.4E-56
973	106-31-0	butyric anhydride	158	-45	4.8E+01	3.0E+03	2.5E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.4E+02	3.4E+00	1.3E+02	-9.36	-9.22	-10.52	-0.91	0.58	0.0%	0.0%	4.1E-43
974	1653-19-6	2,3-dichlorobuta-1,3-diene	123	-89	6.2E+03	5.2E+02	1.0E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.5E+02	2.1E+00	7.5E+01	-10.06	-9.68	-12.09	-2.69	0.19	0.0%	0.0%	2.1E-41
975	869-24-9	2-chloroethyldiethylammonium chloride	172	87	9.9E-03	1.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	9.1E+01	-6.77	-7.07	-8.72	-1.21	0.47	0.0%	0.0%	3.6E-27
976	1247119-31-8	(2R,5R)-1,6-Diphenylhexane-2,5-diamine dihydrochloride	341	87	9.9E-03	2.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	9.1E+01	-6.76	-7.07	-8.73	-1.84	0.64	0.0%	0.0%	3.6E-23
977	71786-67-9	benzyl(3-hydroxyphenacyl)methylammonium chloride	292	87	9.9E-03	2.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	9.1E+01	-6.76	-7.07	-8.73	-1.53	0.64	0.0%	0.0%	4.6E-25
978	123-51-3	3-methylbutan-1-ol	88	-61	5.1E+02	2.7E+04	1.8E+01	14.0	3.5E-06	3.8E-07	3.5E-06	conf	conf	2.1E+02	2.9E+00	1.1E+02	-8.77	-8.52	-9.68	-0.30	0.70	0.0%	0.0%	3.2E-41
979	155-04-4	zinc di(benzothiazol-2-yl) disulphide	398	87	9.9E-03	2.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	9.0E+01	-6.76	-7.08	-8.73	-3.17	0.13	0.0%	0.0%	9.9E-16
980	108-03-2	1-nitropropane	89	-26	1.3E+03	1.5E+04	8.9E+00	8.8	3.5E-06	1.1E-05	3.5E-07	conf	conf	2.4E+02	3.4E+00	1.3E+02	-9.72	-9.54	-11.14	-0.57	0.31	0.0%	0.0%	9.2E-52
981	104-12-1	4-chlorophenyl isocyanate	154	-6	3.3E+01	8.9E+03	1.7E+03	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.0E+02	2.8E+00	1.0E+02	-8.40	-8.15	-9.54	-2.41	0.78	0.0%	0.0%	1.2E-24
982	657-84-1	sodium toluene-4-sulphonate	194	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	9.0E+01	-6.77	-7.08	-8.73	-0.50	0.70	0.0%	0.0%	3.6E-32
983	614-45-9	tert-butyl perbenzoate	194	34	3.1E+00	3.3E+02	7.8E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.2E+02	3.1E+00	1.1E+02	-8.96	-8.75	-10.06	-2.45	0.60	0.0%	0.0%	7.5E-28
984	67-48-1	choline chloride	140	87	9.9E-03	9.6E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	9.0E+01	-6.78	-7.08	-8.73	0.09	1.05	0.0%	0.0%	1.2E-36
985	1912-24-9	atrazine (reach)	216	114	3.8E-03	1.5E+01	6.6E+02	1.7	3.5E-06	2.2E-09	1.1E-07	conf	conf	1.4E+02	1.9E+00	6.7E+01	-6.63	-6.93	-7.88	-2.72	1.13	0.0%	0.0%	8.4E-14
986	618-88-2	5-nitroisophthalic acid	211	169	2.4E-05	3.7E+03	3.7E+01	2.7	3.5E-06	3.5E-06	3.5E-07	conf	conf	2.4E+02	3.3E+00	1.2E+02	-7.40	-8.44	-10.43	0.23	0.57	0.0%	0.0%	1.2E-52
987	38051-10-4	2,2-bis(chloromethyl)trimethylene bis(bis(2-chloroethyl)phosphate)	583	90	2.7E-06	2.4E-01	2.0E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.0E+02	2.8E+00	1.0E+02	-7.64	-7.70	-9.43	-1.42	0.36	0.0%	0.0%	1.2E-30
988	122-51-0	triethyl orthoformate	148	-38	9.3E+02	3.3E+04	2.8E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.0E+02	2.8E+00	1.0E+02	-8.89	-8.65	-9.90	-0.54	0.42	0.0%	0.0%	4.2E-41
989	102-01-2	acetoacetanilide	177	124	4.1E-03	7.7E+03	1.0E+01	0.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.3E+02	3.2E+00	1.2E+02	-6.87	-7.94	-9.91	-0.66	0.24	0.0%	0.0%	3.9E-40
990	101-37-1	2,4,6-triallyloxy-1,3,5-triazine	249	124	2.8E-02	1.8E+02	1.9E+05	2.3	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.3E+02	3.1E+00	1.2E+02	-7.54	-8.28	-9.98	-1.89	0.29	0.0%	0.0%	3.5E-31
991	91-17-8	decahydronaphthalene	138	-29	1.3E+02	1.9E+00	1.6E+04	14.0	3.5E-06	5.8E-09	3.5E-07	conf	conf	1.4E+02	1.9E+00	6.5E+01	-10.22	-9.91	-12.45	-2.65	0.70	0.0%	0.0%	7.6E-45
992	2943-75-1	triethoxyoctylsilane	276	53	1.9E-01	7.9E+00	1.7E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.0E+02	2.8E+00	1.0E+02	-9.35	-9.13	-10.32	-2.40	1.39	0.0%	0.0%	5.6E-30
993	110-12-3	5-methylhexan-2-one	114	-54	8.9E+02	4.0E+03	4.6E+01	14.0	3.5E-06	5.3E-07	1.1E-06	conf	conf	2.0E+02	2.8E+00	1.0E+02	-9.45	-9.19	-10.59	-0.54	0.46	0.0%	0.0%	4.1E-47
994	865-48-5	sodium 2-methylpropan-2-olate	96	87	9.9E-03	6.6E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+02	2.4E+00	8.7E+01	-6.80	-7.10	-8.74	-1.39	0.64	0.0%	0.0%	4.7E-26
995	306-83-2	2,2-dichloro-1,1,1-trifluoroethane	153	-100	9.4E+04	1.7E+03	1.5E+02	14.0	3.5E-06	3.5E-08	1.1E-08	conf	conf	1.3E+02	1.9E+00	6.5E+01	-10.05	-9.18	-11.89	-1.37	0.32	0.0%	0.0%	2.4E-51
996	3277-26-7	1,1,3,3-tetramethyldisiloxane	132	-111	5.3E+03	7.4E+02	1.4E+04	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	1.3E+02	1.8E+00	6.4E+01	-9.87	-9.26	-11.70	-0.32	0.32	0.0%	0.0%	9.7E-60
997	88-60-8	6-tert-butyl-m-cresol	164	52	1.1E+00	5.5E+02	9.3E+03	10.8	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.1E+02	2.9E+00	1.1E+02	-9.37	-9.21	-10.59	-2.54	0.21	0.0%	0.0%	6.7E-31
998	150-76-5	mequinol	124	25	1.1E+00	6.7E+04	3.9E+01	10.1	3.5E-06	7.2E-07	1.1E-06	conf	conf	2.1E+02	3.0E+00	1.1E+02	-7.81	-8.03	-9.76	-1.51	0.84	0.0%	0.0%	2.5E-32
999	105-95-3	1,4-dioxacycloheptadecane-5,17-dione	270	71	5.8E-05	1.8E+01	5.1E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.9E+02	2.6E+00	9.4E+01	-7.91	-8.60	-10.08	-2.54	0.42	0.0%	0.0%	2.6E-27
1000	7085-85-0	ethyl 2-cyanoacrylate	125	-9	3.9E+01	5.6E+03	2.6E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.3E+02	3.2E+00	1.2E+02	-9.23	-9.09	-10.47	-3.13	1.70	0.0%	0.0%	4.8E-26
1001	104-67-6	undecan-4-olide	184	11	5.5E-01	5.8E+01	1.1E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.9E+02	2.7E+00	9.6E+01	-8.56	-8.32	-9.62	-1.83	0.44	0.0%	0.0%	4.4E-29
1002	5766-67-6	ethylenediaminetetraacetonitrile	216	159	2.2E-05	1.0E+06	6.8E-03	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.0E+02	2.7E+00	1.0E+02	-6.22	-7.28	-9.20	-0.67	0.38	0.0%	0.0%	1.7E-34
1003	124-26-5	stearamide	284	152	8.9E-05	3.4E-03	5.0E+06	-0.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.5E+02	2.1E+00	7.8E+01	-7.69	-8.35	-10.15	-3.48	0.28	0.0%	0.0%	8.3E-22
1004	64-67-5	diethyl sulphate	154	38	3.2E+01	2.0E+04	1.4E+01	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	2.3E+02	3.2E+00	1.2E+02	-9.21	-9.04	-10.51	-1.81	1.12	0.0%	0.0%	7.9E-36
1005	111-55-7	ethylene di(acetate)	146	-95	7.9E+01	2.0E+05	2.5E+00	14.0	3.5E-06	4.8E-07	1.1E-06	conf	conf	2.0E+02	2.8E+00	1.0E+02	-8.04	-7.81	-9.54	-1.11	0.14	0.0%	0.0%	1.2E-33
1006	494799-38-1	Methyl 3-cyclopentyl-1-methyl-1H-indole-6-carboxylate	257	125	5.5E-04	1.6E+01	5.8E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+02	2.5E+00	9.2E+01	-8.52	-8.63	-10.10	-2.97	0.81	0.0%	0.0%	1.3E-24
1007	141-02-6	bis(2-ethylhexyl) fumarate	341	29	2.6E-01	9.8E-03	8.7E+07	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.3E+02	1.8E+00	6.4E+01	-9.56	-9.52	-11.46	-3.59	0.89	0.0%	0.0%	1.3E-29
1008	56-89-3	cystine	240	301	3.5E-08	1.2E+03	4.6E-05	1.4	3.5E-06	3.0E-07	1.1E-06	conf	conf	1.9E+02	2.7E+00	9.6E+01	-6.30	-7.44	-9.22	0.44	1.29	0.0%	0.0%	1.3E-43
1009	37763-23-8	methyl (R)-amino(4-hydroxyphenyl)acetate	181	88	2.0E-02	3.1E+04	1.1E+00	1.6	3.5E-06	1.1E-05	3.5E-06	conf	conf	2.3E+02	3.2E+00	1.2E+02	-8.12	-9.47	-11.00	-2.10	0.59	0.0%	0.0%	2.5E-37
1010	123-96-6	octan-2-ol	130	-27	3.2E+01	1.8E+03	5.4E+02	14.0	3.5E-06	4.2E-07	3.5E-07	conf	conf	1.9E+02	2.7E+00	9.8E+01	-8.82	-8.58	-9.77	-1.39	0.27	0.0%	0.0%	2.7E-33
1011	111-65-9	octane	114	-68	2.0E+03	8.2E+00	1.9E+04	14.0	3.5E-06	3.1E-07	1.1E-07	conf	conf	1.4E+02	1.9E+00	6.6E+01	-10.31	-9.97	-12.74	-3.65	0.70	0.0%	0.0%	6.6E-39
1012	96-69-5	6,6'-di-tert-butyl-4,4'-thiodi-m-cresol	359	197	2.9E-08	1.3E-02	1.7E+08	10.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.4E+02	1.9E+00	6.6E+01	-8.45	-9.05	-9.35	-2.97	0.98	0.0%	0.0%	4.0E-20
1013	41253-21-8	1H-1,2,4-triazole, sodium salt	91	87	9.9E-03	6.3E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+02	2.3E+00	8.4E+01	-6.82	-7.11	-8.75	-1.12	0.64	0.0%	0.0%	5.5E-28
1014	97-52-9	4-nitro-o-anisidine	168	97	1.4E-02	1.0E+03	3.5E+01	1.1	3.5E-06	3.5E-06	3.5E-07	conf	conf	2.2E+02	3.1E+00	1.1E+02	-7.49	-8.50	-10.47	-1.64	0.45	0.0%	0.0%	8.8E-37
1015	111-17-1	3,3'-thiodi(propionic acid)	178	127	1.9E-03	6.9E+04	6.6E-01	4.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.2E+02	3.1E+00	1.1E+02	-7.36	-8.67	-10.48	-0.89	1.13	0.0%	0.0%	4.7E-43
1016	95-68-1	2,4-xylidine	121	29	2.4E+01	1.0E+03	1.5E+02	14.0	3.5E-06	2.8E-07	1.1E-07	conf	conf	1.9E+02	2.6E+00	9.4E+01	-8.71	-8.47	-9.68	-1.46	0.73	0.0%	0.0%	3.8E-32
1017	89-63-4	4-chloro-2-nitroaniline	173	93	3.7E-02	4.1E+02	4.6E+02	-1.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	1.3E+02	1.8E+00	6.2E+01	-6.81	-7.01	-7.95	-2.08	0.70	0.0%	0.0%	2.6E-17
1018	39515-51-0	m-phenoxybenzaldehyde	198	84	2.2E-02	4.4E+01	5.9E+03	14.0	3.5E-06	4.7E-08	3.5E-07	conf	conf	1.4E+02	2.0E+00	7.0E+01	-7.66	-7.45	-8.73	-2.20	1.18	0.0%	0.0%	5.5E-21
1019	100-69-6	2-vinylpyridine	105	-15	3.4E+02	3.3E+05	5.1E+01	4.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.1E+02	2.9E+00	1.1E+02	-7.47	-8.09	-9.97	-1.71	0.32	0.0%	0.0%	1.9E-32
1020	75-63-8	bromotrifluoromethane	149	-109	1.2E+06	2.1E+02	3.9E+01	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.3E+02	1.9E+00	6.6E+01	-10.26	-9.69	-12.52	-1.31	0.27	0.0%	0.0%	4.6E-58
1021	993-00-0	chloro(methyl)silane	81	-119	3.8E+05	1.2E+04	2.5E+01	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	1.3E+02	1.8E+00	6.1E+01	-9.91	-9.12	-11.65	-0.51	0.25	0.0%	0.0%	2.3E-57
1022	20769-85-1	2-bromo-2-methylpropionyl bromide	230	17	3.8E+02	5.2E+02	6.8E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.8E+02	2.5E+00	9.3E+01	-9.78	-9.48	-11.49	-1.35	0.47	0.0%	0.0%	7.0E-48
1023	6422-99-7	sebacic acid, compound with hexane-1,6-diamine (1:1)	318	87	9.9E-03	2.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+02	2.3E+00	8.2E+01	-6.81	-7.12	-8.77	-1.84	0.64	0.0%	0.0%	1.9E-23
1024	109-92-2	ethyl vinyl ether	72	-103	7.0E+04	7.2E+03	8.1E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.6E+02	2.3E+00	8.1E+01	-10.09	-9.57	-12.08	-1.37	0.12	0.0%	0.0%	4.1E-53
1025	938-18-1	2,4,6-trimethylbenzoyl chloride	183	54	1.4E+00	1.2E+02	1.2E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.8E+02	2.5E+00	9.3E+01	-8.68	-8.44	-9.70	-2.34	0.23	0.0%	0.0%	4.0E-26
1026	122-00-9	4'-methylacetophenone	134	8	1.1E+01	5.8E+02	1.7E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.1E+02	2.9E+00	1.1E+02	-9.07	-8.88	-10.11	-1.50	0.23	0.0%	0.0%	5.1E-35
1027	95-14-7	benzotriazole	119	85	3.3E-03	7.7E+03	1.5E+01	1.6	3.5E-06	5.7E-09	3.5E-07	conf	conf	1.3E+02	1.8E+00	6.2E+01	-6.52	-7.01	-8.00	-1.26	0.50	0.0%	0.0%	2.9E-22
1028	52556-42-0	sodium 3-(allyloxy)-2-hydroxypropanesulphonate	218	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+02	2.3E+00	8.1E+01	-6.82	-7.12	-8.77	-1.84	0.64	0.0%	0.0%	1.8E-23
1029	125971-95-1	tert-butyl [(4R,6R)-6-{2-[2-(4-fluorophenyl)-3-phenyl-4-(phenylcarbamoyl)-5-(propan-2-yl)-1H-pyrrol-1-yl]ethyl}-2,2-	655	348	1.7E-17	1.7E-06	3.0E+10	-1.9	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.8E+02	2.5E+00	9.3E+01	-8.77	-8.77	-9.12	-5.69	0.89	0.0%	0.0%	4.9E-07
1030	98-16-8	α,α,α-trifluoro-m-toluidine	161	10	9.1E+01	4.4E+03	1.1E+02	3.0	3.5E-06	2.1E-08	1.1E-06	conf	conf	1.3E+02	1.9E+00	6.5E+01	-6.90	-7.13	-8.30	-2.31	0.36	0.0%	0.0%	6.2E-18
1031	560-62-3	9-hydroxyandrost-4-ene-3,17-dione	302	173	2.7E-07	6.8E+01	1.8E+01	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.9E+02	2.6E+00	9.4E+01	-6.48	-7.44	-9.32	-1.48	0.55	0.0%	0.0%	1.9E-29
1032	128-69-8	perylene-3,4:9,10-tetracarboxylic dianhydride	392	265	1.1E-11	3.1E-02	1.8E+06	14.0	3.5E-06	3.5E-07	3.5E-08	conf	conf	1.4E+02	1.9E+00	6.8E+01	-7.87	-8.46	-9.62	-0.87	2.03	0.0%	0.0%	3.7E-36
1033	105-39-5	ethyl chloroacetate	123	-49	7.0E+02	2.1E+04	1.3E+01	14.0	3.5E-06	2.4E-07	1.1E-06	conf	conf	1.7E+02	2.4E+00	8.8E+01	-8.91	-8.66	-9.86	-2.53	0.44	0.0%	0.0%	5.9E-26
1034	86-28-2	9-ethylcarbazole	195	103	4.7E-03	9.7E+00	1.9E+04	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	1.8E+02	2.5E+00	9.3E+01	-8.70	-8.51	-10.10	-2.83	0.26	0.0%	0.0%	1.3E-25
1035	106-51-4	p-benzoquinone	108	24	3.4E+00	1.2E+04	1.8E+00	14.0	3.5E-06	1.9E-06	1.1E-06	conf	conf	2.1E+02	2.9E+00	1.1E+02	-8.51	-8.35	-10.18	-3.93	0.68	0.0%	0.0%	2.2E-19
1036	22984-54-9	butan-2-one O,O',O''-(methylsilylidyne)trioxime	301	3	5.5E-02	7.0E-01	6.8E+09	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.2E+02	1.7E+00	5.9E+01	-8.55	-8.67	-8.85	-0.89	0.76	0.0%	0.0%	2.9E-30
1037	2905-62-6	3,5-dichlorobenzoyl chloride	209	54	1.2E+00	1.0E+01	5.4E+02	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	1.5E+02	2.1E+00	7.4E+01	-9.04	-8.76	-10.27	-2.47	0.12	0.0%	0.0%	3.6E-29
1038	457-68-1	1,1'-methylenebis[4-fluorobenzene]	204	41	1.4E+00	8.3E-01	2.6E+04	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	1.5E+02	2.2E+00	7.7E+01	-10.07	-9.80	-11.68	-2.87	0.12	0.0%	0.0%	1.2E-36
1039	58670-89-6	2-decyltetradecanol	355	131	6.5E-07	5.4E-06	3.9E+10	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+02	1.7E+00	5.9E+01	-8.49	-8.50	-8.65	-1.96	2.17	0.0%	0.0%	5.4E-22
1040	78-86-4	2-chlorobutane	93	-101	1.9E+04	5.4E+02	3.1E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.3E+02	1.8E+00	6.4E+01	-10.24	-9.87	-12.43	-0.88	0.41	0.0%	0.0%	1.7E-61
1041	20592-85-2	[nitrilotris(methylene)]trisphosphonic acid, sodium salt	299	90	2.7E-09	1.0E+06	3.5E-06	2.3	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.8E+02	2.5E+00	9.3E+01	-6.19	-7.29	-9.22	-0.38	0.42	0.0%	0.0%	8.3E-37
1042	56718-71-9	p-(2-methoxyethyl)phenol	152	47	1.0E+00	1.8E+03	6.2E+01	10.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.1E+02	2.9E+00	1.1E+02	-9.15	-8.97	-10.53	-0.90	0.62	0.0%	0.0%	1.9E-43
1043	71-41-0	pentan-1-ol	88	-50	3.5E+02	3.0E+04	2.1E+01	14.0	3.5E-06	4.0E-06	3.5E-06	conf	conf	2.1E+02	2.9E+00	1.1E+02	-9.46	-9.30	-10.57	-0.35	0.14	0.0%	0.0%	1.6E-48
1044	1115-20-4	3-hydroxy-2,2-dimethylpropyl 3-hydroxy-2,2-dimethylpropionate	204	81	2.2E-03	4.6E+03	1.2E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	2.1E+02	2.9E+00	1.1E+02	-6.26	-7.04	-8.68	-1.60	0.92	0.0%	0.0%	2.2E-24
1045	21351-39-3	uronium hydrogen sulphate	158	87	9.9E-03	1.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+02	2.2E+00	7.9E+01	-6.84	-7.14	-8.79	0.48	0.93	0.0%	0.0%	2.9E-40
1046	121-17-5	4-chloro-α,α,α-trifluoro-3-nitrotoluene	226	52	1.6E+01	5.7E+01	2.6E+03	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	1.8E+02	2.5E+00	9.2E+01	-9.72	-9.47	-11.07	-2.39	0.38	0.0%	0.0%	1.3E-35
1047	98-11-3	benzenesulphonic acid	158	89	2.3E-03	7.1E+03	6.8E-02	0.7	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.8E+02	2.5E+00	9.2E+01	-6.31	-7.37	-9.28	-0.30	0.84	0.0%	0.0%	5.7E-38
1048	2494-89-5	2-[(p-aminophenyl)sulphonyl]ethyl hydrogensulphate	281	204	1.2E-09	5.2E+03	2.1E-04	-3.4	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.0E+02	2.8E+00	1.0E+02	-6.65	-7.99	-9.92	-1.42	1.17	0.0%	0.0%	3.0E-34
1049	875-74-1	D-(-)-α-phenylglycine	151	239	3.7E-06	4.4E+04	1.7E-02	1.8	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.1E+02	2.9E+00	1.1E+02	-7.08	-8.55	-10.45	-1.32	0.94	0.0%	0.0%	3.5E-39
1050	141-97-9	ethyl acetoacetate	130	-19	1.2E+02	2.0E+04	6.3E-01	10.6	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.0E+02	2.8E+00	1.0E+02	-8.69	-8.51	-9.98	-0.40	0.19	0.0%	0.0%	5.6E-43
1051	1583-59-1	2,2-difluoro-1,3-benzodioxole	158	10	1.4E+02	7.3E+02	4.3E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.8E+02	2.6E+00	9.3E+01	-9.77	-9.52	-10.86	-2.08	0.53	0.0%	0.0%	2.3E-36
1052	35435-21-3	triethoxy(2,4,4-trimethylpentyl)silane	276	40	9.9E-01	8.3E+00	1.1E+04	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.6E+02	2.2E+00	8.0E+01	-9.42	-9.15	-10.55	-1.82	1.14	0.0%	0.0%	6.2E-36
1053	895525-72-1	{[2-(trifluoromethyl)benzoyl]amino}methyl acetate	220	56	3.2E-01	2.1E+02	6.8E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.9E+02	2.6E+00	9.5E+01	-8.82	-8.61	-10.14	-2.23	0.68	0.0%	0.0%	6.0E-30
1054	107-95-9	β-alanine	89	256	3.2E-05	6.6E+05	8.1E-05	3.7	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.1E+02	2.9E+00	1.1E+02	-7.06	-8.46	-10.45	-0.78	1.11	0.0%	0.0%	1.1E-43
1055	120-55-8	oxydiethylene dibenzoate	314	60	1.1E+01	7.2E+01	1.1E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+02	2.5E+00	9.3E+01	-9.68	-9.44	-10.97	-2.24	0.24	0.0%	0.0%	5.1E-36
1056	583-78-8	2,5-dichlorophenol	163	47	6.1E+00	3.6E+03	6.3E+02	7.5	3.5E-06	1.3E-08	1.1E-07	conf	conf	1.2E+02	1.7E+00	6.0E+01	-7.70	-7.42	-8.38	-2.50	0.84	0.0%	0.0%	2.3E-17
1057	98-52-2	4-tert-butylcyclohexanol	156	4	1.4E+00	8.1E+01	2.6E+03	14.0	3.5E-06	2.6E-07	3.5E-07	conf	conf	1.6E+02	2.3E+00	8.3E+01	-8.77	-8.51	-9.71	-1.57	0.40	0.0%	0.0%	1.3E-31
1058	585-07-9	tert-butyl methacrylate	142	-48	8.2E+02	4.5E+03	4.4E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.9E+02	2.6E+00	9.6E+01	-9.72	-9.47	-10.82	-2.62	0.87	0.0%	0.0%	5.4E-32
1059	96-34-4	methyl chloroacetate	109	-61	1.4E+03	5.8E+04	4.3E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.1E+02	2.9E+00	1.1E+02	-9.40	-9.27	-10.58	-2.36	0.64	0.0%	0.0%	4.0E-32
1060	5308-25-8	1-ethylpiperazine	114	10	1.6E+02	7.2E+05	7.9E-01	9.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.1E+02	2.9E+00	1.1E+02	-8.74	-8.60	-10.47	-0.50	0.16	0.0%	0.0%	2.4E-46
1061	28479-22-3	3-chloro-p-tolyl isocyanate	168	11	2.7E+01	2.5E+03	6.0E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+02	2.6E+00	9.3E+01	-9.15	-8.93	-10.18	-2.28	0.60	0.0%	0.0%	8.0E-30
1062	533-68-6	ethyl 2-bromobutyrate	195	-18	1.5E+02	1.8E+03	1.3E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.0E+02	2.8E+00	1.0E+02	-9.88	-9.70	-10.98	-1.69	1.21	0.0%	0.0%	1.6E-40
1063	150-78-7	1,4-dimethoxybenzene	138	-6	1.1E+01	2.7E+03	1.4E+02	14.0	3.5E-06	7.3E-07	1.1E-06	conf	conf	1.9E+02	2.6E+00	9.6E+01	-8.67	-8.44	-9.88	-1.16	0.70	0.0%	0.0%	6.3E-36
1064	3290-92-4	propylidynetrimethyl trimethacrylate	338	-9	1.8E-02	2.3E+01	3.2E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.8E+02	2.5E+00	9.0E+01	-9.46	-9.32	-10.72	-2.43	0.70	0.0%	0.0%	1.2E-32
1065	120-71-8	6-methoxy-m-toluidine	137	46	4.2E+00	8.3E+03	5.0E+01	4.6	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.9E+02	2.7E+00	1.0E+02	-7.45	-8.28	-10.05	-2.16	0.67	0.0%	0.0%	9.1E-30
1066	141-05-9	diethyl maleate	172	-72	2.4E+01	3.6E+03	1.6E+02	14.0	3.5E-06	1.2E-06	1.1E-06	conf	conf	1.9E+02	2.7E+00	9.9E+01	-8.99	-8.77	-10.13	-1.39	0.36	0.0%	0.0%	4.1E-36
1067	115-84-4	2-butyl-2-ethylpropanediol	160	43	8.1E-02	3.2E+04	1.3E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.9E+02	2.7E+00	9.9E+01	-7.70	-8.37	-10.04	-1.07	0.31	0.0%	0.0%	7.1E-38
1068	92-69-3	biphenyl-4-ol	170	87	2.3E-03	2.0E+02	1.9E+03	9.2	3.5E-06	5.1E-08	3.5E-08	conf	conf	1.3E+02	1.9E+00	6.6E+01	-7.12	-7.22	-8.56	-2.52	0.34	0.0%	0.0%	3.1E-18
1069	100-47-0	benzonitrile	103	-7	7.5E+01	4.2E+03	3.5E+01	14.0	3.5E-06	4.0E-07	1.1E-07	conf	conf	1.7E+02	2.4E+00	8.9E+01	-8.68	-8.44	-9.72	-1.09	0.70	0.0%	0.0%	2.9E-35
1070	115-21-9	trichloro(ethyl)silane	164	-64	4.9E+03	1.9E+04	3.2E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.8E+02	2.5E+00	9.2E+01	-9.79	-9.53	-11.05	-0.45	0.29	0.0%	0.0%	4.1E-52
1071	106904-09-0	2-chloro-3-methyl-4-(methylsulfonyl)benzoic acid	249	157	7.3E-05	3.9E+02	1.9E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.9E+02	2.7E+00	9.9E+01	-7.08	-8.08	-10.01	-1.42	0.43	0.0%	0.0%	6.3E-35
1072	115-46-8	azacyclonol	267	151	1.1E-06	4.6E+02	2.8E+03	10.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+02	2.6E+00	9.4E+01	-7.39	-8.42	-10.02	-2.64	0.59	0.0%	0.0%	2.8E-26
1073	75-89-8	2,2,2-trifluoroethanol	100	-91	1.0E+04	6.0E+05	1.9E+00	12.3	3.5E-06	7.2E-07	3.5E-06	conf	conf	1.9E+02	2.6E+00	9.5E+01	-9.02	-8.80	-9.98	-0.21	0.49	0.0%	0.0%	1.4E-44

1074	95-23-8	5-amino-1,3-dihydro-2H-benzimidazol-2-one	149	130	1.6E-03	9.4E+03	1.9E+00	6.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.7E+02	2.4E+00	8.8E+01	-6.58	-7.53	-9.38	-1.83	0.84	0.0%	0.0%	2.1E-27
1075	112-42-5	undecan-1-ol	172	19	6.8E-01	2.0E+01	1.9E+04	14.0	3.5E-06	3.7E-06	3.5E-07	conf	conf	1.8E+02	2.5E+00	9.0E+01	-9.78	-9.62	-10.77	-2.79	0.28	0.0%	0.0%	1.9E-30
1076	81-25-4	cholic acid	409	233	1.3E-12	1.1E+02	3.3E+03	4.9	3.5E-06	3.1E-07	3.5E-07	conf	conf	1.7E+02	2.4E+00	8.6E+01	-7.04	-7.62	-9.35	-0.63	0.22	0.0%	0.0%	7.1E-36
1077	98-53-3	4-tert-butylcyclohexanone	154	8	2.3E+01	3.4E+02	8.1E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.8E+02	2.6E+00	9.4E+01	-9.54	-9.31	-10.47	-1.78	0.44	0.0%	0.0%	1.1E-35
1078	90-80-2	D-glucono-1,5-lactone	178	137	3.7E-07	1.5E+05	1.0E-02	11.4	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.0E+02	2.8E+00	1.0E+02	-7.09	-8.30	-10.45	-0.32	0.28	0.0%	0.0%	8.8E-48
1079	6041-94-7	4-[(2,5-dichlorophenyl)azo]-3-hydroxy-N-phenylnaphthalene-2-carboxamide	436	276	1.3E-13	1.0E-02	3.8E+08	9.3	3.5E-06	1.1E-07	1.1E-08	conf	conf	1.1E+02	1.6E+00	5.6E+01	-8.39	-8.49	-8.75	-0.93	1.38	0.0%	0.0%	3.2E-29
1080	897671-34-0	Methyl 5-methyl-4-[(oxomethylene)sulfamoyl]thiophene-3-carboxylate	261	152	1.7E-04	8.7E+02	1.0E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.9E+02	2.6E+00	9.7E+01	-7.27	-8.23	-10.04	-1.75	1.21	0.0%	0.0%	1.1E-32
1081	500011-86-9	3-Bromo-1-(3-chloropyridin-2-yl)-1H-pyrazole-5-carboxylic acid	303	171	1.8E-05	1.6E+02	1.1E+02	0.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.9E+02	2.6E+00	9.7E+01	-7.15	-8.04	-9.98	-2.87	0.73	0.0%	0.0%	1.5E-24
1082	56962-04-0	3-Bromo-5-chlorophenol	207	56	4.0E-01	1.3E+03	1.1E+03	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	1.8E+02	2.6E+00	9.4E+01	-8.54	-8.32	-10.06	-2.56	0.36	0.0%	0.0%	4.3E-27
1083	7023-61-2	calcium 4-[(5-chloro-4-methyl-2-sulphonatophenyl)azo]-3-hydroxy-2-naphthoate	459	87	9.9E-03	3.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+02	2.0E+00	7.4E+01	-6.85	-7.16	-8.82	-0.95	0.91	0.0%	0.0%	1.2E-29
1084	5188-07-8	sodium methanethiolate	70	87	9.9E-03	4.8E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+02	2.0E+00	7.4E+01	-6.88	-7.17	-8.81	-2.42	0.39	0.0%	0.0%	3.4E-20
1085	623-03-0	4-chlorobenzonitrile	138	23	2.9E+00	2.5E+03	1.5E+02	14.0	3.5E-06	5.3E-09	3.5E-08	conf	conf	1.2E+02	1.6E+00	5.6E+01	-7.56	-7.28	-8.32	-1.32	0.34	0.0%	0.0%	8.4E-24
1086	80286-58-4	2-[(1R,4R,4aS,8aR)-4,7-dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-1-yl]acrylic acid	248	124	7.2E-04	4.5E+01	3.3E+05	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.8E+02	2.5E+00	9.1E+01	-8.43	-8.86	-10.09	-2.28	0.08	0.0%	0.0%	3.2E-29
1087	600-00-0	ethyl 2-bromo-2-methylpropionate	195	-11	2.9E+02	1.5E+03	1.2E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.9E+02	2.6E+00	9.7E+01	-10.04	-9.83	-11.31	-1.60	1.32	0.0%	0.0%	4.7E-44
1088	110-25-8	(Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine	354	196	2.3E-07	6.0E-02	6.8E+06	3.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.9E+02	2.6E+00	9.5E+01	-7.43	-8.29	-10.00	-2.53	0.63	0.0%	0.0%	6.3E-27
1089	72714-62-6	615-790-8	330	43	2.7E+00	1.6E+00	2.5E+05	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.4E+02	2.0E+00	7.0E+01	-10.52	-10.27	-12.32	-4.22	2.33	0.0%	0.0%	2.9E-31
1090	595-37-9	2,2-dimethylbutyric acid	116	22	9.6E+01	3.1E+04	8.7E+01	14.0	3.5E-06	2.2E-09	1.1E-06	conf	conf	1.1E+02	1.6E+00	5.5E+01	-7.91	-7.63	-8.71	-1.03	0.37	0.0%	0.0%	2.5E-28
1091	76114-73-3	Carbamic acid, N-butyl-, 2-propyn-1-yl ester	155	30	1.9E+01	7.8E+02	4.4E+01	12.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.9E+02	2.7E+00	9.9E+01	-9.55	-9.41	-10.65	-0.88	0.31	0.0%	0.0%	1.4E-44
1092	456-04-2	α-chloro-4-fluoroacetophenone	173	25	6.8E+00	1.6E+03	1.3E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.8E+02	2.6E+00	9.4E+01	-8.89	-8.67	-10.11	-3.75	0.47	0.0%	0.0%	5.1E-20
1093	3687-46-5	decyl oleate	423	161	1.7E-06	2.3E-07	2.8E+12	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E+02	1.5E+00	5.4E+01	-9.64	-9.64	-9.64	-6.52	1.44	0.0%	0.0%	3.4E-29
1094	274693-53-7	Benzyl [(3aS,4R,6S,6aR)-6-hydroxy-2,2-dimethyltetrahydro-3aH-cyclopenta[d][1,3]dioxol-4-yl]carbamate	307	155	6.2E-07	1.1E+03	1.6E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.8E+02	2.6E+00	9.4E+01	-7.36	-8.38	-10.02	-1.74	0.75	0.0%	0.0%	1.3E-32
1095	59-67-6	nicotinic acid	123	63	1.2E-02	4.1E+04	4.9E+00	2.0	3.5E-06	6.3E-07	3.5E-07	conf	conf	1.8E+02	2.5E+00	9.1E+01	-6.78	-7.80	-9.71	-0.71	0.61	0.0%	0.0%	4.1E-38
1096	74860-00-7	2-(11H-dibenzo[b,e]azepin-6-ylmethyl)-1H-isoindole-1,3(2H)-dione	352	254	6.4E-11	2.0E-01	1.9E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+02	2.5E+00	9.1E+01	-7.67	-8.72	-10.04	-3.12	0.46	0.0%	0.0%	2.5E-23
1097	360-64-5	o-(trifluoromethyl)benzamide	189	90	8.0E-02	4.2E+02	9.3E+00	12.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+02	2.6E+00	9.5E+01	-8.30	-8.10	-10.00	-2.14	0.94	0.0%	0.0%	1.5E-29
1098	1307233-94-8	Ethyl N-{[2-(chloromethyl)-1-methyl-1H-benzimidazol-5-yl]carbonyl}-N-pyridin-2-yl-ß-alaninate	401	254	5.8E-11	1.5E+01	5.5E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+02	2.6E+00	9.3E+01	-7.41	-8.45	-10.02	-2.86	0.64	0.0%	0.0%	7.5E-25
1099	13290-96-5	dimethyl 5-nitroisophthalate	239	77	2.5E-02	1.6E+02	3.0E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+02	2.6E+00	9.4E+01	-8.38	-8.19	-10.03	-1.91	0.64	0.0%	0.0%	1.9E-31
1100	21535-43-3	N-(2-benzylphenyl)-2-chloroacetamide	260	170	5.5E-06	3.6E+00	1.4E+03	12.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+02	2.6E+00	9.4E+01	-7.64	-8.41	-10.07	-3.08	0.08	0.0%	0.0%	8.3E-24
1101	96-99-1	4-chloro-3-nitrobenzoic acid	202	126	5.8E-04	5.0E+02	2.2E+02	3.2	3.5E-06	1.1E-06	1.1E-07	conf	conf	1.8E+02	2.6E+00	9.4E+01	-7.10	-7.92	-9.99	-1.77	0.35	0.0%	0.0%	4.2E-32
1102	87-60-5	3-chloro-o-toluidine	142	42	4.7E+00	5.1E+02	1.9E+02	3.5	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.8E+02	2.6E+00	9.4E+01	-7.56	-8.34	-10.11	-2.41	0.71	0.0%	0.0%	2.0E-28
1103	102-77-2	2-(morpholinothio)benzothiazole	252	151	6.8E-04	9.6E+01	1.0E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	1.8E+02	2.5E+00	9.1E+01	-6.78	-7.10	-8.74	-2.63	0.56	0.0%	0.0%	1.2E-18
1104	36768-62-4	2,2,6,6-tetramethyl-4-piperidylamine	156	52	8.5E+01	1.3E+05	8.7E+00	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	1.8E+02	2.5E+00	9.1E+01	-7.61	-7.33	-8.86	-0.84	0.33	0.0%	0.0%	1.2E-30
1105	132335-44-5	(1S)-3-(dimethylamino)-1-(2-thienyl)propan-1-ol	185	70	1.7E-02	2.4E+04	1.0E+01	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	1.8E+02	2.6E+00	9.4E+01	-6.91	-7.88	-9.98	-1.79	0.78	0.0%	0.0%	7.0E-32
1106	2436-29-5	3-(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)propanal	203	177	7.3E-06	2.1E+03	1.0E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+02	2.6E+00	9.4E+01	-6.97	-8.03	-10.00	-1.61	1.19	0.0%	0.0%	2.2E-33
1107	109-59-1	2-isopropoxyethanol	104	-44	2.4E+02	2.5E+05	1.0E+00	14.0	3.5E-06	4.3E-09	1.1E-06	conf	conf	1.1E+02	1.6E+00	5.4E+01	-7.58	-7.31	-8.32	0.31	0.52	0.0%	0.0%	3.1E-35
1108	94-04-2	vinyl 2-ethylhexanoate	170	-22	5.5E+01	2.0E+02	4.0E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.7E+02	2.4E+00	8.9E+01	-10.19	-9.96	-11.35	-2.90	0.44	0.0%	0.0%	7.8E-34
1109	2146-71-6	vinyl laurate	226	24	7.1E-01	3.8E+00	4.4E+05	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	1.4E+02	1.9E+00	6.6E+01	-9.20	-8.85	-10.47	-1.27	1.51	0.0%	0.0%	9.5E-40
1110	85480-89-3	[ethylenebis[nitrilobis(methylene)]]tetrakisphosphonic acid, calcium sodium salt	499	87	9.9E-03	3.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+02	2.0E+00	7.1E+01	-6.86	-7.18	-8.84	-0.42	0.42	0.0%	0.0%	1.3E-33
1111	1647-12-7	Ethyl 2-methylbut-3-enoate	128	-57	1.2E+03	4.5E+03	1.3E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.8E+02	2.6E+00	9.4E+01	-10.08	-9.87	-11.27	-2.09	0.65	0.0%	0.0%	1.3E-39
1112	109-77-3	malononitrile	66	-12	1.5E+01	6.9E+04	2.5E-01	14.0	3.5E-06	4.0E-07	3.5E-07	conf	conf	1.7E+02	2.3E+00	8.5E+01	-7.69	-7.55	-9.41	-2.98	0.25	0.0%	0.0%	2.0E-20
1113	116-02-9	3,3,5-trimethylcyclohexanol	142	3	6.1E+00	9.3E+02	8.5E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+02	2.5E+00	9.0E+01	-8.94	-8.73	-10.11	-1.24	0.29	0.0%	0.0%	4.5E-37
1114	101-43-9	cyclohexyl methacrylate	168	-13	2.9E+01	7.1E+02	3.5E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.8E+02	2.5E+00	9.1E+01	-9.85	-9.66	-10.83	-1.20	0.87	0.0%	0.0%	2.6E-43
1115	15968-01-1	disodium phthalate	210	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+02	2.0E+00	7.0E+01	-6.88	-7.19	-8.84	-0.65	0.60	0.0%	0.0%	7.3E-32
1116	1843-05-6	octabenzone	326	177	9.2E-06	2.3E-01	9.1E+06	9.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+02	1.7E+00	6.0E+01	-8.79	-9.31	-10.08	-3.95	0.51	0.0%	0.0%	9.5E-19
1117	106-20-7	bis(2-ethylhexyl)amine	241	28	7.1E-01	1.7E-03	3.6E+06	10.9	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.1E+02	1.5E+00	5.3E+01	-10.38	-10.14	-12.81	-2.71	0.51	0.0%	0.0%	1.7E-47
1118	938063-63-9	Methyl 3-[(2,2-dimethylbutanoyl)thio]propanoate	218	54	4.5E-01	3.9E+02	1.3E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.9E+02	2.6E+00	9.6E+01	-9.29	-9.11	-10.63	-1.98	0.77	0.0%	0.0%	2.3E-35
1119	123-92-2	isopentyl acetate	130	-56	7.6E+02	3.5E+03	1.8E+02	14.0	3.5E-06	5.1E-07	1.1E-06	conf	conf	1.6E+02	2.2E+00	8.0E+01	-9.56	-9.30	-10.73	-1.00	0.38	0.0%	0.0%	3.1E-44
1120	110-89-4	piperidine	85	-25	3.9E+03	3.2E+05	1.5E+01	11.0	3.5E-06	5.3E-07	3.5E-07	conf	conf	1.7E+02	2.3E+00	8.5E+01	-8.75	-8.54	-9.80	-1.37	0.70	0.0%	0.0%	1.2E-33
1121	31024-26-7	3-[methoxy(dimethyl)silyl]propan-1-amine	147	-12	3.8E+02	2.2E+04	2.2E+01	10.3	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.8E+02	2.6E+00	9.5E+01	-9.60	-9.44	-10.66	-2.48	0.38	0.0%	0.0%	7.1E-32
1122	494799-36-9	3-cyclopentyl-1H-indole-6-carboxylic acid	229	163	1.9E-05	4.9E+01	1.8E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.8E+02	2.6E+00	9.3E+01	-8.07	-9.21	-10.56	-2.61	1.19	0.0%	0.0%	3.4E-30
1123	430-67-1	2,2-Difluoroethanamine	81	-95	9.7E+04	9.1E+05	4.6E-01	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.8E+02	2.6E+00	9.5E+01	-9.81	-9.64	-10.91	-1.86	0.70	0.0%	0.0%	1.6E-38
1124	25260-60-0	(2Z)-but-2-ene-1,4-diyl diacetate	172	-72	6.7E+01	1.2E+04	1.5E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.8E+02	2.6E+00	9.5E+01	-9.30	-9.17	-10.59	-2.45	0.85	0.0%	0.0%	1.7E-31
1125	103041-38-9	Ethyl N-pyridin-2-yl-beta-alaninate	194	78	1.4E-01	2.9E+03	4.0E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	1.8E+02	2.5E+00	9.1E+01	-7.31	-7.16	-8.77	-1.59	0.92	0.0%	0.0%	5.4E-25
1126	41263-74-5	4-(Methylamino)-3-nitrobenzoic acid	196	139	8.0E-04	1.5E+03	7.9E+01	4.1	3.5E-06	3.5E-06	1.1E-07	conf	conf	1.8E+02	2.6E+00	9.5E+01	-7.41	-8.39	-10.55	-1.05	0.70	0.0%	0.0%	3.2E-42
1127	618-83-7	5-hydroxyisophthalic acid	182	159	5.6E-07	7.6E+03	1.9E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.8E+02	2.6E+00	9.5E+01	-7.59	-8.81	-10.52	-1.33	0.27	0.0%	0.0%	1.1E-39
1128	88-95-9	phthaloyl dichloride	203	68	7.1E-01	7.2E+02	7.6E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.8E+02	2.6E+00	9.5E+01	-9.11	-8.94	-10.58	-1.65	0.92	0.0%	0.0%	1.4E-37
1129	103-69-5	N-ethylaniline	121	-9	4.1E+01	1.5E+03	1.3E+02	5.0	3.5E-06	6.0E-09	3.5E-07	conf	conf	1.1E+02	1.5E+00	5.2E+01	-7.48	-7.21	-8.15	-1.61	0.65	0.0%	0.0%	4.7E-21
1130	32257-57-1	tetrasodium 4,4'-{ethene-1,2-diylbis[(3-sulfonato-4,1-phenylene)imino{6-[bis(2-hydroxyethyl)amino]-1,3,5-triazine-	1093	87	9.9E-03	7.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+02	1.9E+00	6.8E+01	-6.87	-7.19	-8.86	-6.00	0.64	0.0%	0.0%	5.5E-24
1131	75128-73-3	2-[(2-acetamido-6,9-dihydro-6-oxo-1H-purin-9-yl]methoxy]ethyl acetate	309	288	3.2E-12	3.3E+04	1.8E-01	5.1	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.8E+02	2.6E+00	9.5E+01	-7.20	-8.62	-10.51	-0.99	1.35	0.0%	0.0%	2.1E-42
1132	1555-62-0	605-014-6	291	147	2.7E-05	2.4E+01	3.0E+04	4.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.7E+02	2.4E+00	8.9E+01	-7.58	-8.28	-10.07	-1.83	0.64	0.0%	0.0%	2.9E-32
1133	617-45-8	acid D,L-aspart	133	218	3.5E-05	1.9E+05	4.8E-05	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.8E+02	2.6E+00	9.5E+01	-7.13	-8.33	-10.49	-0.34	1.19	0.0%	0.0%	5.5E-48
1134	10420-33-4	dimethyl acetylsuccinate	188	-46	2.4E+01	8.9E+04	1.8E-01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.8E+02	2.6E+00	9.5E+01	-8.76	-8.62	-10.53	-1.07	0.50	0.0%	0.0%	5.5E-42
1135	517-23-7	α-acetyl-γ-butyrolactone	128	13	4.1E+00	3.5E+04	3.5E-02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.8E+02	2.6E+00	9.5E+01	-8.53	-8.49	-10.52	-1.09	1.15	0.0%	0.0%	1.3E-41
1136	2370-88-9	2,4,6,8-tetramethylcyclotetrasiloxane	236	-43	1.1E+03	4.1E+03	4.0E+04	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	1.1E+02	1.5E+00	5.1E+01	-9.31	-8.99	-10.83	2.24	0.65	0.0%	0.0%	4.1E-38
1137	50-78-2	O-acetylsalicylic acid	180	93	8.7E-03	2.3E+03	1.3E+01	3.5	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.7E+02	2.4E+00	8.9E+01	-7.30	-8.24	-10.03	-0.75	0.48	0.0%	0.0%	1.7E-40
1138	35037-73-1	p-(trifluoromethoxy)phenyl isocyanate	203	-4	9.6E+01	5.1E+01	4.4E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.4E+02	1.9E+00	6.8E+01	-10.12	-9.84	-11.87	-2.46	0.37	0.0%	0.0%	1.6E-41
1139	128-08-5	N-bromosuccinimide	178	121	9.2E-04	1.3E+05	6.5E-02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.8E+02	2.5E+00	9.4E+01	-7.32	-8.45	-10.55	-2.96	0.08	0.0%	0.0%	1.1E-27
1140	18171-19-2	(3-chloropropyl)dimethoxymethylsilane	183	-21	1.3E+02	5.6E+02	6.6E+01	14.0	3.5E-06	1.1E-07	1.1E-07	conf	conf	1.2E+02	1.7E+00	6.1E+01	-9.26	-8.97	-10.66	-0.80	0.43	0.0%	0.0%	2.5E-45
1141	98-29-3	4-tert-butylpyrocatechol	166	83	4.4E-02	8.6E+02	8.7E+02	10.0	3.5E-06	1.1E-05	3.5E-06	conf	conf	1.8E+02	2.5E+00	9.2E+01	-9.64	-9.82	-11.11	-2.96	0.64	0.0%	0.0%	1.4E-31
1142	3380-34-5	triclosan	290	137	6.2E-04	3.0E+00	4.6E+04	8.8	3.5E-06	2.2E-09	3.5E-08	conf	conf	1.0E+02	1.4E+00	5.0E+01	-7.65	-7.45	-8.39	-3.95	1.03	0.0%	0.0%	1.2E-10
1143	117-08-8	tetrachlorophthalic anhydride	286	111	6.9E-05	6.6E+00	4.5E+04	14.0	3.5E-06	1.1E-07	1.1E-07	conf	conf	1.2E+02	1.7E+00	6.0E+01	-7.63	-7.75	-9.16	-0.37	0.51	0.0%	0.0%	2.0E-36
1144	2536-05-2	2,2'-methylenediphenyl diisocyanate	250	99	6.3E-03	3.5E+01	1.7E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.4E+02	1.9E+00	6.9E+01	-8.91	-8.87	-10.25	0.37	0.26	0.0%	0.0%	2.6E-52
1145	7585-39-9	cycloheptapentylose	1137	87	9.9E-03	7.9E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.9E+00	6.7E+01	-6.88	-7.20	-8.87	-0.11	0.83	0.0%	0.0%	3.4E-36
1146	89-72-5	2-sec-butylphenol	150	39	5.3E+00	9.6E+02	2.9E+03	10.8	3.5E-06	3.3E-08	3.5E-07	conf	conf	1.1E+02	1.6E+00	5.5E+01	-8.23	-7.96	-9.14	-2.44	0.84	0.0%	0.0%	5.1E-22
1147	157577-99-6	Disodium 4-amino-3-[{4-[({4-[(2,4-diaminophenyl)diazenyl]phenyl}sulfonyl)amino]phenyl}diazenyl]-5-hydroxy-6-[ph	861	87	9.9E-03	5.9E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.6E+01	-6.88	-7.21	-8.87	-0.55	1.40	0.0%	0.0%	6.6E-33
1148	67-43-6	N-carboxymethyliminobis(ethylenenitrilo)tetra(acetic acid)	393	334	1.6E-14	2.0E+00	1.2E-05	1.0	3.5E-06	8.8E-08	3.5E-07	conf	conf	1.3E+02	1.8E+00	6.3E+01	-6.18	-7.16	-8.68	-0.81	0.99	0.0%	0.0%	1.3E-29
1149	103-71-9	phenyl isocyanate	119	-37	2.9E+02	4.0E+04	3.9E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.7E+02	2.3E+00	8.5E+01	-9.06	-8.84	-10.16	-1.58	1.22	0.0%	0.0%	7.0E-35
1150	80584-91-4	6,6',6''-(1,3,5-triazine-2,4,6-triyltriimino)trihexanoic acid	469	301	3.6E-14	2.0E-06	2.1E+04	4.2	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.7E+02	2.3E+00	8.6E+01	-8.71	-8.71	-10.04	-2.34	0.87	0.0%	0.0%	2.0E-28
1151	115-27-5	1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	371	130	8.6E-05	7.1E-01	2.3E+04	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	1.1E+02	1.5E+00	5.4E+01	-7.63	-7.34	-8.97	-0.72	0.28	0.0%	0.0%	2.2E-32
1152	103-49-1	dibenzylamine	197	74	1.3E-01	1.2E+01	1.7E+03	8.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.6E+02	2.2E+00	8.2E+01	-9.12	-8.91	-10.20	-2.11	0.82	0.0%	0.0%	3.1E-31
1153	504-29-0	2-pyridylamine	94	27	1.3E+01	1.6E+04	3.4E+00	7.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	1.0E+02	1.4E+00	4.9E+01	-7.44	-7.19	-8.07	-1.71	0.75	0.0%	0.0%	5.0E-20
1154	83066-88-0	(2R)-2-[4-[[5-(trifluoromethyl)-2-pyridinyl]oxy]phenoxy]propanoic acid	327	163	3.7E-05	5.6E+01	3.8E+03	1.0	3.5E-06	2.2E-09	1.1E-06	conf	conf	1.0E+02	1.4E+00	4.9E+01	-7.04	-7.16	-8.09	-1.63	0.83	0.0%	0.0%	1.4E-20
1155	1569-01-3	1-propoxypropan-2-ol	118	-34	1.8E+02	5.0E+04	3.1E+00	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.5E+02	2.1E+00	7.6E+01	-8.31	-8.08	-9.55	-0.63	0.66	0.0%	0.0%	1.6E-37
1156	96-05-9	allyl methacrylate	126	-56	8.9E+02	2.6E+03	1.3E+02	14.0	3.5E-06	7.2E-07	1.1E-06	conf	conf	1.5E+02	2.1E+00	7.6E+01	-9.74	-9.47	-10.99	-2.54	0.73	0.0%	0.0%	7.7E-34
1157	108-67-8	mesitylene	120	-22	2.7E+02	8.5E+01	4.3E+03	14.0	3.5E-06	6.3E-09	1.1E-07	conf	conf	9.9E+01	1.4E+00	4.8E+01	-9.93	-9.63	-11.58	-1.88	0.70	0.0%	0.0%	5.6E-44
1158	156-87-6	3-aminopropan-1-ol	75	-15	2.1E+01	1.0E+06	7.6E-02	10.0	3.5E-06	4.7E-07	3.5E-06	conf	conf	1.5E+02	2.1E+00	7.8E+01	-7.58	-7.84	-9.63	-0.75	0.75	0.0%	0.0%	3.6E-37
1159	140-90-9	sodium O-ethyl dithiocarbonate	144	87	9.9E-03	1.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.4E+01	-6.93	-7.23	-8.87	-2.27	1.06	0.0%	0.0%	2.0E-21
1160	3452-07-1	icos-1-ene	281	50	5.5E-02	5.7E-05	1.1E+10	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.9E+01	1.4E+00	4.8E+01	-9.05	-8.99	-10.18	0.38	0.27	0.0%	0.0%	1.1E-51
1161	27344-41-8	disodium 2,2'-([1,1'-biphenyl]-4,4'-diyldivinylene)bis(benzenesulphonate)	563	87	9.9E-03	3.9E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.4E+01	-6.90	-7.22	-8.88	-1.16	0.44	0.0%	0.0%	1.4E-28
1162	7048-04-6	L-Cysteine, hydrochloride, hydrate	158	87	9.9E-03	1.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.4E+01	-6.93	-7.23	-8.87	-1.84	0.64	0.0%	0.0%	4.4E-24
1163	515-74-2	sodium sulphanilate	195	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.4E+01	-6.92	-7.23	-8.88	-1.84	0.64	0.0%	0.0%	4.2E-24
1164	102-69-2	tripropylamine	143	-34	4.0E+02	1.6E+03	9.8E+02	11.0	3.5E-06	7.1E-08	3.5E-07	conf	conf	1.1E+02	1.6E+00	5.5E+01	-9.33	-9.04	-10.65	-1.21	0.70	0.0%	0.0%	1.0E-41
1165	139-89-9	trisodium 2-(carboxylatomethyl(2-hydroxyethyl)amino)ethyliminodi(acetate)	344	87	9.9E-03	2.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.4E+01	-6.91	-7.23	-8.88	-0.95	1.05	0.0%	0.0%	4.4E-30
1166	2437-25-4	dodecanenitrile	181	25	8.4E-01	6.4E+00	5.9E+04	14.0	3.5E-06	6.0E-07	1.1E-07	conf	conf	1.3E+02	1.8E+00	6.5E+01	-9.67	-9.43	-10.61	-3.47	0.55	0.0%	0.0%	1.0E-24
1167	932742-30-8	3-((5-(3-(Dodecanoyloxy)-2,2-dimethylpropylideneamino)-1,3,3-trimethylcyclohexyl)methylimino)-2,2-dimethylpro	703	273	1.2E-12	1.7E-10	9.3E+16	6.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.7E+01	1.4E+00	4.7E+01	-12.78	-12.78	-12.78	-1.46	0.73	0.0%	0.0%	3.6E-59
1168	99-87-6	p-cymene	134	-28	1.5E+02	4.1E+01	1.0E+04	14.0	3.5E-06	5.8E-07	1.1E-07	conf	conf	1.1E+02	1.6E+00	5.7E+01	-10.14	-9.84	-11.87	-1.67	0.70	0.0%	0.0%	1.8E-48
1169	62-23-7	4-nitrobenzoic acid	167	116	3.4E-04	3.8E+02	4.9E+01	3.3	3.5E-06	2.3E-07	3.5E-07	conf	conf	1.4E+02	1.9E+00	7.0E+01	-6.88	-7.54	-9.27	-0.71	0.70	0.0%	0.0%	1.0E-34
1170	88-44-8	4-aminotoluene-3-sulphonic acid	187	139	9.4E-06	8.4E+03	3.0E-02	-0.9	3.5E-06	3.5E-06	3.5E-07	conf	conf	1.7E+02	2.4E+00	8.7E+01	-7.04	-8.41	-10.53	-1.08	0.63	0.0%	0.0%	8.5E-42
1171	961-69-3	potassium (R)-[(3-ethoxy-1-methyl-3-oxoprop-1-enyl)amino]phenylacetate	301	87	9.9E-03	2.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.3E+01	-6.92	-7.23	-8.89	-1.84	0.64	0.0%	0.0%	3.7E-24
1172	10563-26-5	N,N'-bis(3-aminopropyl)ethylenediamine	174	88	9.2E-02	1.0E+06	2.2E-02	10.5	3.5E-06	1.1E-05	1.1E-06	conf	conf	1.7E+02	2.4E+00	8.9E+01	-7.84	-8.97	-11.11	-0.69	0.27	0.0%	0.0%	2.0E-50
1173	96-20-8	2-aminobutan-1-ol	89	-15	3.6E+01	8.3E+05	2.0E-01	9.5	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.7E+02	2.4E+00	8.7E+01	-8.59	-8.79	-10.58	-1.32	0.99	0.0%	0.0%	3.2E-40
1174	70356-09-1	1-[4-(1,1-dimethylethyl)phenyl]-3-(4-methoxyphenyl)propane-1,3-dione	310	155	1.8E-04	1.8E+00	3.2E+04	8.2	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.4E+02	1.9E+00	7.1E+01	-8.80	-8.70	-10.23	-2.76	2.48	0.0%	0.0%	7.4E-27
1175	5888-33-5	exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acrylate	208	44	1.0E+00	8.7E+01	1.6E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.5E+02	2.1E+00	7.6E+01	-9.74	-9.56	-10.82	-2.93	0.27	0.0%	0.0%	8.2E-30
1176	112-29-8	1-bromodecane	221	5	9.5E+00	1.7E-01	4.0E+05	14.0	3.5E-06	5.0E-07	1.1E-07	conf	conf	1.0E+02	1.4E+00	4.9E+01	-10.47	-10.19	-12.83	-2.43	1.24	0.0%	0.0%	3.4E-50
1177	6166-86-5	2,4,6,8,10-pentamethylcyclopentasiloxane	296	-22	2.2E+02	1.2E+03	1.6E+05	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	9.6E+01	1.3E+00	4.6E+01	-9.38	-9.09	-10.81	2.24	0.65	0.0%	0.0%	6.9E-38
1178	873-32-5	2-chlorobenzonitrile	138	23	5.7E+00	2.3E+03	1.5E+02	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	1.2E+02	1.7E+00	6.1E+01	-7.98	-7.72	-9.10	-1.23	0.08	0.0%	0.0%	1.3E-29
1179	350-46-9	1-fluoro-4-nitrobenzene	141	25	3.7E+01	1.4E+03	1.0E+02	14.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	9.6E+01	1.3E+00	4.6E+01	-8.67	-8.39	-9.63	-1.15	0.70	0.0%	0.0%	4.5E-34
1180	124-30-1	octadecylamine	270	94	1.2E-02	9.7E-04	5.1E+07	10.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.9E+01	1.4E+00	4.8E+01	-9.92	-9.91	-11.90	-3.75	0.78	0.0%	0.0%	1.2E-31
1181	2163-00-0	1,6-dichlorohexane	155	-28	3.9E+01	2.1E+02	6.3E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.3E+02	1.8E+00	6.4E+01	-9.53	-9.27	-10.67	-1.98	0.61	0.0%	0.0%	1.1E-35
1182	6289-46-9	dimethyl 2,5-dioxocyclohexane-1,4-dicarboxylate	228	36	7.4E-02	5.1E+04	1.0E-02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.7E+02	2.3E+00	8.5E+01	-7.54	-8.46	-10.60	-1.04	1.27	0.0%	0.0%	9.2E-43
1183	2807-30-9	2-(propyloxy)ethanol	104	-32	1.8E+02	1.9E+05	1.2E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.6E+02	2.2E+00	8.1E+01	-8.53	-8.34	-10.06	-0.39	0.86	0.0%	0.0%	1.2E-43
1184	65-45-2	salicylamide	137	118	4.0E+00	7.5E+03	1.1E+01	8.3	3.5E-06	2.6E-07	1.1E-06	conf	conf	1.4E+02	1.9E+00	6.9E+01	-8.05	-7.80	-9.42	-1.66	1.14	0.0%	0.0%	7.2E-29
1185	590-19-2	buta-1,2-diene	54	-118	1.7E+05	3.3E+03	1.1E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E+02	1.6E+00	5.6E+01	-10.46	-10.03	-12.58	-1.73	0.34	0.0%	0.0%	2.0E-54
1186	62889-66-1	613-099-6	316	137	8.0E-07	5.4E-02	1.7E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.3E+02	1.8E+00	6.4E+01	-8.45	-8.88	-10.25	-3.00	1.04	0.0%	0.0%	1.9E-25
1187	56-40-6	glycine	75	246	1.1E-05	1.8E+05	3.9E-04	2.3	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.6E+02	2.3E+00	8.4E+01	-7.16	-8.59	-10.56	-0.71	1.14	0.0%	0.0%	3.0E-45
1188	97-63-2	ethyl methacrylate	114	-67	2.4E+03	1.1E+04	5.9E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.6E+02	2.2E+00	8.1E+01	-10.09	-9.89	-11.25	-1.43	1.14	0.0%	0.0%	4.5E-45
1189	123-28-4	didodecyl 3,3'-thiodipropionate	515	155	8.7E-07	9.6E-07	6.2E+11	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.3E+01	1.3E+00	4.5E+01	-9.02	-9.02	-9.02	-1.11	0.78	0.0%	0.0%	6.5E-30
1190	3081-14-9	N,N'-bis(1,4-dimethylpentyl)-p-phenylenediamine	305	113	1.1E-03	4.3E-02	2.0E+06	6.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+02	1.6E+00	5.9E+01	-9.27	-9.13	-10.41	-2.56	1.45	0.0%	0.0%	1.9E-29
1191	93-58-3	methyl benzoate	136	-12	5.1E+01	2.1E+03	6.8E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.6E+02	2.2E+00	8.2E+01	-9.65	-9.50	-10.72	-1.15	0.66	0.0%	0.0%	7.9E-43
1192	91-64-5	coumarin	146	33	8.8E-02	1.4E+03	3.2E+01	14.0	3.5E-06	6.2E-07	1.1E-06	conf	conf	1.5E+02	2.0E+00	7.5E+01	-8.19	-8.11	-9.84	-2.08	0.75	0.0%	0.0%	6.8E-29
1193	15356-60-2	(+)-menthol	156	-6	1.0E+00	9.4E+02	2.4E+03	14.0	3.5E-06	3.2E-07	3.5E-07	conf	conf	1.3E+02	1.8E+00	6.6E+01	-8.29	-8.05	-9.62	-1.33	0.15	0.0%	0.0%	1.2E-32
1194	39605-45-3	6-chloro-N,N,N',N'-tetrabutyl-1,3,5-triazine-2,4-diamine	370	180	5.1E-06	7.1E-03	2.6E+08	1.7	3.5E-06	1.1E-07	1.1E-07	conf	conf	1.2E+02	1.6E+00	5.8E+01	-6.96	-7.43	-8.96	-5.46	1.12	1.6%	0.2%	3.0E-07
1195	64354-92-3	3-(isodecyloxy)propiononitrile	211	48	1.7E-01	1.0E+01	8.5E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.3E+02	1.8E+00	6.4E+01	-8.96	-8.72	-9.92	-2.40	0.22	0.0%	0.0%	3.1E-27
1196	18996-35-5	sodium dihydrogen citrate	214	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	6.0E+01	-6.95	-7.26	-8.91	0.34	0.41	0.0%	0.0%	4.1E-40
1197	110-77-0	2-(ethylthio)ethanol	106	-27	2.5E+01	1.5E+04	2.8E+00	14.0	3.5E-06	3.0E-08	3.5E-06	conf	conf	1.0E+02	1.4E+00	5.0E+01	-7.85	-7.58	-8.76	-1.19	0.59	0.0%	0.0%	1.4E-27
1198	60-12-8	2-phenylethanol	122	6	3.2E+00	5.3E+03	3.7E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.5E+02	2.1E+00	7.8E+01	-8.69	-8.47	-10.14	-0.37	0.28	0.0%	0.0%	1.6E-44
1199	14025-15-1	disodium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4-)-N,N',O,O',ON,ON']cuprate(2-)	384	87	9.9E-03	2.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	5.9E+01	-6.94	-7.26	-8.91	-0.42	0.71	0.0%	0.0%	3.7E-34
1200	599-04-2	α-hydroxy-β,β-dimethyl-γ-butyrolactone	130	31	5.5E-02	1.8E+05	1.1E-01	12.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.6E+02	2.2E+00	8.2E+01	-7.45	-8.54	-10.60	-0.50	0.66	0.0%	0.0%	1.5E-47
1201	19766-89-3	sodium 2-ethylhexanoate	166	87	9.9E-03	1.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	5.9E+01	-6.96	-7.26	-8.91	-0.72	0.45	0.0%	0.0%	6.3E-32
1202	74351-78-3	616-083-7	669	350	3.7E-22	1.3E-03	1.0E+05	0.7	3.5E-06	3.5E-08	3.5E-08	conf	conf	1.0E+02	1.4E+00	5.0E+01	-6.91	-7.11	-8.38	-3.15	1.02	0.0%	0.0%	3.8E-14
1203	100-01-6	4-nitroaniline	138	72	2.8E-03	1.2E+03	3.0E+01	1.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.4E+01	-6.72	-7.14	-8.08	-1.33	0.84	0.0%	0.0%	2.7E-22
1204	21850-44-2	1,1'-(isopropylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)benzene]	944	281	8.5E-13	5.1E-10	3.3E+11	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.4E+01	-12.30	-12.30	-12.30	-5.34	2.87	0.0%	0.0%	1.3E-23
1205	48076-38-6	icosyl acrylate	353	117	1.9E-04	1.7E-05	1.1E+10	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	9.1E+01	1.3E+00	4.4E+01	-8.79	-8.51	-9.40	-5.36	1.80	0.0%	0.0%	3.9E-09
1206	2210-79-9	2,3-epoxypropyl o-tolyl ether	164	30	5.8E+00	1.5E+03	1.4E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.6E+02	2.2E+00	8.1E+01	-9.43	-9.27	-10.68	-2.13	0.29	0.0%	0.0%	1.4E-34
1207	80-08-0	dapsone	248	183	3.6E-06	2.1E+03	5.9E+00	1.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.5E+02	2.1E+00	7.8E+01	-7.14	-8.28	-10.08	-2.00	0.81	0.0%	0.0%	3.8E-31
1208	7585-20-8	zirconium acetate	327	87	9.9E-03	2.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.6E+00	5.9E+01	-6.95	-7.26	-8.92	-1.23	0.64	0.0%	0.0%	2.4E-28
1209	7235-40-7	β,β-carotene	537	237	2.4E-09	1.5E-10	4.2E+17	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-12.81	-12.81	-12.81	-10.55	2.21	0.0%	0.0%	1.0E-55
1210	110-00-9	furan	68	-87	7.9E+04	8.1E+03	2.3E+01	14.0	3.5E-06	2.2E-09	3.5E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.12	-9.72	-11.96	-1.00	0.25	0.0%	0.0%	1.4E-55
1211	40039-93-8	2,2',6,6'-Tetrabromo-4,4'-isopropylidenediphenol, oligomeric reaction products with 1-chloro-2,3-epoxypropane	636	87	9.9E-03	4.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.6E+00	5.9E+01	-6.94	-7.26	-8.92	-6.00	0.64	0.0%	0.0%	2.2E-24
1212	732-26-3	2,4,6-tri-tert-butylphenol	262	104	2.7E-02	2.6E-01	2.5E+06	12.1	3.5E-06	2.2E-09	1.1E-06	conf	conf	9.0E+01	1.3E+00	4.4E+01	-9.60	-9.46	-10.63	-4.22	0.84	0.0%	0.0%	2.6E-20
1213	74-96-4	bromoethane	109	-92	6.2E+04	6.7E+03	4.7E+01	14.0	3.5E-06	9.7E-09	3.5E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.15	-9.76	-12.08	-0.69	0.75	0.0%	0.0%	7.8E-60
1214	87-61-6	1,2,3-trichlorobenzene	181	16	9.6E+00	2.7E+01	8.5E+03	14.0	3.5E-06	2.9E-09	3.5E-08	conf	conf	9.0E+01	1.3E+00	4.4E+01	-9.41	-9.13	-10.78	-2.64	0.70	0.0%	0.0%	1.5E-31
1215	3710-84-7	N,N-diethylhydroxylamine	89	8	4.6E+02	1.2E+05	2.7E+00	5.1	3.5E-06	1.1E-05	1.1E-06	conf	conf	1.6E+02	2.2E+00	8.2E+01	-8.94	-9.50	-11.13	-1.19	0.71	0.0%	0.0%	4.4E-46
1216	111-78-4	cycloocta-1,5-diene	108	-58	6.6E+02	8.4E+01	5.4E+03	14.0	3.5E-06	1.5E-08	3.5E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.19	-9.90	-11.98	-2.14	0.55	0.0%	0.0%	3.4E-45
1217	354-58-5	trichlorotrifluoroethane	187	-75	4.5E+04	3.0E+02	1.2E+03	14.0	3.5E-06	3.5E-08	1.1E-08	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.30	-9.50	-12.21	-1.90	0.10	0.0%	0.0%	2.4E-49
1218	83-42-1	2-chloro-6-nitrotoluene	172	56	5.0E+00	1.1E+02	1.0E+03	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.5E+01	-9.02	-8.72	-10.12	-2.13	0.70	0.0%	0.0%	1.7E-30
1219	108-83-8	2,6-dimethylheptan-4-one	142	-41	2.9E+02	1.1E+03	3.6E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.4E+02	2.0E+00	7.2E+01	-9.88	-9.62	-11.04	-1.38	0.24	0.0%	0.0%	1.2E-43
1220	87-59-2	2,3-xylidine	121	29	1.6E+01	1.0E+03	1.5E+02	5.0	3.5E-06	2.2E-09	1.1E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-7.43	-7.19	-8.10	-1.67	0.84	0.0%	0.0%	2.0E-20
1221	554-00-7	2,4-dichloroaniline	162	46	2.0E+00	1.8E+02	2.3E+02	2.0	3.5E-06	2.2E-09	3.5E-08	conf	conf	9.0E+01	1.3E+00	4.4E+01	-6.32	-7.08	-8.04	-2.31	0.62	0.0%	0.0%	1.4E-16
1222	534-52-1	2-methyl-4,6-dinitro-phenol	198	121	2.3E-04	4.7E+03	1.9E+02	4.2	3.5E-06	2.2E-09	1.1E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-6.68	-7.10	-8.05	-2.89	0.54	0.0%	0.0%	8.6E-14
1223	623-84-7	propane-1,2-diyl diacetate	160	-95	7.7E+01	5.0E+04	6.6E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.6E+02	2.2E+00	8.1E+01	-9.19	-9.04	-10.63	-0.81	0.27	0.0%	0.0%	5.7E-45
1224	14726-36-4	zinc bis(dibenzyldithiocarbamate)	610	87	9.9E-03	4.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.6E+00	5.8E+01	-6.94	-7.26	-8.93	-3.32	0.71	0.0%	0.0%	5.7E-16
1225	1506-02-1	1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthyl)ethan-1-one	258	107	2.5E-02	6.1E-01	2.2E+06	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.0E+02	1.4E+00	4.9E+01	-9.59	-9.43	-10.38	-3.08	0.39	0.0%	0.0%	8.8E-26
1226	23235-61-2	2,2'-[oxybis(methylene)]bis[2-ethylpropane-1,3-diol]	250	147	4.7E-07	3.0E+06	2.0E-01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.5E+02	2.1E+00	7.7E+01	-6.88	-8.03	-10.04	0.09	1.19	0.0%	0.0%	1.0E-47
1227	25306-75-6	sodium O-isobutyl dithiocarbonate	172	87	9.9E-03	1.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.6E+00	5.8E+01	-6.97	-7.27	-8.92	-1.60	0.77	0.0%	0.0%	6.9E-26
1228	36631-30-8	triisodecyl benzene-1,2,4-tricarboxylate	631	246	2.1E-11	1.3E-07	3.5E+14	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	8.9E+01	1.2E+00	4.3E+01	-9.90	-9.90	-9.90	-8.51	2.62	0.0%	0.0%	5.6E-31
1229	68971-49-3	hexasodium 2,2'-[vinylenebis[(3-sulphonato-4,1-phenylene)imino[6-[bis(2-hydroxyethyl)amino]-1,3,5-triazine-4,2-d	1369	87	9.9E-03	9.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.6E+00	5.8E+01	-6.94	-7.26	-8.93	-6.00	0.64	0.0%	0.0%	1.9E-24
1230	34443-12-4	OO-tert-butyl O-(2-ethylhexyl) peroxycarbonate	246	-4	5.7E-01	7.7E+01	4.6E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.3E+02	1.8E+00	6.7E+01	-9.76	-9.60	-10.89	-2.97	0.06	0.0%	0.0%	6.0E-30
1231	110-02-1	thiophene	84	-46	9.8E+03	1.9E+03	6.5E+01	14.0	3.5E-06	3.0E-08	1.1E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-9.99	-9.56	-11.75	-1.22	0.53	0.0%	0.0%	2.1E-51
1232	618-62-2	3,5-dichloronitrobenzene	192	66	6.8E-01	8.0E+01	1.3E+03	14.0	3.5E-06	4.6E-09	3.5E-08	conf	conf	9.0E+01	1.3E+00	4.4E+01	-8.33	-8.06	-9.23	-2.64	0.70	0.0%	0.0%	2.5E-21
1233	60-80-0	phenazone	188	119	3.7E-02	4.2E+05	3.9E+00	1.8	3.5E-06	4.1E-09	1.1E-06	conf	conf	9.0E+01	1.3E+00	4.4E+01	-6.76	-7.19	-8.15	-5.60	0.64	4.9%	1.2%	1.4E-04
1234	68413-60-5	diammonium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4-)-N,N',O,O',ON,ON']hydroxyferrate(2-)	397	87	9.9E-03	2.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.6E+00	5.8E+01	-6.95	-7.27	-8.93	-0.73	0.24	0.0%	0.0%	5.4E-32
1235	50594-82-6	1,2,3-trichloro-5-(trifluoromethyl)benzene	249	25	2.5E+01	1.3E+00	7.8E+04	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.33	-9.99	-12.45	-3.01	0.11	0.0%	0.0%	9.6E-42
1236	7299-99-2	2,2-bis[[(2-ethyl-1-oxohexyl)oxy]methyl]propane-1,3-diyl bis(2-ethylhexanoate)	641	220	2.7E-10	4.5E-07	2.2E+12	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	8.9E+01	1.2E+00	4.3E+01	-9.34	-9.34	-9.34	-5.91	1.56	0.0%	0.0%	4.5E-07
1237	320-60-5	2,4-dichloro-α,α,α-trifluorotoluene	215	1	1.5E+02	8.3E+00	1.7E+04	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.28	-9.90	-12.38	-2.70	0.30	0.0%	0.0%	1.0E-43
1238	109-78-4	3-hydroxypropiononitrile	71	-16	2.7E+00	2.0E+05	7.6E-02	13.9	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.5E+02	2.1E+00	7.6E+01	-7.51	-8.08	-10.07	-0.71	1.10	0.0%	0.0%	4.4E-41
1239	66682-07-3	1,2,3-Trichloro-5-(trichloromethyl)benzene	299	77	1.4E-01	8.7E-02	6.8E+05	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.13	-9.87	-11.63	-1.39	0.64	0.0%	0.0%	8.8E-49
1240	100930-72-1	3,3'-Diisopropyl-5,5',6,6'-tetramethylbiphenyl-2,2'-diol	326	184	1.7E-08	1.8E-02	1.1E+08	7.6	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-8.53	-9.02	-9.24	-4.40	1.20	0.0%	0.0%	2.3E-12
1241	617-48-1	DL-malic acid	134	113	3.9E-04	3.4E+05	2.1E-02	3.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.5E+02	2.1E+00	7.9E+01	-7.29	-8.72	-10.61	-0.36	0.44	0.0%	0.0%	7.7E-49
1242	2495-39-8	sodium prop-2-enesulphonate	144	87	9.9E-03	1.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+02	1.6E+00	5.7E+01	-6.98	-7.28	-8.92	0.66	0.64	0.0%	0.0%	6.0E-43
1243	3698-89-3	dodecyl methyl sulphide	216	22	9.4E-01	9.5E-03	2.1E+06	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.50	-10.24	-12.85	-4.05	0.64	0.0%	0.0%	1.5E-36
1244	121-33-5	vanillin	152	72	6.0E-02	6.6E+03	1.1E+01	7.3	3.5E-06	6.4E-07	1.1E-06	conf	conf	1.4E+02	2.0E+00	7.2E+01	-7.61	-8.09	-9.87	-1.07	0.21	0.0%	0.0%	1.5E-36
1245	78-08-0	triethoxy(vinyl)silane	190	-13	9.6E+01	5.3E+04	1.4E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.5E+02	2.0E+00	7.5E+01	-8.81	-8.61	-10.17	0.21	1.07	0.0%	0.0%	4.3E-50
1246	504-63-2	propane-1,3-diol	76	-20	2.8E+00	1.4E+06	1.9E-01	14.0	3.5E-06	4.3E-06	3.5E-06	conf	conf	1.5E+02	2.1E+00	8.0E+01	-7.92	-8.92	-10.71	0.67	0.30	0.0%	0.0%	1.2E-59
1247	354-32-5	trifluoroacetyl chloride	132	-84	3.0E+04	1.9E+05	8.7E-01	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	1.1E+02	1.5E+00	5.4E+01	-9.17	-8.81	-10.57	-1.20	0.56	0.0%	0.0%	4.0E-41
1248	75-44-5	phosgene	99	-67	1.8E+05	9.7E+03	1.9E-01	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.04	-9.27	-11.89	-1.17	0.59	0.0%	0.0%	3.8E-53
1249	338-65-8	2-Chloro-1,1-difluoroethane	101	-121	9.5E+04	5.4E+03	2.5E+01	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.15	-9.41	-12.05	-1.52	0.52	0.0%	0.0%	1.7E-51
1250	4253-34-3	methylsilanetriyl triacetate	220	-45	1.8E+01	6.6E+03	1.8E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.5E+02	2.1E+00	7.9E+01	-9.18	-9.05	-10.66	-0.35	0.90	0.0%	0.0%	2.1E-49
1251	61203-94-9	612-101-2	202	24	6.2E-01	4.4E-02	1.6E+06	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.46	-10.21	-12.40	-3.42	0.13	0.0%	0.0%	5.3E-38
1252	434-16-2	7,8-didehydrocholesterol	385	167	1.1E-07	7.4E-03	4.5E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-8.59	-9.09	-9.30	-5.11	0.45	0.0%	0.0%	1.0E-09
1253	68127-98-0	614-284-4	261	28	3.3E+01	6.2E+01	1.9E+03	14.0	3.5E-06	3.5E-08	1.1E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-9.61	-9.33	-11.16	-1.56	0.76	0.0%	0.0%	4.6E-43
1254	72-18-4	L-valine	117	252	1.2E-06	4.0E+04	8.3E-03	2.3	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.5E+02	2.1E+00	7.9E+01	-7.21	-8.68	-10.59	-0.99	1.04	0.0%	0.0%	4.0E-43
1255	139147-73-2	604-112-6	237	22	7.0E+00	1.5E-01	6.3E+05	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.22	-9.32	-11.99	-1.92	0.64	0.0%	0.0%	3.0E-47
1256	594-42-3	trichloromethanesulphenyl chloride	186	-22	6.0E+02	1.2E+02	3.0E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.09	-9.69	-11.96	-1.94	0.15	0.0%	0.0%	8.5E-47

1257	10605-40-0	chloro(3-chloropropyl)dimethylsilane	171	-44	6.4E+02	1.7E+02	5.2E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.05	-9.70	-11.87	-1.91	0.16	0.0%	0.0%	3.5E-46
1258	7651-02-7	N-[3-(dimethylamino)propyl]stearamide	369	196	2.2E-07	5.8E-04	2.2E+07	9.2	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.6E+01	1.3E+00	4.7E+01	-8.91	-9.43	-10.09	-3.59	0.23	0.0%	0.0%	8.6E-21
1259	593-85-1	diguanidinium carbonate	180	87	9.9E-03	1.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+02	1.6E+00	5.6E+01	-6.98	-7.29	-8.93	-0.98	0.81	0.0%	0.0%	3.4E-30
1260	26272-90-2	hexadecyl chloroformate	305	84	7.1E-03	5.7E-04	3.2E+07	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.10	-10.05	-12.14	-2.63	1.13	0.0%	0.0%	2.0E-42
1261	7378-99-6	dimethyl(octyl)amine	157	-22	7.5E+01	3.0E+01	3.0E+03	10.0	3.5E-06	1.0E-07	3.5E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.02	-9.73	-11.66	-3.08	0.41	0.0%	0.0%	7.2E-35
1262	95149-35-2	1-[4-(trans-4-propylcyclohexyl)phenyl]pentan-1-one	286	119	5.7E-04	7.4E-01	2.3E+07	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-8.69	-9.13	-9.77	-4.16	0.33	0.0%	0.0%	5.9E-16
1263	644-97-3	dichloro(phenyl)phosphine	179	-5	1.3E+01	3.1E+02	1.0E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.2E+02	1.7E+00	6.2E+01	-9.21	-8.97	-10.21	-1.63	0.21	0.0%	0.0%	7.7E-35
1264	111-44-4	bis(2-chloroethyl) ether	143	-34	1.4E+02	4.2E+03	3.6E+01	14.0	3.5E-06	1.7E-08	1.1E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-8.78	-8.50	-9.80	-0.42	0.70	0.0%	0.0%	2.8E-41
1265	34452-51-2	potassium mercaptoacetate	130	87	9.9E-03	9.0E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+02	1.6E+00	5.6E+01	-6.99	-7.29	-8.93	-0.93	0.89	0.0%	0.0%	1.3E-30
1266	329-01-1	α,α,α-trifluoro-3-tolyl isocyanate	187	-21	2.8E+02	1.2E+03	3.6E+03	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.4E+02	1.9E+00	7.0E+01	-10.32	-10.07	-11.49	-2.01	0.43	0.0%	0.0%	4.3E-42
1267	135590-91-9	1-(2,4-Dichlorophenyl)-4,5-dihydro-5-methyl-1H-pyrazole-3,5-dicarboxylic acid 3,5-diethyl ester	373	150	4.4E-04	2.4E+00	6.6E+04	14.0	3.5E-06	8.8E-08	3.5E-07	conf	conf	9.8E+01	1.4E+00	4.8E+01	-8.02	-7.98	-9.29	-2.16	0.44	0.0%	0.0%	1.1E-24
1268	927-07-1	tert-butyl peroxypivalate	174	-13	2.0E+02	2.2E+02	6.3E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.2E+02	1.7E+00	6.2E+01	-10.09	-9.81	-11.63	-2.33	0.73	0.0%	0.0%	1.4E-40
1269	402-31-3	α,α,α,β,β,β-hexafluoro-m-xylene	214	-46	2.5E+03	6.0E+01	8.3E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.38	-10.03	-12.70	-2.66	0.73	0.0%	0.0%	5.4E-47
1270	5421-46-5	ammonium mercaptoacetate	109	87	9.9E-03	7.5E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+02	1.5E+00	5.5E+01	-7.00	-7.29	-8.94	-0.93	0.89	0.0%	0.0%	1.3E-30
1271	72162-46-0	N-[3-(isodecyloxy)propyl]propane-1,3-diamine	272	105	3.7E-03	6.9E-01	7.9E+03	10.3	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.2E+02	1.7E+00	6.0E+01	-8.69	-8.45	-9.82	-2.73	0.57	0.0%	0.0%	2.0E-24
1272	1558-33-4	dichloro(chloromethyl)methylsilane	164	-56	1.9E+03	1.1E+03	3.2E+02	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.0E+01	1.3E+00	4.4E+01	-9.83	-9.41	-11.57	-1.89	0.64	0.0%	0.0%	8.3E-44
1273	2629-68-7	1,4-bis[chloro(difluoro)methyl]benzene	247	3	1.2E+02	1.8E+01	3.5E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.0E+01	1.3E+00	4.4E+01	-10.30	-10.01	-12.30	-2.76	0.64	0.0%	0.0%	1.5E-42
1274	2082-81-7	tetramethylene dimethacrylate	226	-46	2.5E-02	1.7E+02	1.5E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.4E+02	2.0E+00	7.3E+01	-9.37	-9.26	-10.72	-1.49	0.52	0.0%	0.0%	6.1E-40
1275	99-62-7	1,3-diisopropylbenzene	162	-16	4.1E+01	1.2E+00	7.9E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	8.9E+01	1.2E+00	4.3E+01	-10.47	-10.16	-12.67	-3.08	0.37	0.0%	0.0%	4.8E-43
1276	89-04-3	trioctyl benzene-1,2,4-tricarboxylate	547	226	6.9E-10	2.0E-05	6.5E+11	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	8.4E+01	1.2E+00	4.1E+01	-8.61	-8.52	-8.65	-1.24	0.68	0.0%	0.0%	1.8E-26
1277	4009-98-7	(methoxymethyl)triphenylphosphonium chloride	343	87	9.9E-03	2.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+02	1.5E+00	5.5E+01	-6.98	-7.29	-8.95	-2.66	0.64	0.0%	0.0%	1.3E-19
1278	110-83-8	cyclohexene	82	-81	1.1E+04	2.6E+02	9.1E+02	14.0	3.5E-06	8.2E-08	3.5E-07	conf	conf	8.6E+01	1.2E+00	4.2E+01	-10.40	-10.07	-12.56	-2.10	0.74	0.0%	0.0%	8.1E-51
1279	2235-00-9	1-vinylhexahydro-2H-azepin-2-one	139	55	1.2E+00	1.1E+04	1.7E+01	-0.4	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.4E+02	2.0E+00	7.2E+01	-7.44	-8.37	-10.16	-0.74	0.45	0.0%	0.0%	1.6E-41
1280	106-63-8	isobutyl acrylate	128	-57	1.2E+03	4.0E+03	1.3E+02	14.0	3.5E-06	4.3E-07	1.1E-06	conf	conf	1.2E+02	1.7E+00	6.1E+01	-9.68	-9.40	-10.94	-2.43	0.41	0.0%	0.0%	2.7E-34
1281	49562-28-9	fenofibrate	361	158	8.3E-05	5.3E-02	1.5E+05	14.0	3.5E-06	6.0E-08	1.1E-06	conf	conf	9.1E+01	1.3E+00	4.4E+01	-8.29	-8.24	-9.44	-1.58	1.04	0.0%	0.0%	1.5E-29
1282	124-70-9	dichloro(methyl)(vinyl)silane	141	-78	6.9E+03	7.0E+02	4.0E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+02	1.4E+00	5.1E+01	-10.37	-10.02	-12.51	-0.26	0.60	0.0%	0.0%	6.0E-69
1283	42221-52-3	2,3,4,5-tetrachlorobenzoylchloride	278	93	3.5E-02	1.9E+00	1.0E+04	14.0	3.5E-06	3.5E-08	3.5E-08	conf	conf	9.1E+01	1.3E+00	4.4E+01	-8.75	-8.49	-9.72	-3.17	0.14	0.0%	0.0%	4.1E-21
1284	119-53-9	benzoin	212	107	7.7E-05	1.1E+03	6.9E+01	12.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.4E+02	1.9E+00	7.1E+01	-7.34	-8.33	-10.17	-1.68	0.22	0.0%	0.0%	3.7E-34
1285	110-53-2	1-bromopentane	151	-54	1.7E+03	1.7E+02	1.4E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.4E+01	-10.26	-9.90	-12.28	-2.09	0.64	0.0%	0.0%	2.9E-48
1286	87-99-0	xylitol	152	103	2.6E-01	1.0E+06	2.8E-03	13.4	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.5E+02	2.0E+00	7.5E+01	-7.65	-8.73	-10.66	1.94	0.51	0.0%	0.0%	9.9E-37
1287	111-82-0	methyl laurate	214	23	1.5E+00	1.5E+00	1.9E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+02	1.4E+00	5.1E+01	-10.30	-10.05	-11.67	-2.23	1.53	0.0%	0.0%	9.0E-42
1288	624-65-7	3-chloropropyne	75	-72	2.8E+04	1.1E+04	2.0E+01	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.1E+01	1.3E+00	4.4E+01	-9.76	-9.27	-11.46	-1.74	0.64	0.0%	0.0%	4.3E-44
1289	5510-99-6	di-sec-butylphenol, mixed isomers	206	76	9.8E-01	5.4E+01	3.6E+04	11.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+02	1.7E+00	6.0E+01	-9.51	-9.30	-10.47	-3.36	0.32	0.0%	0.0%	1.4E-24
1290	4355-11-7	cyclohexanediacetic acid	200	133	8.8E-04	2.2E+03	9.3E+01	3.6	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.4E+02	1.9E+00	7.1E+01	-7.59	-8.41	-10.18	-1.61	0.24	0.0%	0.0%	9.8E-35
1291	92-88-6	biphenyl-4,4'-diol	186	127	1.5E-06	2.2E+02	6.3E+02	8.9	3.5E-06	6.9E-08	3.5E-08	conf	conf	9.8E+01	1.4E+00	4.9E+01	-6.55	-7.32	-8.75	-2.39	0.44	0.0%	0.0%	5.0E-20
1292	88-99-3	phthalic acid	166	127	1.0E-04	2.8E+03	1.2E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.4E+02	1.9E+00	7.1E+01	-7.41	-8.38	-10.17	-0.42	0.60	0.0%	0.0%	2.5E-44
1293	6642-31-5	6-amino-1,3-dimethyluracil	155	137	1.0E-03	9.0E+03	5.5E-02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.4E+02	1.9E+00	7.1E+01	-6.91	-7.95	-10.08	-2.78	0.64	0.0%	0.0%	9.0E-26
1294	443-83-4	2-chloro-6-fluorotoluene	145	-22	4.4E+02	7.7E+01	2.5E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.4E+01	-10.21	-9.88	-12.09	-2.14	0.11	0.0%	0.0%	3.5E-46
1295	646-25-3	decamethylenediamine	172	60	7.1E-01	1.1E+03	2.0E+02	10.8	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.2E+02	1.7E+00	6.2E+01	-8.17	-7.92	-9.60	-3.02	0.83	0.0%	0.0%	2.8E-21
1296	51867-77-7	4-[(2,5-dichlorophenyl)azo]-3-hydroxy-2-naphthoic acid	361	225	6.5E-10	3.9E+00	3.4E+07	14.0	3.5E-06	3.5E-08	1.1E-08	conf	conf	9.0E+01	1.3E+00	4.4E+01	-8.34	-8.75	-9.20	-3.29	1.02	0.0%	0.0%	1.5E-17
1297	130755-46-3	603-434-4	704	340	6.6E-17	6.4E-08	6.8E+06	1.5	3.5E-06	3.5E-08	3.5E-08	conf	conf	9.1E+01	1.3E+00	4.4E+01	-10.20	-10.20	-10.20	-3.61	1.16	0.0%	0.0%	2.4E-21
1298	5894-60-0	trichloro(hexadecyl)silane	360	90	7.3E-03	2.6E-01	2.3E+09	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	8.3E+01	1.2E+00	4.0E+01	-8.75	-8.97	-9.17	-3.58	0.55	0.0%	0.0%	6.7E-16
1299	60728-43-0	612-012-9	690	350	2.4E-22	6.0E-04	1.3E+05	14.0	3.5E-06	3.5E-08	3.5E-08	conf	conf	9.0E+01	1.3E+00	4.4E+01	-7.04	-7.73	-8.85	-3.20	1.05	0.0%	0.0%	3.2E-16
1300	2915-57-3	bis(2-ethylhexyl) succinate	343	-12	1.3E-02	2.9E-01	1.3E+07	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-9.75	-9.78	-10.67	-0.99	0.78	0.0%	0.0%	9.4E-44
1301	2156-97-0	dodecyl acrylate	240	34	2.7E-01	4.3E-02	1.3E+06	14.0	3.5E-06	5.6E-07	3.5E-07	conf	conf	8.6E+01	1.2E+00	4.2E+01	-10.48	-10.25	-12.28	-1.40	0.92	0.0%	0.0%	9.7E-55
1302	13122-18-4	tert-butyl 3,5,5-trimethylperoxyhexanoate	230	21	7.0E+00	2.6E+00	4.9E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.1E+02	1.5E+00	5.4E+01	-10.64	-10.36	-12.48	-2.94	0.80	0.0%	0.0%	1.5E-42
1303	75-52-5	nitromethane	61	-52	4.8E+03	7.2E+04	9.1E-01	10.1	3.5E-06	2.2E-09	3.5E-07	conf	conf	8.1E+01	1.1E+00	3.9E+01	-8.89	-8.60	-9.86	-0.63	0.54	0.0%	0.0%	5.1E-40
1304	32768-54-0	2,3-dichlorotoluene	161	4	3.3E+01	6.1E+01	6.8E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.1E+01	1.3E+00	4.5E+01	-9.63	-9.34	-11.05	-2.57	0.26	0.0%	0.0%	4.4E-34
1305	126-98-7	methacrylonitrile	67	-69	7.5E+03	9.3E+04	5.8E+00	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.2E+02	1.7E+00	6.1E+01	-9.26	-9.00	-10.22	-0.99	0.57	0.0%	0.0%	5.5E-40
1306	1779-49-3	methyltriphenylphosphonium bromide	357	87	9.9E-03	2.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+02	1.5E+00	5.2E+01	-7.00	-7.31	-8.97	-2.45	0.64	0.0%	0.0%	6.5E-21
1307	5160-02-1	barium bis[2-chloro-5-[(2-hydroxy-1-naphthyl)azo]toluene-4-sulphonate]	889	87	9.9E-03	6.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+02	1.5E+00	5.2E+01	-6.99	-7.31	-8.97	-1.03	1.01	0.0%	0.0%	3.9E-30
1308	352-70-5	3-fluorotoluene	110	-54	2.6E+03	4.9E+02	5.5E+02	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-10.16	-9.79	-11.99	-1.90	0.37	0.0%	0.0%	2.1E-47
1309	6850-63-1	2,6-dimethylcyclohexylamine	127	-11	1.6E+02	5.7E+01	3.0E+02	14.0	3.5E-06	2.6E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-10.00	-9.66	-11.70	-1.44	0.07	0.0%	0.0%	5.6E-49
1310	330-54-1	diuron (reach)	233	126	6.2E-04	6.4E+01	4.7E+02	-1.6	3.5E-06	9.0E-09	1.1E-07	conf	conf	8.3E+01	1.2E+00	4.0E+01	-6.72	-7.15	-8.19	-3.18	1.26	0.0%	0.0%	4.3E-13
1311	77-75-8	methylpentynol	98	-23	7.5E+02	8.0E+04	8.7E+00	13.6	3.5E-06	2.2E-08	1.1E-06	conf	conf	8.6E+01	1.2E+00	4.2E+01	-8.42	-8.15	-9.29	-0.15	0.74	0.0%	0.0%	2.9E-39
1312	101-96-2	N,N'-di-sec-butyl-p-phenylenediamine	220	76	2.1E-01	1.2E+01	3.2E+03	6.3	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.2E+02	1.6E+00	5.9E+01	-8.52	-8.25	-9.67	-3.24	0.39	0.0%	0.0%	1.9E-20
1313	20120-33-6	dimethyl [3-[(hydroxymethyl)amino]-3-oxopropyl]phosphonate	211	84	1.7E-05	3.2E+05	8.1E-04	12.7	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.3E+02	1.9E+00	6.9E+01	-6.84	-7.99	-10.07	-0.03	0.73	0.0%	0.0%	6.6E-47
1314	22036-77-7	[ethylenebis[nitrilobis(methylene)]]tetrakisphosphonic acid, sodium salt	524	87	9.9E-03	3.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+02	1.4E+00	5.2E+01	-7.00	-7.32	-8.97	0.11	0.64	0.0%	0.0%	7.7E-39
1315	647-42-7	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctan-1-ol	364	-16	1.3E+02	2.1E-01	2.6E+04	13.5	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.0E+02	1.4E+00	5.1E+01	-10.71	-10.42	-13.68	-2.15	0.16	0.0%	0.0%	3.1E-61
1316	95149-34-1	1-[4-(trans-4-propylcyclohexyl)phenyl]butan-1-one	272	110	1.3E-03	1.8E+00	7.4E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-9.12	-9.47	-10.34	-3.78	0.21	0.0%	0.0%	3.4E-21
1317	6386-38-5	methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	292	131	1.8E-04	2.8E+00	1.1E+05	11.9	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.0E+02	1.4E+00	5.0E+01	-8.39	-8.43	-9.84	-2.18	0.56	0.0%	0.0%	3.2E-28
1318	3234-85-3	tetradecyl myristate	425	163	2.1E-06	1.3E-07	4.5E+12	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.9E+01	1.1E+00	3.8E+01	-9.89	-9.89	-9.89	-3.24	2.87	0.0%	0.0%	1.0E-21
1319	5468-75-7	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2-methylphenyl)-3-oxobutyramide]	658	350	2.7E-20	1.4E-05	1.0E+07	0.6	3.5E-06	3.5E-07	3.5E-08	conf	conf	1.2E+02	1.6E+00	6.0E+01	-7.87	-7.87	-9.47	-0.74	1.21	0.0%	0.0%	6.1E-36
1320	112-05-0	nonanoic acid	158	59	2.9E+00	4.1E+02	3.3E+03	4.9	3.5E-06	3.8E-06	1.1E-06	conf	conf	1.4E+02	1.9E+00	7.1E+01	-9.09	-9.21	-10.80	-1.19	0.47	0.0%	0.0%	3.4E-43
1321	123-62-6	propionic anhydride	130	-69	2.1E+02	1.3E+04	2.5E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.4E+02	1.9E+00	7.1E+01	-9.47	-9.35	-10.73	-1.35	0.21	0.0%	0.0%	2.8E-41
1322	371771-07-2	N-[4-(1,1,1,2,3,3,3-heptafluoropropan-2-yl)-2-methylphenyl]-N'-[2-methyl-1-(methylsulfinyl)propan-2-yl]phthalamic	541	275	2.9E-15	8.9E-04	6.0E+05	13.2	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.9E+01	1.4E+00	4.9E+01	-8.01	-9.12	-10.30	-2.18	0.64	0.0%	0.0%	2.0E-31
1323	112-54-9	dodecanal	184	14	2.1E+00	4.0E+00	5.6E+04	14.0	3.5E-06	3.7E-06	1.1E-07	conf	conf	1.1E+02	1.6E+00	5.7E+01	-10.42	-10.21	-11.71	-3.48	0.75	0.0%	0.0%	3.4E-32
1324	142-87-0	sodium decyl sulphate	260	87	9.9E-03	1.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+02	1.4E+00	5.1E+01	-7.01	-7.32	-8.97	-1.13	1.23	0.0%	0.0%	2.0E-29
1325	16530-71-5	ammonium myristate	245	87	9.9E-03	1.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+02	1.4E+00	5.1E+01	-7.01	-7.32	-8.97	-1.84	0.64	0.0%	0.0%	1.0E-24
1326	488-98-2	o-fluoro-α,α,α-trichlorotoluene	213	16	4.5E+01	3.2E+01	1.3E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-10.04	-9.76	-11.66	-2.83	0.67	0.0%	0.0%	8.3E-37
1327	112-31-2	decanal	156	-8	3.1E+01	5.2E+01	5.8E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.0E+02	1.4E+00	5.0E+01	-9.81	-9.54	-11.19	-2.67	0.17	0.0%	0.0%	2.1E-34
1328	111-48-8	thiodiglycol	122	25	3.2E-02	1.5E+05	2.4E-01	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.4E+02	1.9E+00	7.1E+01	-7.78	-8.88	-10.68	0.12	0.57	0.0%	0.0%	5.1E-54
1329	460-00-4	1-bromo-4-fluorobenzene	175	-19	5.0E+02	2.3E+02	1.2E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-10.04	-9.73	-11.80	-2.28	0.18	0.0%	0.0%	2.1E-42
1330	138401-24-8	4'-((2-butyl-4-oxo-1,3-diazaspiro[4.4]non-1-ene-3-yl)methyl)(1,1'-biphenyl)-2-carbonitrile	386	244	3.2E-10	5.6E-03	4.6E+06	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-8.69	-9.24	-10.25	-2.64	0.16	0.0%	0.0%	8.6E-28
1331	91745-35-6	Amines, bis(hydrogenated tallow alkyl), 2-[[bis(hydrogenated tallow alkyl)amino]carbonyl]benzoates	1191	87	9.9E-03	8.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+02	1.4E+00	5.1E+01	-6.99	-7.32	-8.99	-0.50	0.64	0.0%	0.0%	4.0E-34
1332	2627-95-4	1,1,3,3-tetramethyl-1,3-divinyldisiloxane	186	-57	6.0E+04	7.7E-02	9.1E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	8.5E+01	1.2E+00	4.1E+01	-10.68	-10.43	-13.40	-3.34	0.23	0.0%	0.0%	3.9E-47
1333	3851-87-4	bis(3,5,5-trimethylhexanoyl) peroxide	314	7	2.0E-01	1.8E-01	1.1E+07	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	8.5E+01	1.2E+00	4.2E+01	-10.25	-10.17	-11.78	-1.65	0.37	0.0%	0.0%	1.0E-47
1334	629-03-8	1,6-dibromohexane	244	8	7.4E+00	1.5E+01	9.3E+03	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.6E+01	1.3E+00	4.8E+01	-9.86	-9.58	-11.27	-2.85	0.64	0.0%	0.0%	1.3E-33
1335	119-17-5	m-(4,5-dihydro-3-methyl-5-oxo-1H-pyrazol-1-yl)benzenesulphonic acid	254	197	4.3E-09	1.1E+04	2.5E-01	0.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.3E+02	1.8E+00	6.7E+01	-6.77	-8.07	-10.09	-0.65	0.61	0.0%	0.0%	8.9E-42
1336	64754-95-6	Castor oil, hydrogenated, lithium salt	945	87	9.9E-03	6.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+02	1.4E+00	5.1E+01	-7.00	-7.32	-8.99	-0.48	0.64	0.0%	0.0%	2.5E-34
1337	142-92-7	hexyl acetate	144	-33	1.9E+02	9.4E+02	6.8E+02	14.0	3.5E-06	9.2E-07	1.1E-06	conf	conf	1.2E+02	1.7E+00	6.1E+01	-9.86	-9.60	-10.97	-2.27	0.36	0.0%	0.0%	9.2E-36
1338	15396-00-6	3-(trimethoxysilyl)propyl isocyanate	205	33	1.2E+01	7.0E+05	1.8E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.3E+02	1.8E+00	6.7E+01	-8.10	-8.28	-10.18	-0.88	0.90	0.0%	0.0%	1.5E-40
1339	505-65-7	1,3-dioxepane	102	-52	1.8E+03	6.7E+04	4.7E+00	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.2E+02	1.6E+00	5.9E+01	-9.01	-8.77	-10.01	-0.67	1.45	0.0%	0.0%	7.3E-41
1340	707-72-2	615-161-8	229	2	2.9E+01	2.9E+01	8.7E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-9.98	-9.70	-11.56	-3.71	0.64	0.0%	0.0%	1.7E-29
1341	29901-62-0	potassium sulphanilate	211	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+02	1.4E+00	5.0E+01	-7.03	-7.33	-8.98	-1.84	0.64	0.0%	0.0%	8.9E-25
1342	28783-41-7	4,5,6,7-tetrahydrothieno[3,2-c]pyridinium chloride	176	87	9.9E-03	1.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+02	1.4E+00	5.0E+01	-7.03	-7.33	-8.98	-1.00	0.64	0.0%	0.0%	1.9E-30
1343	36443-68-2	ethylenebis(oxyethylene) bis[3-(5-tert-butyl-4-hydroxy-m-tolyl)propionate]	587	274	1.5E-14	3.3E-04	1.6E+08	11.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	8.1E+01	1.1E+00	4.0E+01	-8.67	-9.28	-9.59	-0.73	0.45	0.0%	0.0%	5.3E-37
1344	42125-46-2	4-tert-butylcyclohexyl chloroformate	219	23	5.7E+00	6.6E-01	1.5E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-10.46	-10.17	-12.54	-2.59	0.79	0.0%	0.0%	3.9E-46
1345	104358-16-9	600-558-0	236	59	4.6E-02	2.1E-01	1.5E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-10.20	-10.01	-11.17	-3.40	0.09	0.0%	0.0%	6.4E-29
1346	56-86-0	glutamic acid	147	228	1.5E-04	3.3E+05	1.5E-04	2.1	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.3E+02	1.9E+00	6.9E+01	-7.25	-8.67	-10.64	-0.76	0.43	0.0%	0.0%	1.5E-45
1347	104-83-6	α,4-dichlorotoluene	161	3	1.2E+01	8.6E+01	2.8E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.2E+01	1.3E+00	4.6E+01	-9.33	-9.06	-10.52	-2.93	0.81	0.0%	0.0%	1.2E-27
1348	99-61-6	3-nitrobenzaldehyde	151	69	6.0E-01	1.1E+03	3.4E+01	14.0	3.5E-06	6.6E-08	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-7.75	-7.49	-8.85	-1.52	0.22	0.0%	0.0%	6.1E-26
1349	19529-38-5	disodium [N,N-bis[2-[bis(carboxymethyl)amino]ethyl]glycinato(5-)]ferrate(2-)	495	87	9.9E-03	3.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.9E+01	1.4E+00	5.0E+01	-7.02	-7.33	-8.99	-0.66	1.09	0.0%	0.0%	5.1E-33
1350	2612-57-9	2,4-dichlorophenyl isocyanate	188	24	1.5E+01	1.6E+02	7.6E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.1E+01	1.3E+00	4.5E+01	-9.30	-9.04	-10.43	-1.94	0.92	0.0%	0.0%	3.2E-34
1351	142-96-1	dibutyl ether	130	-50	1.0E+03	4.2E+02	1.0E+03	14.0	3.5E-06	3.1E-08	3.5E-07	conf	conf	7.7E+01	1.1E+00	3.7E+01	-10.00	-9.71	-11.66	-1.16	0.45	0.0%	0.0%	3.5E-51
1352	77-76-9	acetone-dimethyl acetal	104	-75	1.1E+04	2.8E+04	2.4E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	1.0E+02	1.5E+00	5.2E+01	-9.41	-9.06	-10.86	-0.94	0.71	0.0%	0.0%	7.1E-46
1353	81646-13-1	docosyltrimethylammonium methyl sulphate	480	87	9.9E-03	3.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.8E+01	1.4E+00	4.9E+01	-7.02	-7.34	-9.00	-2.79	0.56	0.0%	0.0%	3.7E-19
1354	1026785-65-8	methyl 3-{1,4-dioxaspiro[4.5]dec-8-yl[(trans-4-methylcyclohexyl)carbonyl]amino}-5-iodothiophene-2-carboxylate	547	243	3.4E-10	4.4E-02	1.4E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-8.45	-9.27	-10.32	-3.29	0.31	0.0%	0.0%	4.7E-24
1355	1724-39-6	cyclododecanol	184	25	1.7E-02	1.0E+01	3.8E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E+02	1.5E+00	5.5E+01	-9.07	-8.90	-10.38	-2.29	0.15	0.0%	0.0%	3.5E-31
1356	102-36-3	3,4-dichlorophenyl isocyanate	188	24	9.5E+00	1.6E+02	7.6E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.1E+01	1.3E+00	4.5E+01	-9.20	-8.94	-10.25	-2.02	1.19	0.0%	0.0%	3.0E-32
1357	130841-23-5	620-459-6	358	95	6.3E-02	2.5E-01	3.0E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.4E+01	1.3E+00	4.7E+01	-10.21	-9.97	-11.40	-3.71	0.45	0.0%	0.0%	2.3E-28
1358	143390-89-0	Kresoxim-Methyl	313	137	1.7E-04	4.2E+00	7.6E+05	14.0	3.5E-06	7.1E-07	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-8.75	-9.03	-10.20	-3.80	0.46	0.0%	0.0%	3.0E-20
1359	15086-94-9	2-(3,6-dihydroxy-2,4,5,7-tetrabromoxanthen-9-yl)-benzoic acid	648	284	1.9E-15	5.3E-05	8.1E+06	6.1	3.5E-06	1.1E-06	3.5E-08	conf	conf	9.1E+01	1.3E+00	4.5E+01	-8.10	-8.92	-10.30	-3.85	1.08	0.0%	0.0%	1.6E-20
1360	7139-02-8	2,6-dichloro-4,8-dipiperidinopyrimido[5,4-d]pyrimidine	367	202	1.9E-07	1.2E-01	2.8E+05	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-7.86	-8.49	-9.84	-2.27	0.07	0.0%	0.0%	1.4E-27
1361	597-82-0	O,O,O-triphenyl phosphorothioate	342	86	3.4E-05	1.1E-01	3.0E+06	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	8.3E+01	1.2E+00	4.1E+01	-8.72	-8.97	-9.99	-3.64	0.12	0.0%	0.0%	5.5E-20
1362	35113-48-5	609-063-4	274	23	2.3E-01	1.1E+03	2.9E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.3E+02	1.8E+00	6.7E+01	-9.29	-9.11	-10.76	-1.82	0.87	0.0%	0.0%	1.2E-37
1363	26544-23-0	isodecyl diphenyl phosphite	374	155	7.0E-06	5.8E-03	3.3E+08	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	7.6E+01	1.1E+00	3.7E+01	-8.67	-9.18	-9.36	-4.59	0.36	0.0%	0.0%	4.7E-12
1364	85187-23-1	1,3,5-triisopropyl-2,4-dinitrobenzene	294	136	2.4E-04	2.7E-02	1.0E+06	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	9.1E+01	1.3E+00	4.4E+01	-8.67	-8.40	-9.58	-3.65	0.49	0.0%	0.0%	1.2E-17
1365	50-89-5	thymidine	242	227	1.8E-11	5.2E+03	2.3E-01	9.7	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.3E+02	1.8E+00	6.7E+01	-7.36	-8.58	-10.65	-0.67	1.62	0.0%	0.0%	2.2E-46
1366	57693-14-8	trisodium bis[3-hydroxy-4-[(2-hydroxy-1-naphthyl)azo]-7-nitronaphthalene-1-sulphonato(3-)]chromate(3-)	1004	87	9.9E-03	6.9E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.7E+01	1.3E+00	4.8E+01	-7.02	-7.34	-9.01	-1.63	0.51	0.0%	0.0%	3.0E-26
1367	1025-15-6	1,3,5-triallyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	249	195	3.3E-05	9.2E+02	1.3E+05	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	1.0E+02	1.4E+00	4.9E+01	-6.76	-7.37	-8.99	-2.05	1.11	0.0%	0.0%	1.8E-23
1368	2873-97-4	N-(1,1-dimethyl-3-oxobutyl)acrylamide	169	96	7.7E-02	1.1E+04	8.9E-01	-0.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.2E+02	1.7E+00	6.4E+01	-7.15	-8.36	-10.19	-1.40	0.08	0.0%	0.0%	1.8E-36
1369	194608-78-1	2-Propylheptan-1-amine	157	2	3.4E+01	3.3E+01	5.1E+03	10.5	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.0E+01	1.3E+00	4.5E+01	-9.95	-9.67	-11.45	-2.85	0.55	0.0%	0.0%	5.6E-35
1370	125-65-5	pleuromulin	379	201	1.6E-09	9.2E-01	8.5E+02	12.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+02	1.7E+00	6.2E+01	-7.50	-8.54	-10.20	-1.93	0.70	0.0%	0.0%	1.5E-32
1371	35948-25-5	6H-dibenz[c,e][1,2]oxaphosphorin 6-oxide	216	84	3.8E-03	1.9E+02	7.4E+01	14.0	3.5E-06	3.5E-07	3.5E-08	conf	conf	1.1E+02	1.5E+00	5.6E+01	-7.52	-7.64	-9.53	-0.86	0.57	0.0%	0.0%	1.6E-35
1372	52-89-1	cysteine hydrochloride	158	87	9.9E-03	1.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.6E+01	1.3E+00	4.8E+01	-7.05	-7.35	-9.00	-0.78	0.50	0.0%	0.0%	3.7E-32
1373	127-68-4	sodium 3-nitrobenzenesulphonate	225	87	9.9E-03	1.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.6E+01	1.3E+00	4.8E+01	-7.04	-7.35	-9.00	0.64	0.35	0.0%	0.0%	1.7E-43
1374	2373-38-8	sodium 1,4-bis(1,3-dimethylbutyl) sulphonatosuccinate	388	87	9.9E-03	2.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.6E+01	1.3E+00	4.8E+01	-7.04	-7.35	-9.01	0.06	0.64	0.0%	0.0%	1.2E-38
1375	957-68-6	3-acetoxymethylen-7-amino-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid	272	305	5.1E-09	1.1E+04	4.7E-02	2.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.3E+02	1.8E+00	6.6E+01	-7.31	-8.79	-10.66	-1.51	0.77	0.0%	0.0%	2.2E-39
1376	20292-08-4	2-ethylhexyl laurate	313	81	4.2E-03	6.0E-03	4.5E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.6E+01	1.1E+00	3.7E+01	-9.33	-9.49	-10.51	-0.55	0.78	0.0%	0.0%	3.1E-46
1377	111974-73-3	601-145-8	321	169	2.5E-06	7.1E-01	1.9E+05	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-7.92	-8.43	-9.85	-3.02	0.65	0.0%	0.0%	8.8E-23
1378	65405-84-7	α,2,2,6-tetramethylcyclohexene-1-butyraldehyde	208	43	8.3E-01	2.5E+01	1.6E+05	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-9.48	-9.26	-10.36	-2.82	0.23	0.0%	0.0%	2.3E-27
1379	123-11-5	anisaldehyde	136	13	4.0E+00	4.8E+03	6.2E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.2E+02	1.7E+00	6.3E+01	-8.84	-8.62	-10.25	-1.00	0.15	0.0%	0.0%	3.7E-40
1380	2135-17-3	flumetasone	410	216	1.4E-11	3.3E+01	3.9E+01	13.0	3.5E-06	1.1E-07	1.1E-06	conf	conf	9.3E+01	1.3E+00	4.6E+01	-6.96	-7.56	-9.05	-1.00	0.64	0.0%	0.0%	7.0E-31
1381	30125-47-4	3,4,5,6-tetrachloro-N-[2-(4,5,6,7-tetrachloro-2,3-dihydro-1,3-dioxo-1H-inden-2-yl)-8-quinolyl]phthalimide	694	350	2.3E-19	1.4E-07	1.5E+10	1.5	3.5E-06	3.5E-09	3.5E-09	conf	conf	7.4E+01	1.0E+00	3.6E+01	-9.86	-9.86	-9.86	-5.62	0.69	0.0%	0.0%	6.6E-10
1382	98-60-2	4-chlorobenzenesulphonyl chloride	211	85	1.6E-01	5.2E+02	3.9E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.1E+01	1.3E+00	4.5E+01	-7.92	-7.66	-9.14	-1.75	0.52	0.0%	0.0%	2.4E-26
1383	13402-02-3	hexadecyl acrylate	297	80	5.8E-03	6.3E-03	1.2E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.7E+01	1.1E+00	3.7E+01	-9.65	-9.75	-11.00	-0.85	0.26	0.0%	0.0%	5.7E-48
1384	79-03-8	propionyl chloride	93	-68	1.3E+04	1.9E+04	1.0E+00	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.2E+02	1.7E+00	6.3E+01	-10.28	-10.03	-11.72	-2.27	1.06	0.0%	0.0%	7.5E-42
1385	31335-74-7	2,2-dimethyl-1,3-propanediyl dioctanoate	357	26	5.8E-03	5.3E-02	4.6E+07	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.8E+01	1.1E+00	3.8E+01	-9.70	-9.79	-10.69	-4.32	0.57	0.0%	0.0%	4.7E-20
1386	122-01-0	4-chlorobenzoyl chloride	175	33	1.6E+01	3.3E+02	1.2E+02	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.1E+01	1.3E+00	4.5E+01	-9.03	-8.75	-10.13	-0.98	0.36	0.0%	0.0%	2.4E-39
1387	53056-20-5	610-950-3	223	64	4.0E-01	1.4E+01	3.3E+02	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.1E+01	1.3E+00	4.5E+01	-8.90	-8.63	-9.95	-2.31	0.29	0.0%	0.0%	4.8E-28
1388	543-39-5	2-methyl-6-methyleneoct-7-en-2-ol	154	-12	1.2E+01	3.8E+02	2.9E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E+02	1.6E+00	5.8E+01	-9.56	-9.34	-10.49	-2.04	0.15	0.0%	0.0%	7.7E-34
1389	3621-82-7	2,6-dichlorobenzoxazole	188	66	6.4E-01	9.0E+01	1.0E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.1E+01	1.3E+00	4.5E+01	-8.50	-8.24	-9.51	-2.06	0.14	0.0%	0.0%	9.7E-27
1390	91-66-7	N,N-diethylaniline	149	-1	2.1E+01	1.6E+03	1.4E+03	6.0	3.5E-06	1.7E-08	3.5E-07	conf	conf	7.6E+01	1.1E+00	3.7E+01	-7.93	-7.65	-8.59	-1.96	0.70	0.0%	0.0%	1.4E-21
1391	82966-34-5	[(2R*, 4R*) -2-(bromomethyl)-2-(2,4-dichlorophenyl)-1,3-dioxolan-4-yl]methyl methanesulfonate	420	189	1.3E-06	3.2E+00	1.1E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.1E+01	1.3E+00	4.5E+01	-6.85	-7.50	-9.06	-2.08	0.33	0.0%	0.0%	9.2E-24
1392	1400584-86-	sodium (5s,8s)-8-methoxy-2,4-dioxo-1,3-diazaspiro[4.5]decan-3-ide	221	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.4E+01	1.3E+00	4.7E+01	-7.06	-7.36	-9.01	-1.84	0.64	0.0%	0.0%	5.7E-25
1393	75330-75-5	(1S,3R,7S,8S,8aR)-8-{2-[(2R,4R)-4-hydroxy-6-oxotetrahydro-2H-pyran-2-yl]ethyl}-3,7-dimethyl-1,2,3,7,8,8a-hexahydr	405	198	1.8E-10	5.2E-01	5.5E+04	14.0	3.5E-06	2.5E-07	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-7.40	-8.23	-9.64	-2.62	0.45	0.0%	0.0%	5.6E-24
1394	1247119-36-	Ethyl (2S)-2-({[(2-isopropyl-1,3-thiazol-4-yl)methyl](methyl)carbamoyl}amino)-4-(morpholin-4-yl)butanoate ethane	503	87	9.9E-03	3.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.3E+01	1.3E+00	4.7E+01	-7.04	-7.36	-9.02	-1.84	0.64	0.0%	0.0%	5.2E-25
1395	84029-45-8	sodium 4-(4-methyl-3-nitrobenzoylamino)benzenesulphonate	358	87	9.9E-03	2.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.3E+01	1.3E+00	4.7E+01	-7.05	-7.36	-9.02	-1.84	0.64	0.0%	0.0%	5.4E-25
1396	64131-85-7	O,O,O-tris(4-nitrophenyl) thiophosphate	477	90	2.7E-06	1.1E-01	8.3E+05	14.0	3.5E-06	3.5E-06	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.5E+01	-9.33	-9.60	-10.88	-2.96	0.37	0.0%	0.0%	5.7E-30
1397	227197-72-0	607-145-4	154	49	3.9E+00	6.3E+02	2.3E+02	-0.1	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.1E+01	1.3E+00	4.6E+01	-6.66	-7.35	-8.95	-1.53	0.23	0.0%	0.0%	1.4E-26
1398	10081-67-1	4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)phenyl]aniline	406	215	2.3E-08	2.1E-04	3.2E+08	0.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.2E+02	1.6E+00	6.0E+01	-7.50	-8.60	-10.21	-1.00	0.12	0.0%	0.0%	7.7E-40
1399	70714-66-8	[[(phosphonomethyl)imino]bis[ethylenenitrilobis(methylene)]]tetrakisphosphonic acid, ammonium salt	590	87	9.9E-03	4.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.3E+01	1.3E+00	4.6E+01	-7.04	-7.36	-9.02	0.07	0.64	0.0%	0.0%	7.1E-39
1400	4672-38-2	propylphosphonic acid	124	28	1.1E-02	1.5E+05	9.5E-01	2.6	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.2E+02	1.7E+00	6.1E+01	-7.24	-8.40	-10.22	-1.00	0.00	0.0%	0.0%	7.0E-40
1401	6331-96-0	2-amino-4,5-dichlorobenzenesulfonic acid	242	157	1.1E-06	3.5E+01	1.6E-01	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.2E+01	1.3E+00	4.6E+01	-6.45	-7.31	-8.92	-0.54	0.13	0.0%	0.0%	2.2E-33
1402	2212-81-9	[1,3-phenylenebis(1-methylethylidene)]bis[tert-butyl] peroxide	338	113	2.3E-03	5.4E-02	2.2E+07	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	7.5E+01	1.0E+00	3.6E+01	-9.55	-9.54	-10.35	-3.27	0.56	0.0%	0.0%	2.4E-24
1403	26567-10-2	3,3',5,5'-tetramethylbiphenyl-2,2'-diol	242	161	2.2E-06	1.5E+00	9.8E+04	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	9.1E+01	1.3E+00	4.5E+01	-6.85	-7.41	-9.04	-3.06	0.14	0.0%	0.0%	6.9E-18
1404	103-24-2	bis(2-ethylhexyl) azelate	413	41	5.0E-04	1.6E-03	3.9E+09	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.2E+01	1.0E+00	3.5E+01	-9.03	-9.12	-9.60	-4.66	0.57	0.0%	0.0%	8.4E-13
1405	2402-77-9	2,3-dichloropyridine	148	19	4.0E+01	1.1E+03	1.2E+02	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.1E+01	1.3E+00	4.5E+01	-8.94	-8.66	-9.98	-3.04	0.97	0.0%	0.0%	1.9E-23
1406	10291-28-8	2,5-bis(p-toluidino)terephthalic acid	376	253	7.4E-11	9.4E-01	3.7E+05	-0.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+02	1.6E+00	6.0E+01	-7.66	-8.37	-10.18	-3.59	0.68	0.0%	0.0%	2.4E-21
1407	88-50-6	4-amino-2,5-dichlorobenzenesulphonic acid	242	157	1.1E-06	3.5E+01	1.6E-01	-1.1	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.1E+01	1.3E+00	4.6E+01	-6.29	-7.28	-8.89	-1.81	0.77	0.0%	0.0%	2.3E-24
1408	25953-19-9	cefazolin	455	333	2.0E-16	2.6E+01	2.5E-03	2.6	3.5E-06	1.1E-07	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-6.35	-7.39	-8.96	-1.04	1.35	0.0%	0.0%	5.5E-30
1409	90-02-8	salicylaldehyde	122	43	3.0E+01	8.8E+03	1.0E+02	8.4	3.5E-06	1.6E-06	3.5E-06	conf	conf	1.2E+02	1.7E+00	6.2E+01	-9.21	-9.01	-10.45	-2.24	0.38	0.0%	0.0%	4.6E-32
1410	4584-46-7	2-chloroethyldimethylammonium chloride	144	87	9.9E-03	9.9E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.2E+01	1.3E+00	4.6E+01	-7.07	-7.37	-9.02	-1.84	0.64	0.0%	0.0%	5.4E-25
1411	127337-60-4	2-(chloromethyl)-3-methyl-4-(2,2,2-trifluoroethoxy)pyridine hydrochloride (1:1)	276	87	9.9E-03	1.9E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.2E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.02	-1.84	0.64	0.0%	0.0%	5.0E-25
1412	5407-04-5	3-chloropropyldimethylammonium chloride	158	87	9.9E-03	1.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.2E+01	1.3E+00	4.6E+01	-7.07	-7.37	-9.02	-0.88	0.64	0.0%	0.0%	1.4E-31
1413	694-83-7	cyclohex-1,2-ylenediamine	114	27	5.4E+01	1.0E+06	1.2E+00	10.0	3.5E-06	4.2E-08	3.5E-07	conf	conf	8.0E+01	1.1E+00	4.0E+01	-7.45	-7.32	-8.62	-1.00	0.77	0.0%	0.0%	7.0E-28
1414	18516-18-2	3-hydroxy-2-(hydroxymethyl)-2-methylpropionaldehyde	118	34	3.3E-01	3.1E+05	4.7E-02	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.2E+02	1.7E+00	6.4E+01	-7.83	-8.86	-10.72	-0.41	0.38	0.0%	0.0%	1.9E-49
1415	96441-14-4	N-[2-(3-carbamoyl-4-hydroxyphenyl)-2-oxoethyl]-N-(4-phenylbut-2-yl)ammonium chloride	363	87	9.9E-03	2.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.2E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.8E-25
1416	2996-92-1	trimethoxyphenylsilane	198	20	9.7E+00	7.9E+02	3.5E+00	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.1E+02	1.5E+00	5.3E+01	-8.85	-8.61	-9.96	-0.33	0.54	0.0%	0.0%	2.5E-43
1417	73978-41-3	(2,4-diaminopteridin-6-yl)methanol monohydrochloride	229	87	9.9E-03	1.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.2E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.02	-1.84	0.64	0.0%	0.0%	4.9E-25
1418	50-24-8	prednisolone	360	215	9.1E-12	4.4E+02	2.5E+01	13.2	3.5E-06	1.4E-07	1.1E-06	conf	conf	9.3E+01	1.3E+00	4.6E+01	-6.96	-7.63	-9.17	-1.70	1.42	0.0%	0.0%	6.0E-27
1419	5208-93-5	3-methyl-1-(2,6,6-trimethylcyclohex-1-en-1-yl)penta-1,4-dien-3-ol	220	72	9.8E-03	4.7E+00	2.8E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-9.25	-9.18	-10.49	-2.38	0.41	0.0%	0.0%	2.4E-31
1420	133647-88-8	Propanoic acid, 2-(4-hydroxyphenoxy)-, sodium salt (1:1), (2R)-	204	87	9.9E-03	1.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.37	-9.02	-0.70	0.27	0.0%	0.0%	6.9E-33
1421	13222-26-9	2-Chloro-2-methylpropanoyl chloride	141	-35	2.0E+03	2.8E+03	4.5E+00	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	9.1E+01	1.3E+00	4.5E+01	-9.55	-9.13	-11.18	-1.32	0.52	0.0%	0.0%	2.6E-45
1422	6425-39-4	2,2'-dimorpholinyldiethyl ether	244	106	1.0E-02	2.8E+05	4.9E-02	6.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+02	1.6E+00	6.0E+01	-6.95	-8.08	-10.18	-0.22	0.63	0.0%	0.0%	3.3E-46
1423	24085-08-3	2-[tert-butyl(phenylmethyl)amino]-1-[4-hydroxy-3-(hydroxymethyl)phenyl] hydrochloride	364	87	9.9E-03	2.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.70	0.64	0.0%	0.0%	6.3E-26
1424	6640-22-8	disodium 4,4'-methylenebis[3-hydroxy-2-naphthoate]	432	87	9.9E-03	3.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.5E-25
1425	30018-16-7	(2-ethoxy-1-methyl-2-oxoethyl)triphenylphosphonium bromide	443	87	9.9E-03	3.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.5E-25
1426	27511-79-1	5-aminopyrazole-4-carboxamide hemisulphate	350	87	9.9E-03	2.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.6E-25
1427	139893-43-9	604-165-5	454	87	9.9E-03	3.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.05	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.5E-25
1428	88046-01-9	(2-carbamimidamido-1,3-thiazol-4-yl)methyl carbamimidothioate dihydrochloride	303	87	9.9E-03	2.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.6E-25
1429	754186-36-2	(2S)-N-[(diethylamino)methyl]-2-(2-oxopyrrolidin-1-yl)butanamide (2R,3R)-tartrate	405	87	9.9E-03	2.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.5E-25
1430	1184182-45-	Salt of N-acetyl-L-glutamic acid and 1-[(7S)-3,4-dimethoxybicyclo[4.2.0]octa-1,3,5-trien-7-yl]methanamine (1:1), mo	400	87	9.9E-03	2.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.5E-25
1431	19294-29-2	Potassium 4-methylbenzenesulfinate	194	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.37	-9.02	-1.84	0.64	0.0%	0.0%	4.9E-25
1432	62476-59-9	sodium 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoate	384	87	9.9E-03	2.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.20	0.62	0.0%	0.0%	2.5E-29
1433	86386-77-8	1-{[2-(2,4-difluorophenyl)oxiran-2-yl]methyl}-1H-1,2,4-triazole monomethanesulfonate	333	87	9.9E-03	2.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.6E-25
1434	4316-74-9	sodium N-methyltaurinate	161	87	9.9E-03	1.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.38	-9.02	1.24	1.03	0.0%	0.0%	5.0E-25
1435	1115-70-4	metformin hydrochloride	166	87	9.9E-03	1.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.38	-9.02	-6.00	0.64	0.0%	0.0%	5.0E-25
1436	5344-48-9	611-000-0	285	87	9.9E-03	2.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.7E-25
1437	220380-44-9	691-746-1	1618	87	9.9E-03	1.1E+04	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.04	-7.37	-9.04	-1.84	0.64	0.0%	0.0%	4.1E-25
1438	46830-22-2	benzyldimethyl[2-[(1-oxoallyl)oxy]ethyl]ammonium chloride	270	87	9.9E-03	1.9E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.34	0.56	0.0%	0.0%	2.3E-28
1439	3598-16-1	sodium phenoxyacetate hemihydrate	174	87	9.9E-03	1.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.38	-9.02	-1.84	0.64	0.0%	0.0%	4.9E-25

1440	1192015-20-	[2-(4-benzyl-2-phenylpiperazin-1-yl)phenyl]methanol (2E)-but-2-enedioate (1:1)	475	87	9.9E-03	3.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.05	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.5E-25
1441	114-49-8	hyoscine hydrobromide	384	87	9.9E-03	2.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.5E-25
1442	7400-27-3	tert-butylhydrazine monohydrochloride	125	87	9.9E-03	8.6E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.08	-7.38	-9.02	-1.84	0.64	0.0%	0.0%	5.1E-25
1443	121627-17-6	6,6'-[(3,3'-di-tert-butyl-5,5'-dimethoxybiphenyl-2,2'-diyl)bis(oxy)]bis(dibenzo[d,f][1,3,2]dioxaphosphepine)	787	87	9.9E-03	5.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.05	-7.37	-9.03	-1.62	0.64	0.0%	0.0%	1.7E-26
1444	86604-75-3	Pyridine, 2-(chloromethyl)-4-methoxy-3,5-dimethyl-, hydrochloride (1:1)	222	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.37	-9.03	-2.61	0.35	0.0%	0.0%	2.6E-20
1445	98231-71-1	619-328-6	252	87	9.9E-03	1.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.7E-25
1446	155-41-9	N-methylhyoscinium bromide	398	87	9.9E-03	2.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.5E-25
1447	1124-64-7	620-019-3	172	87	9.9E-03	1.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.38	-9.02	-1.84	0.64	0.0%	0.0%	4.9E-25
1448	132335-47-8	(3S)-N,N-dimethyl-3-(naphthalen-1-yloxy)-3-(thiophen-2-yl)propan-1-amine ethanedioate	401	87	9.9E-03	2.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.5E-25
1449	15295-77-9	(3S)-2-Oxotetrahydrofuran-3-ammonium bromide	182	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.38	-9.02	-1.84	0.64	0.0%	0.0%	4.9E-25
1450	252317-48-9	607-657-8	489	87	9.9E-03	3.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.05	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.4E-25
1451	78628-80-5	1-Naphthalenemethanamine, N-[(2E)-6,6-dimethyl-2-hepten-4-yn-1-yl]-N-methyl-, hydrochloride (1:1)	328	87	9.9E-03	2.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-4.22	0.64	0.0%	0.0%	3.2E-12
1452	106649-95-0	N-(aminosulfonyl)-3-chloropropanimidamide hydrochloride	222	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.8E-25
1453	83393-23-1	8-benzyl-3-oxo-8-azoniabicyclo[3.2.1]octane chloride	252	87	9.9E-03	1.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.7E-25
1454	859-18-7	methyl (2S-trans)-6,8-dideoxy-6-[[(1-methyl-4-propylpyrrolidin-2-yl)carbonyl]amino]-1-thio-D-erythro-α-D-galacto-c	443	87	9.9E-03	3.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-2.62	1.29	0.0%	0.0%	2.8E-20
1455	886588-62-1	692-713-4	380	87	9.9E-03	2.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.5E-25
1456	581076-67-7	Benzamide, N-[3-[(aminoiminomethyl)amino]-4-methylphenyl]-4-[(4-methyl-1-piperazinyl)methyl]-, hydrochloride (	417	87	9.9E-03	2.9E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.25	0.60	0.0%	0.0%	5.4E-29
1457	128346-46-3	N,N,N-trimethyladamantan-1-aminium chloride	230	87	9.9E-03	1.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.8E-25
1458	657-27-2	lysine hydrochloride	183	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.38	-9.02	-1.84	0.64	0.0%	0.0%	4.9E-25
1459	104617-50-7	600-588-4	292	87	9.9E-03	2.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.7E-25
1460	69477-29-8	614-977-1	1194	87	9.9E-03	8.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.04	-7.37	-9.04	-1.84	0.64	0.0%	0.0%	4.1E-25
1461	1185167-55-	1-(2-isopropyl-1,3-thiazol-4-yl)-N-methylmethanamine dihydrochloride	243	87	9.9E-03	1.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.37	-9.03	-1.84	0.64	0.0%	0.0%	4.8E-25
1462	66-84-2	glucosamine hydrochloride	216	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.37	-9.02	-1.84	0.64	0.0%	0.0%	4.8E-25
1463	3724-43-4	609-368-2	128	87	9.9E-03	8.8E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.08	-7.38	-9.02	-1.84	0.64	0.0%	0.0%	5.1E-25
1464	33719-11-8	(3aR,8aS,8bS)-1,3-Dibenzyl-2-oxodecahydrothieno[1',2':1,2]thieno[3,4-d]imidazol-5-ium bromide	445	87	9.9E-03	3.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.06	-7.37	-9.03	-1.55	0.64	0.0%	0.0%	6.2E-27
1465	10545-99-0	sulphur dichloride	103	87	9.9E-03	7.1E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.08	-7.38	-9.02	-1.84	0.64	0.0%	0.0%	5.2E-25
1466	22252-43-3	(6R-trans)-7-amino-3-methyl-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid	214	298	1.1E-07	8.4E+03	1.3E-01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+02	1.6E+00	6.0E+01	-6.81	-7.96	-10.10	-0.91	1.11	0.0%	0.0%	1.1E-39
1467	31291-60-8	di-sec-butylphenol	206	76	4.2E-02	4.3E+01	2.6E+05	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	9.1E+01	1.3E+00	4.5E+01	-8.04	-7.76	-9.21	-3.36	0.32	0.0%	0.0%	3.1E-17
1468	3452-97-9	3,5,5-trimethylhexan-1-ol	144	-19	1.4E+01	1.2E+02	1.3E+03	14.0	3.5E-06	1.4E-07	3.5E-06	conf	conf	8.8E+01	1.2E+00	4.4E+01	-9.39	-9.11	-10.49	-1.88	0.18	0.0%	0.0%	5.2E-35
1469	345-92-6	bis(4-fluorophenyl) ketone	218	75	6.6E-02	1.5E+01	3.5E+03	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	1.1E+02	1.5E+00	5.6E+01	-9.07	-8.87	-10.32	-2.39	0.48	0.0%	0.0%	4.9E-30
1470	26576-46-5	N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxobutyramide	233	199	2.7E-07	1.3E+04	1.7E+00	2.3	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.0E+02	1.5E+00	5.3E+01	-6.49	-7.60	-9.50	-1.33	1.33	0.0%	0.0%	9.7E-32
1471	62518-65-4	3-(m-tert-butylphenyl)-2-methylpropionaldehyde	204	46	4.8E-01	4.0E+00	2.3E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-9.64	-9.38	-10.66	-2.84	0.23	0.0%	0.0%	2.8E-29
1472	139-40-2	propazine (reach)	230	116	9.7E-04	6.4E+00	1.7E+03	2.0	3.5E-06	2.2E-09	1.1E-07	conf	conf	7.0E+01	9.8E-01	3.4E+01	-7.01	-7.22	-8.17	-2.00	1.05	0.0%	0.0%	6.1E-19
1473	1927-95-3	4-bromophenyl acetate	215	39	3.3E+00	6.4E+01	3.0E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.0E+02	1.4E+00	5.1E+01	-9.36	-9.11	-10.39	-2.10	0.72	0.0%	0.0%	1.1E-32
1474	5856-77-9	2,2-dimethylbutyryl chloride	135	-36	1.5E+03	3.1E+03	2.4E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.1E+02	1.5E+00	5.4E+01	-10.01	-9.75	-11.41	-1.66	0.45	0.0%	0.0%	2.3E-44
1475	21643-42-5	tetradecyl acrylate	268	62	3.3E-02	7.6E-02	1.3E+07	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.6E+01	1.1E+00	3.7E+01	-10.18	-10.09	-11.34	-1.40	0.92	0.0%	0.0%	4.3E-46
1476	36483-57-5	2,2-dimethylpropan-1-ol, tribromo derivative	325	74	1.6E-02	9.8E+01	7.1E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.1E+02	1.6E+00	5.8E+01	-8.89	-8.69	-10.33	-1.47	0.55	0.0%	0.0%	4.5E-37
1477	110-71-4	1,2-dimethoxyethane	90	-82	1.1E+04	3.4E+05	6.2E-01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E+02	1.6E+00	5.9E+01	-9.26	-9.01	-10.40	0.92	0.30	0.0%	0.0%	3.3E-59
1478	55117-15-2	alpha,2-dichloro-6-fluorotoluene	179	9	2.7E+01	9.6E+01	4.4E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-9.73	-9.46	-11.00	-2.68	0.64	0.0%	0.0%	7.3E-33
1479	92-77-3	3-hydroxy-2-naphthanilide	263	205	5.0E-09	1.1E+01	3.0E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.39	-8.20	-9.76	-2.78	0.13	0.0%	0.0%	1.1E-23
1480	107-29-9	acetaldehyde oxime	59	-74	7.4E+02	7.4E+04	6.2E-01	11.9	3.5E-06	4.2E-07	3.5E-07	conf	conf	1.0E+02	1.4E+00	5.3E+01	-8.64	-8.40	-9.78	-0.95	0.52	0.0%	0.0%	8.0E-37
1481	1135-22-4	3-Thiophenebutanol, 2,5-dihydro-.alpha.,.alpha.-dimethyl-, 1,1-dioxide	218	103	4.7E-04	8.7E+03	9.5E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E+02	1.6E+00	5.8E+01	-7.22	-8.25	-10.23	-0.61	0.64	0.0%	0.0%	3.0E-43
1482	7173-51-5	didecyldimethylammonium chloride	362	87	9.9E-03	2.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.8E+01	1.2E+00	4.4E+01	-7.07	-7.39	-9.04	-3.58	0.67	0.0%	0.0%	3.1E-15
1483	6443-69-2	3,4,5-trimethoxytoluene	182	46	2.3E+00	1.1E+03	1.1E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E+02	1.6E+00	5.7E+01	-8.90	-8.70	-10.28	-2.93	1.38	0.0%	0.0%	4.6E-26
1484	141-75-3	butyryl chloride	107	-55	5.3E+03	5.2E+03	3.2E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.0E+02	1.4E+00	5.2E+01	-10.06	-9.75	-11.63	-1.67	1.12	0.0%	0.0%	3.1E-46
1485	50-23-7	hydrocortisone	362	215	1.6E-11	4.7E+02	4.2E+01	13.2	3.5E-06	2.1E-07	3.5E-07	conf	conf	9.5E+01	1.3E+00	4.8E+01	-6.84	-7.69	-9.37	-1.12	0.30	0.0%	0.0%	2.4E-32
1486	928-70-1	potassium isopentyl dithiocarbonate	202	87	9.9E-03	1.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.8E+01	1.2E+00	4.4E+01	-7.08	-7.39	-9.04	-2.15	1.06	0.0%	0.0%	3.6E-23
1487	76-05-1	trifluoroacetic acid	114	-24	1.5E+04	1.1E+07	3.2E+00	0.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.2E+02	1.6E+00	6.1E+01	-7.78	-8.98	-10.75	-0.49	1.29	0.0%	0.0%	5.6E-49
1488	107-10-8	propylamine	59	-72	4.1E+04	1.0E+06	2.2E+00	10.0	3.5E-06	4.1E-07	3.5E-06	conf	conf	1.0E+02	1.4E+00	5.2E+01	-9.30	-9.06	-10.14	-1.24	0.70	0.0%	0.0%	2.7E-37
1489	5292-45-5	dimethyl 2-nitroterephthalate	239	77	2.5E-02	1.6E+02	3.0E+01	14.0	3.5E-06	7.5E-07	3.5E-07	conf	conf	1.1E+02	1.5E+00	5.6E+01	-8.43	-8.22	-10.05	-2.27	0.72	0.0%	0.0%	5.1E-29
1490	59721-67-4	611-869-6	216	76	3.5E-02	8.4E-01	9.5E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-9.81	-9.61	-10.70	-2.65	0.11	0.0%	0.0%	5.9E-31
1491	2049-95-8	tert-pentylbenzene	148	-16	7.0E+01	7.9E+00	2.5E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	7.2E+01	1.0E+00	3.5E+01	-10.42	-10.12	-12.33	-2.75	0.16	0.0%	0.0%	6.4E-43
1492	32388-55-9	[3R-(3α,3aβ,7β,8aα)]-1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)ethan-1-one	246	92	7.6E-02	1.1E+01	1.0E+05	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	9.1E+01	1.3E+00	4.5E+01	-8.49	-8.18	-9.53	-2.73	0.25	0.0%	0.0%	1.3E-22
1493	97-72-3	isobutyric anhydride	158	-68	1.1E+02	3.5E+03	1.7E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.2E+02	1.6E+00	5.9E+01	-9.81	-9.67	-10.94	-1.04	0.45	0.0%	0.0%	1.2E-45
1494	118-92-3	anthranilic acid	137	94	1.0E-02	1.4E+04	2.3E+01	2.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E+02	1.5E+00	5.7E+01	-7.32	-8.28	-10.23	-1.08	0.59	0.0%	0.0%	2.7E-39
1495	947-19-3	hydroxycyclohexyl phenyl ketone	204	93	9.4E-04	4.9E+01	2.8E+02	13.4	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.1E+02	1.6E+00	5.9E+01	-8.91	-9.27	-10.79	-1.59	0.53	0.0%	0.0%	1.0E-39
1496	100-39-0	α-bromotoluene	171	-9	4.6E+01	2.0E+02	7.6E+02	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-9.65	-9.39	-10.93	-2.19	1.09	0.0%	0.0%	4.2E-36
1497	88069-93-6	618-109-2	216	67	5.4E-02	1.5E+01	1.4E+04	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-8.76	-8.54	-9.95	-2.40	0.38	0.0%	0.0%	2.0E-27
1498	344348-40-9	608-991-7	216	67	5.4E-02	1.5E+01	1.4E+04	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-8.76	-8.54	-9.95	-2.40	0.38	0.0%	0.0%	2.0E-27
1499	27489-62-9	trans-4-aminocyclohexan-1-ol	115	20	5.3E+00	5.7E+04	1.2E+00	10.0	3.5E-06	2.0E-07	3.5E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.97	-7.78	-9.41	-1.45	0.93	0.0%	0.0%	3.3E-30
1500	31027-31-3	p-isopropylphenyl isocyanate	161	-7	3.3E+01	1.2E+03	1.1E+04	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-9.34	-9.09	-10.24	-2.06	0.76	0.0%	0.0%	6.9E-32
1501	923-02-4	N-(hydroxymethyl)methacrylamide	115	80	2.7E+03	2.6E+05	5.5E-02	-1.3	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.2E+02	1.6E+00	6.0E+01	-7.55	-8.91	-10.75	-0.16	0.52	0.0%	0.0%	4.4E-52
1502	24424-99-5	di(tert-butyl) carbonate	218	-13	3.8E+00	1.9E+02	7.4E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E+02	1.5E+00	5.6E+01	-9.38	-9.19	-10.48	-0.95	0.31	0.0%	0.0%	1.6E-42
1503	312-94-7	α,α,α-trifluoro-o-toluoyl chloride	209	18	3.6E+01	2.5E+02	2.5E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+02	1.5E+00	5.4E+01	-9.86	-9.63	-11.06	-2.52	0.99	0.0%	0.0%	1.7E-34
1504	7473-98-5	2-hydroxy-2-methylpropiophenone	164	54	9.8E-02	8.6E+03	1.2E+01	13.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E+02	1.5E+00	5.6E+01	-7.87	-8.29	-10.24	-1.39	1.39	0.0%	0.0%	6.0E-37
1505	119618-67-6	Bis (acetato-κO)[7-chloro-1-cyclopropyl-6-fluoro-4-(oxo-κO)-1,4-dihydroquinoline-3-carboxylato-&#954	410	173	2.3E-06	2.3E+04	5.4E+01	-1.6	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.8E+01	1.4E+00	5.0E+01	-6.95	-7.80	-9.60	-3.11	0.64	0.0%	0.0%	8.9E-21
1506	6962-44-3	N-(2-methoxy-5-methylphenyl)acetamide	179	118	3.4E-03	2.0E+03	1.4E+01	0.3	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.8E+01	1.4E+00	5.0E+01	-6.95	-7.82	-9.64	-2.13	1.04	0.0%	0.0%	3.8E-27
1507	84-61-7	dicyclohexyl phthalate	330	61	6.1E-04	1.6E+02	1.6E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.9E+01	1.1E+00	3.9E+01	-8.79	-9.34	-10.40	-2.99	0.25	0.0%	0.0%	1.7E-26
1508	110-41-8	2-methylundecanal	184	3	2.0E+02	2.9E+00	4.7E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	6.9E+01	9.6E-01	3.3E+01	-10.57	-10.25	-12.93	-3.67	0.23	0.0%	0.0%	3.3E-40
1509	6381-77-7	2,3-didehydro-3-O-sodio-D-erythro-hexono-1,4-lactone	198	87	9.9E-03	1.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.5E+01	1.2E+00	4.3E+01	-7.10	-7.40	-9.05	-0.74	0.25	0.0%	0.0%	7.4E-33
1510	59113-36-9	oxybispropanediol	166	101	7.8E-05	1.0E+06	1.7E-03	13.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.1E+02	1.5E+00	5.6E+01	-6.93	-8.08	-10.16	0.16	1.64	0.0%	0.0%	1.7E-49
1511	116-11-0	isopropenyl methyl ether	72	-112	7.1E+04	2.1E+04	9.3E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.1E+01	1.3E+00	4.6E+01	-10.29	-9.95	-12.03	-0.98	0.36	0.0%	0.0%	2.0E-56
1512	1869-24-5	2-(trifluoromethyl)benzenesulfonamide	225	88	7.7E-02	9.6E+02	2.1E+01	9.4	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.8E+01	1.4E+00	5.0E+01	-7.96	-7.77	-9.61	-1.71	1.19	0.0%	0.0%	7.4E-30
1513	41184-20-7	disodium aniline-2,5-disulphonate	297	87	9.9E-03	2.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.5E+01	1.2E+00	4.2E+01	-7.09	-7.41	-9.06	-1.84	0.64	0.0%	0.0%	2.9E-25
1514	681-84-5	tetramethyl orthosilicate	152	-42	2.0E+03	2.8E+04	1.2E-02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.1E+02	1.5E+00	5.5E+01	-9.54	-9.28	-10.78	-0.28	0.60	0.0%	0.0%	4.2E-51
1515	34841-35-5	3'-chloropropiophenone	169	32	5.2E+00	4.1E+01	6.5E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-9.58	-9.31	-10.66	-2.17	0.48	0.0%	0.0%	3.8E-34
1516	37052-78-1	1,3-dihydro-5-methoxy-2H-benzimidazole-2-thione	180	143	9.0E-05	8.7E+02	1.0E+02	-1.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E+02	1.5E+00	5.5E+01	-7.32	-8.26	-10.19	-1.51	0.76	0.0%	0.0%	1.2E-35
1517	60-34-4	methylhydrazine	46	-58	8.5E+03	6.7E+05	1.0E-01	8.0	3.5E-06	4.5E-06	3.5E-07	conf	conf	1.1E+02	1.6E+00	5.9E+01	-9.24	-9.01	-10.78	-3.06	0.79	0.0%	0.0%	1.4E-28
1518	40137-22-2	3-(methylamino)propane-1,2-diol	105	16	2.8E+00	1.0E+06	1.6E-02	9.5	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.1E+02	1.6E+00	5.8E+01	-7.97	-8.87	-10.76	-0.94	1.06	0.0%	0.0%	6.0E-45
1519	51-21-8	fluorouracil	130	151	9.5E-06	1.0E+04	1.5E-01	7.8	3.5E-06	2.2E-07	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-6.55	-7.52	-9.30	-2.76	3.23	0.0%	0.0%	4.2E-21
1520	761-65-9	N,N-dibutylformamide	157	38	4.2E+00	3.8E+03	1.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.95	-7.63	-9.17	-2.42	0.93	0.0%	0.0%	2.8E-22
1521	6161-65-5	2-Methoxy-6-methylbenzoic acid	166	84	7.7E-02	1.6E+03	2.5E+01	3.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.1E+02	1.5E+00	5.5E+01	-7.58	-8.49	-10.28	-1.28	0.65	0.0%	0.0%	4.0E-38
1522	877179-03-8	620-313-1	298	184	2.7E-06	2.4E+00	6.2E+03	14.0	3.5E-06	3.5E-07	3.5E-08	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.31	-7.98	-9.74	-3.43	0.36	0.0%	0.0%	1.0E-19
1523	959-52-4	hexahydro-1,3,5-tris(1-oxoallyl)-1,3,5-triazine	249	164	2.2E-05	1.1E+04	2.2E-03	14.0	3.5E-06	3.5E-06	3.5E-07	conf	conf	1.1E+02	1.6E+00	5.8E+01	-7.32	-8.45	-10.73	-1.48	0.79	0.0%	0.0%	3.2E-40
1524	141-52-6	sodium ethanolate	68	87	9.9E-03	4.7E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.4E+01	1.2E+00	4.2E+01	-7.13	-7.42	-9.05	0.39	0.82	0.0%	0.0%	8.4E-42
1525	32539-82-5	629-935-8	240	100	5.1E-05	5.5E+00	1.0E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.8E+01	1.4E+00	5.0E+01	-8.36	-8.78	-10.35	-2.81	1.20	0.0%	0.0%	2.3E-27
1526	1917-44-8	4,6-diphenyl-1,3,5-triazin-2(1H)-one	249	215	2.7E-08	8.4E+01	4.8E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+02	1.4E+00	5.1E+01	-7.67	-8.71	-10.28	-2.36	0.64	0.0%	0.0%	5.5E-30
1527	94-58-6	5-propyl-1,3-benzodioxole	164	44	7.4E+00	3.7E+01	3.8E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	8.7E+01	1.2E+00	4.4E+01	-9.68	-9.42	-10.84	-2.14	0.64	0.0%	0.0%	9.2E-36
1528	556-61-6	methyl isothiocyanate	73	-63	1.6E+03	6.6E+03	2.0E+01	14.0	3.5E-06	5.4E-09	1.1E-06	conf	conf	6.5E+01	9.1E-01	3.2E+01	-9.34	-9.06	-10.55	-3.73	0.40	0.0%	0.0%	9.3E-23
1529	91-68-9	3-diethylaminophenol	165	60	1.1E-01	4.0E+02	2.1E+02	4.1	3.5E-06	3.5E-06	3.5E-07	conf	conf	1.1E+02	1.6E+00	5.8E+01	-7.92	-8.88	-10.80	-1.68	0.34	0.0%	0.0%	4.1E-39
1530	107-56-2	O,O-diisopropyl hydrogen dithiophosphate	214	-60	3.7E+00	7.1E+01	1.2E+03	-0.1	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.42	-7.91	-9.71	-1.23	0.42	0.0%	0.0%	4.9E-34
1531	105-58-8	diethyl carbonate	118	-95	1.6E+03	4.2E+04	1.7E+01	14.0	3.5E-06	1.2E-06	3.5E-07	conf	conf	1.1E+02	1.5E+00	5.4E+01	-9.48	-9.28	-10.54	-0.91	0.75	0.0%	0.0%	2.2E-43
1532	7327-60-8	nitrilotriacetonitrile	134	93	8.2E-03	8.9E+05	4.1E-02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.6E+01	1.3E+00	4.9E+01	-6.70	-7.66	-9.56	-2.08	0.64	0.0%	0.0%	5.6E-27
1533	3030-47-5	bis(2-dimethylaminoethyl)(methyl)amine	173	10	3.9E+01	2.0E+05	2.7E-01	9.2	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E+02	1.5E+00	5.5E+01	-8.36	-8.19	-10.19	-1.02	0.26	0.0%	0.0%	1.5E-39
1534	128-44-9	1,2-benzisothiazol-3(2H)-one 1,1-dioxide, sodium salt	205	87	9.9E-03	1.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.3E+01	1.2E+00	4.1E+01	-7.11	-7.42	-9.07	0.07	0.89	0.0%	0.0%	3.0E-39
1535	976-70-5	3-oxopregn-4-ene-21,17α-carbolactone	342	188	1.0E-06	2.6E+01	1.7E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.5E+01	1.3E+00	4.8E+01	-7.79	-8.81	-10.32	-2.20	0.12	0.0%	0.0%	2.0E-31
1536	51368-55-9	isopropyl 2-bromo-2-methylpropionate	209	-11	1.1E+02	2.6E+02	3.2E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.0E+02	1.4E+00	5.3E+01	-10.41	-10.18	-11.84	-1.66	1.27	0.0%	0.0%	3.0E-48
1537	97-90-5	ethylene dimethacrylate	198	-68	1.1E+04	2.0E+03	1.6E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.6E+01	-10.64	-10.33	-12.95	-1.61	0.23	0.0%	0.0%	2.9E-59
1538	18936-17-9	2-methylbutyronitrile	83	-58	1.7E+03	8.5E+03	1.8E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-9.58	-9.31	-10.69	-1.17	0.73	0.0%	0.0%	2.2E-42
1539	78-77-3	1-bromo-2-methylpropane	137	-78	8.3E+03	1.2E+03	3.8E+02	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	9.1E+01	1.3E+00	4.6E+01	-10.71	-10.42	-12.88	-1.39	0.26	0.0%	0.0%	7.3E-61
1540	1119-40-0	dimethyl glutarate	160	-83	2.4E+01	1.2E+04	7.9E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.1E+02	1.5E+00	5.7E+01	-9.37	-9.22	-10.78	-1.24	1.07	0.0%	0.0%	1.3E-42
1541	134-03-2	sodium ascorbate	198	87	9.9E-03	1.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.2E+01	1.1E+00	4.1E+01	-7.11	-7.42	-9.07	-1.13	0.64	0.0%	0.0%	4.1E-30
1542	38632-47-2	Methansulfonic acid (1,6-hexanediyl-diimino)bis[1-oxo, disodium salt	376	87	9.9E-03	2.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.2E+01	1.1E+00	4.1E+01	-7.10	-7.42	-9.07	-1.89	0.99	0.0%	0.0%	5.4E-25
1543	24199-46-0	6-methyloct-5-en-2-one	140	-28	1.4E+02	1.0E+03	3.5E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+02	1.4E+00	5.0E+01	-9.18	-8.84	-10.44	-1.38	0.32	0.0%	0.0%	1.5E-38
1544	7397-62-8	butyl glycollate	132	-3	7.0E+00	2.3E+04	2.4E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.1E+02	1.5E+00	5.7E+01	-9.13	-8.97	-10.76	-0.77	0.55	0.0%	0.0%	1.5E-46
1545	616-30-8	3-aminopropane-1,2-diol	91	25	3.7E+00	1.0E+06	5.6E-03	9.1	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.1E+02	1.5E+00	5.7E+01	-7.99	-8.87	-10.76	-1.47	0.54	0.0%	0.0%	1.6E-40
1546	503-01-5	isometheptene	141	-39	1.5E+02	7.8E+03	1.1E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-9.14	-8.90	-10.09	-2.58	0.66	0.0%	0.0%	3.7E-27
1547	108-69-0	3,5-xylidine	121	29	1.8E+01	5.9E+02	1.5E+02	14.0	3.5E-06	2.8E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-9.08	-8.84	-10.05	-1.90	0.42	0.0%	0.0%	1.1E-31
1548	1760-24-3	N-(3-(trimethoxysilyl)propyl)ethylenediamine	222	69	4.7E-01	2.9E+05	2.1E-02	9.7	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.1E+02	1.5E+00	5.7E+01	-8.00	-8.88	-10.79	-0.94	0.76	0.0%	0.0%	2.6E-45
1549	66309-83-9	2,6-Dimethyl-1-indanone	160	60	7.9E-01	2.5E+02	1.2E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-8.60	-8.36	-9.81	-1.66	0.34	0.0%	0.0%	1.2E-31
1550	79-08-3	bromoacetic acid	139	29	1.7E+01	8.5E+04	2.7E+00	2.9	3.5E-06	3.6E-07	1.1E-06	conf	conf	9.4E+01	1.3E+00	4.8E+01	-7.07	-7.96	-9.72	-2.11	0.68	0.0%	0.0%	7.4E-28
1551	1885-14-9	phenyl chloroformate	157	0	1.0E+02	1.1E+03	2.2E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.0E+02	1.4E+00	5.2E+01	-9.78	-9.56	-10.83	-1.52	0.47	0.0%	0.0%	1.2E-40
1552	97-97-2	2-chloro-1,1-dimethoxyethane	125	-60	1.5E+03	1.8E+04	3.0E+00	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-9.41	-9.13	-10.53	-1.39	0.56	0.0%	0.0%	2.8E-39
1553	718-71-8	ethyl 2-cyano-2-phenyl-butanoate	217	89	1.4E-02	7.4E+01	4.0E+02	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.22	-7.98	-9.72	-3.11	0.73	0.0%	0.0%	1.8E-21
1554	1256387-74-	tert-butyl (1R,3S,4S)-3-(5-bromo-1H-benzimidazol-2-yl)-2-azabicyclo[2.2.1]heptane-2-carboxylate	392	223	7.8E-09	5.3E-02	5.5E+04	6.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-7.82	-8.83	-10.34	-2.67	0.10	0.0%	0.0%	3.2E-28
1555	34184-82-2	17-hydroxypregna-4,9(11)-diene-3,20-dione	328	179	9.0E-08	1.6E+02	1.0E+03	13.9	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-7.08	-7.96	-9.69	-1.47	0.21	0.0%	0.0%	4.3E-32
1556	94695-48-4	2,3,4,5-tetrafluorobenzoyl chloride	213	23	1.2E+02	1.9E+02	1.7E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.6E+01	-10.15	-9.88	-11.69	-2.47	0.94	0.0%	0.0%	6.5E-40
1557	7529-22-8	!4-methylmorpholine 4-oxide! !monohydrate!	117	125	2.4E-03	4.0E+07	7.6E-02	4.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+02	1.5E+00	5.4E+01	-6.85	-8.15	-10.19	-1.14	0.64	0.0%	0.0%	1.7E-38
1558	96-26-4	1,3-dihydroxyacetone	90	17	5.9E-01	3.1E+05	1.9E-01	13.3	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.1E+02	1.5E+00	5.6E+01	-7.99	-8.97	-10.77	0.02	0.76	0.0%	0.0%	6.2E-54
1559	83196-56-9	617-448-3	311	185	3.3E-08	2.1E+02	7.4E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-7.25	-8.05	-9.71	-2.95	0.15	0.0%	0.0%	2.1E-22
1560	26586-02-7	(E)-3-formylbut-2-enyl acetate	142	-17	4.3E+01	3.8E+04	4.9E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.1E+02	1.5E+00	5.6E+01	-9.30	-9.14	-10.78	-2.02	0.22	0.0%	0.0%	3.1E-36
1561	120118-14-1	601-672-3	218	168	4.3E-06	3.8E+01	1.3E+03	-1.6	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.3E+01	1.3E+00	4.7E+01	-7.09	-7.72	-9.58	-2.39	0.72	0.0%	0.0%	4.7E-25
1562	103577-40-8	1H-Benzimidazole, 2-[[[3-methyl-4-(2,2,2-trifluoroethoxy)-2-pyridinyl]methyl]thio]-	353	216	2.3E-08	7.8E-01	2.7E+04	5.5	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-7.41	-8.05	-9.72	-3.18	0.21	0.0%	0.0%	4.9E-21
1563	14367-46-5	N-ethyl-p-methoxy-α-methylphenethylamine	193	47	7.9E-01	2.4E+03	6.2E+02	9.9	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-8.36	-8.12	-9.78	-2.44	0.66	0.0%	0.0%	4.9E-26
1564	14064-10-9	diethyl chloromalonate	195	-67	1.6E+01	2.3E+03	1.2E+01	6.2	3.5E-06	3.1E-07	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.6E+01	-8.37	-8.13	-9.69	-2.12	0.86	0.0%	0.0%	1.5E-27
1565	1012341-48-	(2E,4R)-5-(biphenyl-4-yl)-4-[(tert-butoxycarbonyl)amino]-2-methylpent-2-enoic acid	381	219	1.5E-08	5.0E-01	6.0E+05	4.6	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-7.41	-7.95	-9.68	-3.22	0.89	0.0%	0.0%	1.4E-20
1566	89878-14-8	627-082-6	147	4	5.0E+01	3.3E+02	7.6E+02	5.2	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.3E+01	1.3E+00	4.7E+01	-8.54	-8.22	-9.71	-2.32	0.64	0.0%	0.0%	2.3E-26
1567	141-18-4	bis(2-butoxyethyl) adipate	346	33	4.8E-03	1.6E+01	6.0E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	8.8E+01	1.2E+00	4.4E+01	-8.41	-8.17	-9.84	-2.20	0.36	0.0%	0.0%	5.3E-28
1568	700-13-0	2,3,5-trimethylhydroquinone	152	86	2.7E-02	2.1E+03	4.7E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.20	-7.39	-9.03	-2.57	0.53	0.0%	0.0%	1.4E-20
1569	159276-62-7	diethyl [2-(2,4-difluorophenyl)prop-2-en-1-yl]malonate	312	23	9.0E-02	9.8E+00	2.1E+04	12.8	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-9.47	-9.26	-10.56	-2.50	0.53	0.0%	0.0%	5.8E-31
1570	99-57-0	2-amino-4-nitrophenol	154	110	2.0E-03	6.5E+03	9.8E+00	2.5	3.5E-06	3.5E-06	3.5E-07	conf	conf	1.1E+02	1.5E+00	5.6E+01	-7.66	-8.78	-10.78	-1.17	0.39	0.0%	0.0%	3.1E-43
1571	35303-76-5	4-(2-aminoethyl)benzenesulphonamide	200	127	1.4E-03	1.8E+03	5.2E-01	9.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.3E+01	1.3E+00	4.7E+01	-6.78	-7.64	-9.57	-1.12	0.95	0.0%	0.0%	7.0E-34
1572	89-39-4	1,4-dimethoxy-2-nitrobenzene	183	74	2.8E-01	1.4E+03	9.3E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+02	1.4E+00	5.3E+01	-8.73	-8.53	-10.30	-1.18	1.28	0.0%	0.0%	4.3E-39
1573	689294-28-8	4-methoxybenzyl (6R,7R)-7-{[(2Z)-2-(5-amino-1,2,4-thiadiazol-3-yl)-2-{[(1-tert-butoxy-2-methyl-1-oxopropan-2-yl)ox	681	350	3.9E-19	7.4E-02	1.4E+04	10.1	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-7.39	-8.21	-9.76	-2.40	0.45	0.0%	0.0%	3.7E-26
1574	27298-98-2	(S)-1-(p-tolyl)ethanamine	135	18	2.7E+01	1.5E+03	1.1E+02	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-9.00	-8.77	-10.02	-1.95	0.94	0.0%	0.0%	4.5E-31
1575	4187-38-6	(1R)-1-(4-methylphenyl)ethanamine	135	18	2.7E+01	1.5E+03	1.1E+02	9.3	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-9.00	-8.77	-10.02	-1.95	0.94	0.0%	0.0%	5.1E-31
1576	3159-04-4	2-Chlorodibenzo[b,f][1,4]thiazepin-11(10H)-one	262	182	3.7E-06	5.4E+00	2.5E+03	0.6	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.27	-7.77	-9.63	-3.02	0.56	0.0%	0.0%	1.8E-21
1577	17639-93-9	methyl 2-chloropropionate	123	-64	1.2E+03	1.2E+04	1.1E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.1E+02	1.5E+00	5.5E+01	-10.03	-9.87	-11.18	-1.51	1.90	0.0%	0.0%	1.1E-43
1578	135-61-5	3-hydroxy-2'-methyl-2-naphthanilide	277	211	6.6E-09	4.3E-01	2.9E+04	10.2	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.0E+01	1.3E+00	4.6E+01	-7.74	-8.78	-10.33	-3.05	0.05	0.0%	0.0%	1.3E-25
1579	23357-46-2	(1R)-1,2,3,4-tetrahydronaphthalen-1-amine	147	48	2.7E+00	7.5E+02	2.6E+02	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-8.57	-8.34	-9.79	-2.07	0.73	0.0%	0.0%	1.4E-28
1580	23357-52-0	(1S)-1,2,3,4-tetrahydronaphthalen-1-amine	147	48	2.7E+00	7.5E+02	2.6E+02	9.3	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-8.57	-8.33	-9.79	-2.07	0.73	0.0%	0.0%	1.4E-28
1581	2941-20-0	608-356-4	135	11	2.7E+01	1.5E+03	9.5E+01	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-9.00	-8.76	-10.02	-2.18	0.70	0.0%	0.0%	1.9E-29
1582	3082-64-2	(1R)-1-Phenylpropan-1-amine	135	11	2.7E+01	1.5E+03	9.5E+01	9.3	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-8.99	-8.76	-10.02	-2.18	0.70	0.0%	0.0%	2.2E-29
1583	150-13-0	4-aminobenzoic acid	137	94	3.4E-03	2.0E+04	9.1E+00	2.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+02	1.4E+00	5.3E+01	-7.26	-8.30	-10.26	-1.92	0.80	0.0%	0.0%	5.5E-33
1584	1093205-93-	3-(3-Amino-2-cyanophenoxy)-2,2-dimethyl-N-propylpropanamide	275	196	4.3E-07	9.6E+00	1.2E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.2E+01	1.3E+00	4.6E+01	-6.49	-7.35	-9.01	-2.58	1.80	0.0%	0.0%	2.1E-20
1585	73573-88-3	(1S,7S,8S,8aR)-8-{2-[(2R,4R)-4-hydroxy-6-oxotetrahydro-2H-pyran-2-yl]ethyl}-7-methyl-1,2,3,7,8,8a-hexahydronapht	391	201	1.1E-09	6.5E+00	2.1E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-7.78	-8.83	-10.33	-3.33	1.41	0.0%	0.0%	8.4E-24
1586	18156-74-6	N-(trimethylsilyl)imidazole	140	29	8.0E+00	1.7E+03	2.4E+02	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-8.63	-8.40	-9.81	-2.61	0.73	0.0%	0.0%	4.0E-25
1587	4433-79-8	4'-chloro-2',5'-dimethoxyacetoacetanilide	272	174	1.2E-05	7.2E+02	1.8E+01	-0.7	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.0E+02	1.4E+00	5.3E+01	-7.41	-8.46	-10.24	-1.92	1.05	0.0%	0.0%	6.7E-33
1588	4501-58-0	(R)-2,2,3-trimethylcyclopent-3-ene-1-acetaldehyde	152	11	3.2E+01	5.2E+02	2.0E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.7E+01	1.4E+00	5.0E+01	-9.82	-9.58	-10.74	-1.99	0.19	0.0%	0.0%	4.0E-36
1589	102445-69-2	600-314-3	425	209	1.6E-10	2.4E+00	1.8E+02	13.5	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-6.88	-7.85	-9.64	-1.12	0.22	0.0%	0.0%	2.1E-34
1590	109232-37-3	isobutyl 5-chloro-2,2-dimethylpentanoate	221	16	3.8E+00	1.5E+01	2.3E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.6E+01	-10.50	-10.27	-11.66	-2.61	0.54	0.0%	0.0%	1.5E-38
1591	107-96-0	3-mercaptopropionic acid	106	30	2.1E+01	7.5E+04	3.3E+00	4.3	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.1E+02	1.5E+00	5.5E+01	-7.79	-9.04	-10.80	-1.41	0.59	0.0%	0.0%	2.5E-41
1592	51-03-6	2-(2-butoxyethoxy)ethyl 6-propylpiperonyl ether	338	153	7.0E-04	3.1E+00	1.9E+04	14.0	3.5E-06	5.6E-07	3.5E-07	conf	conf	8.7E+01	1.2E+00	4.4E+01	-8.70	-8.53	-10.13	-2.56	0.55	0.0%	0.0%	1.7E-27
1593	137863-20-8	L-Valine, N-(1-oxopentyl)-N-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, phenylmethyl ester	526	318	2.3E-15	7.9E-05	5.2E+05	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	9.1E+01	1.3E+00	4.4E+01	-7.10	-7.55	-9.11	-1.30	0.39	0.0%	0.0%	3.3E-29
1594	6318-09-8	613-175-9	234	116	1.7E-03	7.8E+00	9.5E+03	5.1	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-7.58	-7.90	-9.72	-1.76	0.29	0.0%	0.0%	3.2E-30
1595	140-29-4	phenylacetonitrile	117	9	8.7E+00	8.3E+02	3.6E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	9.1E+01	1.3E+00	4.6E+01	-8.53	-8.26	-9.53	-0.96	0.63	0.0%	0.0%	8.4E-35
1596	17261-28-8	2-diphenylphosphinobenzoic acid	306	182	1.0E-06	1.3E+00	3.6E+04	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	9.1E+01	1.3E+00	4.5E+01	-6.67	-7.36	-9.01	-3.06	0.25	0.0%	0.0%	9.1E-18
1597	494-19-9	10,11-dihydro-5H-dibenz[b,f]azepine	195	104	9.3E-03	5.5E-02	1.9E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-9.66	-9.40	-10.69	-2.63	0.37	0.0%	0.0%	5.4E-31
1598	1009-22-9	N-(2-bromo-4-fluorophenyl)acetamide	232	119	5.1E-03	3.6E+02	4.3E+01	12.1	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-7.81	-7.93	-9.71	-2.41	0.83	0.0%	0.0%	8.3E-26
1599	666816-98-4	8-bromo-7-(but-2-yn-1-yl)-3-methyl-3,7-dihydro-1H-purine-2,6-dione	297	239	6.0E-10	7.9E+00	3.9E+01	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-6.72	-7.75	-9.60	-3.41	0.58	0.0%	0.0%	4.4E-19
1600	52688-08-1	Octan-2-yl cyanoacetate	197	44	3.4E-01	1.2E+02	7.8E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+02	1.4E+00	5.1E+01	-9.07	-8.86	-10.37	-2.36	0.65	0.0%	0.0%	1.2E-30
1601	256473-05-9	2-(isopropylthio)-3-(2,2,2-trifluoroethoxy)pyridine	251	56	8.0E-01	2.2E+01	5.8E+03	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-9.40	-9.14	-10.38	-2.41	0.13	0.0%	0.0%	2.5E-30
1602	92-54-6	N-phenylpiperazine	162	71	2.1E-03	3.9E+03	3.5E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-7.15	-7.92	-9.70	-2.06	0.76	0.0%	0.0%	4.9E-28
1603	144689-24-7	4-(2-hydroxypropan-2-yl)-2-propyl-1-{[2'-(1H-tetrazol-5-yl)biphenyl-4-yl]methyl}-1H-imidazole-5-carboxylic acid	447	325	2.3E-19	4.2E-03	4.3E+03	2.4	3.5E-06	3.5E-07	3.5E-08	conf	conf	9.2E+01	1.3E+00	4.6E+01	-6.98	-7.62	-9.54	-2.82	0.99	0.0%	0.0%	4.1E-22
1604	54041-17-7	Acetamide, N-(4-fluorophenyl)-2-hydroxy-N-(1-methylethyl)-	211	101	3.7E-04	1.6E+03	3.0E+01	-0.5	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-6.93	-7.82	-9.63	-2.53	1.74	0.0%	0.0%	1.6E-24
1605	93-67-4	5-chloro-2-phenoxyaniline	220	113	3.3E-03	8.6E+00	8.7E+02	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-8.31	-8.06	-9.75	-2.66	0.34	0.0%	0.0%	1.8E-24
1606	615-20-3	2-chlorobenzothiazole	170	73	4.0E+00	1.5E+02	6.5E+02	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+01	1.3E+00	4.6E+01	-9.20	-8.96	-10.18	-2.21	0.15	0.0%	0.0%	2.4E-30
1607	3467-59-2	N-(2,5-dimethoxyphenyl)acetamide	195	129	1.3E-03	4.4E+03	5.0E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+02	1.4E+00	5.2E+01	-7.24	-8.25	-10.26	-1.82	1.16	0.0%	0.0%	8.9E-34
1608	39627-98-0	N-(2,6-dimethylphenyl)pyridine-2-carboxamide	226	167	2.6E-05	7.0E+01	1.3E+02	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.6E+01	-7.04	-7.87	-9.69	-2.57	0.79	0.0%	0.0%	1.4E-24
1609	353497-37-7	609-118-2	281	141	1.6E-04	6.2E+00	1.7E+04	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	9.1E+01	1.3E+00	4.5E+01	-7.44	-7.37	-9.02	-2.46	0.83	0.0%	0.0%	3.7E-21
1610	6401-97-4	2,4-dihydro-5-methyl-2-phenyl-3H-pyrazol-3-imine	173	105	3.3E-02	9.1E+02	1.6E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.91	-7.88	-9.68	-4.29	2.81	0.0%	0.0%	6.5E-15
1611	6291-85-6	3-ethoxypropylamine	103	-28	1.0E+03	1.5E+05	1.2E+00	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.68	-8.43	-9.82	-1.94	0.39	0.0%	0.0%	9.8E-30
1612	848655-78-7	N-(4-amino-2-ethoxyphenyl)acetamide	194	148	1.5E-04	5.0E+03	1.5E+00	4.1	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-6.83	-7.83	-9.67	-1.92	0.82	0.0%	0.0%	8.8E-29
1613	80841-78-7	4-(chloromethyl)-5-methyl-1,3-dioxol-2-one	149	60	8.8E-03	2.1E+03	6.2E+00	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.06	-7.71	-9.60	-2.23	1.35	0.0%	0.0%	3.0E-26
1614	151012-31-6	[1-(4-bromobenzyl)-2-butyl-4-chloro-1H-imidazol-5-yl]methanol	358	199	3.0E-09	2.1E+00	8.9E+04	3.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+02	1.4E+00	5.2E+01	-7.72	-8.46	-10.25	-2.73	0.62	0.0%	0.0%	3.1E-27
1615	53994-69-7	(6R-trans)-7-amino-3-chloro-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid	235	299	7.5E-08	5.0E+03	3.1E-01	6.8	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-6.60	-7.69	-9.57	-1.49	1.89	0.0%	0.0%	3.9E-31
1616	609-66-5	2-chlorobenzamide	156	102	7.9E-03	4.6E+02	4.5E+00	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.43	-7.70	-9.60	-2.48	0.88	0.0%	0.0%	1.4E-24
1617	30246-33-4	(6R-trans)-7-amino-3-[[(5-methyl-1,3,4-thiadiazol-2-yl)thio]methyl]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carb	344	323	2.1E-12	8.0E+01	1.2E-01	2.2	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-6.57	-7.75	-9.60	-1.83	1.36	0.0%	0.0%	5.7E-29
1618	67442-07-3	2-chloro-N-methoxy-N-methylacetamide	138	20	2.2E+01	9.3E+04	2.1E+00	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.01	-7.77	-9.60	-1.76	1.87	0.0%	0.0%	2.0E-29
1619	55314-16-4	611-255-8	176	67	3.7E-01	7.8E+04	9.3E-01	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.11	-7.66	-9.58	-1.23	0.50	0.0%	0.0%	4.2E-33
1620	201733-56-4	5,5,5',5'-tetramethyl-2,2'-bi-1,3,2-dioxaborinane	226	51	2.7E+00	2.2E+06	7.8E-01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.01	-7.74	-9.62	-1.79	0.64	0.0%	0.0%	2.2E-29
1621	1378387-81-	1-(7-bromo-9,9-difluoro-9H-fluoren-2-yl)-2-chloroethanone	420	285	9.9E-17	5.8E+04	5.2E-03	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	9.1E+01	1.3E+00	4.6E+01	-6.31	-7.30	-8.95	-1.22	1.77	0.0%	0.0%	1.1E-28
1622	35092-89-8	methyl hydrogen 2-nitroterephthalate	225	147	2.7E-04	6.6E+02	3.4E+01	3.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+02	1.4E+00	5.2E+01	-7.39	-8.33	-10.28	-1.54	0.94	0.0%	0.0%	4.5E-36

1623	693-98-1	2-methylimidazole	82	36	9.2E-02	5.0E+04	4.1E+00	8.0	3.5E-06	5.0E-07	1.1E-07	conf	conf	9.5E+01	1.3E+00	4.8E+01	-6.93	-7.81	-9.78	-0.63	0.19	0.0%	0.0%	2.4E-39
1624	52298-44-9	4-amino-2,5-dimethoxy-N-phenylbenzenesulphonamide	308	196	4.6E-07	1.8E+02	7.6E+01	1.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+02	1.4E+00	5.2E+01	-7.34	-8.29	-10.23	-2.03	0.77	0.0%	0.0%	5.3E-32
1625	78-26-2	2-methyl-2-propylpropane-1,3-diol	132	21	3.2E-01	1.2E+04	1.4E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.0E+02	1.4E+00	5.2E+01	-8.34	-8.53	-10.30	-0.56	0.50	0.0%	0.0%	2.9E-44
1626	941-69-5	N-phenylmaleimide	173	151	5.3E-04	4.9E+03	7.6E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.0E+02	1.4E+00	5.2E+01	-7.51	-8.49	-10.30	-3.13	0.27	0.0%	0.0%	6.3E-25
1627	74-83-9	bromomethane	95	-105	2.1E+05	1.2E+04	1.5E+01	14.0	3.5E-06	4.3E-08	1.1E-07	conf	conf	6.1E+01	8.5E-01	3.0E+01	-10.36	-9.73	-12.13	-2.55	0.55	0.0%	0.0%	5.4E-43
1628	114882-16-5	601-332-4	355	193	8.5E-09	7.4E+00	1.2E+04	11.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.76	-8.80	-10.32	-2.89	0.15	0.0%	0.0%	1.2E-26
1629	3634-83-1	1,3-bis(isocyanatomethyl)benzene	188	82	1.2E-01	3.5E+03	1.0E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.0E+02	1.4E+00	5.3E+01	-9.23	-9.38	-10.84	-1.45	0.46	0.0%	0.0%	2.7E-41
1630	102-56-7	2,5-dimethoxyaniline	153	54	3.6E-01	9.0E+03	1.7E+01	3.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+02	1.4E+00	5.2E+01	-7.33	-8.32	-10.28	-1.96	0.75	0.0%	0.0%	7.6E-33
1631	49564-57-0	4-amino-5-methoxy-N,2-dimethylbenzenesulphonamide	230	145	2.1E-04	1.2E+04	3.5E+00	1.7	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.0E+02	1.4E+00	5.2E+01	-7.34	-8.47	-10.29	-1.61	0.86	0.0%	0.0%	1.4E-35
1632	48145-04-6	2-phenoxyethyl acrylate	192	36	1.1E+00	5.8E+02	2.9E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.9E+01	1.4E+00	5.1E+01	-8.98	-8.77	-10.35	-2.40	0.41	0.0%	0.0%	3.5E-30
1633	26537-19-9	methyl 4-tert-butylbenzoate	192	35	2.6E+00	4.1E+01	5.5E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.84	-9.61	-10.78	-2.57	0.58	0.0%	0.0%	4.4E-32
1634	1047-16-1	5,12-dihydroquino[2,3-b]acridine-7,14-dione	312	219	1.5E-08	2.4E-02	2.4E+01	5.9	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.0E+02	1.4E+00	5.1E+01	-7.61	-8.54	-10.33	-0.82	0.72	0.0%	0.0%	2.4E-42
1635	834-12-8	ametryn (reach)	227	131	5.7E-03	1.8E+02	2.1E+03	4.0	3.5E-06	2.2E-09	1.1E-07	conf	conf	6.0E+01	8.4E-01	2.9E+01	-7.09	-7.31	-8.26	-2.91	1.19	0.0%	0.0%	1.1E-14
1636	7065-46-5	3,3-dimethylbutyryl chloride	135	-36	1.6E+03	3.1E+03	2.4E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	9.1E+01	1.3E+00	4.5E+01	-9.52	-9.16	-11.06	-1.53	0.48	0.0%	0.0%	1.5E-42
1637	3056-13-1	(2S,3R,5S)-5-(5-methyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-2-[(4-methylbenzoyloxy)methyl]oxolan-3-yl 4-me	479	305	2.0E-14	1.3E-02	7.9E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.73	-8.78	-10.32	-3.12	0.40	0.0%	0.0%	4.2E-25
1638	94-96-2	2-ethylhexane-1,3-diol	146	13	4.0E-01	1.0E+04	4.0E+01	14.0	3.5E-06	4.6E-07	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.22	-8.17	-9.89	-0.27	0.40	0.0%	0.0%	2.7E-43
1639	40306-75-0	3-acetamido-5-amino-4-hydroxybenzenesulphonic acid	246	221	5.8E-11	9.6E+01	3.5E-04	-0.3	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.9E+01	1.4E+00	5.1E+01	-6.79	-7.99	-10.16	-0.61	0.26	0.0%	0.0%	1.2E-42
1640	121-82-4	perhydro-1,3,5-trinitro-1,3,5-triazine	222	133	1.8E-04	1.0E+06	4.8E+00	14.0	3.5E-06	3.9E-07	1.1E-07	conf	conf	9.0E+01	1.3E+00	4.6E+01	-6.64	-7.70	-9.63	-1.77	0.97	0.0%	0.0%	1.4E-29
1641	2224-33-1	butan-2-one O,O',O''-(vinylsilylidyne)trioxime	313	12	2.9E-02	9.5E-07	1.5E+10	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	5.9E+01	8.3E-01	2.9E+01	-9.26	-9.17	-10.33	-0.49	1.07	0.0%	0.0%	3.4E-45
1642	86-84-0	1-naphthyl isocyanate	169	42	1.3E+00	1.7E+02	5.9E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.33	-9.12	-10.45	-1.90	0.81	0.0%	0.0%	1.2E-34
1643	256473-04-8	2-Chloro-3-(2,2,2-trifluoroethoxy)pyridine.	212	22	5.0E+01	2.3E+02	2.8E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.98	-9.74	-11.27	-1.78	0.33	0.0%	0.0%	3.6E-42
1644	328-99-4	3-(trifluoromethyl)benzoyl fluoride	192	-5	1.5E+02	5.6E+02	1.2E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.5E+01	-9.34	-8.96	-10.84	-2.43	1.11	0.0%	0.0%	1.4E-33
1645	50650-75-4	610-555-6	222	62	3.4E-02	2.1E+00	1.3E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.97	-9.79	-11.04	-3.01	0.24	0.0%	0.0%	8.6E-31
1646	118-83-2	5-chloro-α,α,α-trifluoro-2-nitrotoluene	226	52	2.9E+00	5.2E+01	2.6E+03	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.76	-9.55	-10.80	-2.11	0.13	0.0%	0.0%	1.0E-35
1647	179107-88-1	801-014-7	206	45	5.0E-01	1.1E+01	1.3E+05	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	7.9E+01	1.1E+00	3.9E+01	-9.96	-9.75	-10.87	-3.02	0.72	0.0%	0.0%	1.8E-29
1648	164524-02-1	potassium 4-isopropylbenzenesulphonate	238	87	9.9E-03	1.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.6E+01	1.1E+00	3.8E+01	-7.14	-7.45	-9.10	-0.50	0.70	0.0%	0.0%	5.4E-35
1649	66742-57-2	613-982-6	230	99	9.0E-03	2.0E+01	5.0E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.02	-8.82	-10.42	-3.44	1.90	0.0%	0.0%	1.0E-23
1650	6485-40-1	l-p-mentha-1(6),8-dien-2-one	150	10	1.7E+01	1.2E+03	1.2E+03	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.2E+01	1.1E+00	4.1E+01	-8.72	-8.43	-9.73	-1.22	0.66	0.0%	0.0%	2.3E-34
1651	18169-57-8	trichloroisobutylsilane	192	-51	7.3E+02	4.8E+03	2.6E+03	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	9.5E+01	1.3E+00	4.9E+01	-10.43	-10.19	-11.55	0.34	0.67	0.0%	0.0%	4.8E-65
1652	39489-75-3	bis(2,4-dichloro-5-nitrophenyl) carbonate	442	220	1.2E-08	3.4E-02	2.6E+05	14.0	3.5E-06	3.5E-07	3.5E-08	conf	conf	7.1E+01	9.9E-01	3.5E+01	-7.77	-8.46	-9.90	-3.97	0.89	0.0%	0.0%	1.1E-17
1653	96-45-7	imidazolidine-2-thione	102	70	2.7E-04	8.1E+05	3.2E-01	2.0	3.5E-06	6.3E-09	3.5E-06	conf	conf	6.0E+01	8.3E-01	2.9E+01	-6.86	-7.42	-8.42	-0.21	1.22	0.0%	0.0%	4.6E-32
1654	719-80-2	ethyl diphenylphosphinite	230	69	2.7E-02	3.6E+00	4.0E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.32	-9.10	-10.47	-2.63	0.33	0.0%	0.0%	2.1E-29
1655	142-62-1	hexanoic acid	116	26	3.7E+01	1.2E+04	1.1E+02	4.9	3.5E-06	4.0E-06	1.1E-06	conf	conf	1.0E+02	1.4E+00	5.3E+01	-8.85	-9.27	-10.91	-0.95	0.31	0.0%	0.0%	2.8E-46
1656	3033-62-3	N,N,N',N'-tetramethyl-2,2'-oxybis(ethylamine)	160	-6	1.0E+02	2.6E+05	2.9E-01	9.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.8E+01	1.4E+00	5.0E+01	-8.49	-8.29	-10.24	-1.33	0.79	0.0%	0.0%	2.1E-37
1657	96-23-1	1,3-dichloropropan-2-ol	129	-24	4.1E+01	3.9E+04	6.0E+00	13.1	3.5E-06	4.6E-07	1.1E-07	conf	conf	9.0E+01	1.3E+00	4.6E+01	-8.32	-8.06	-9.82	-0.27	0.33	0.0%	0.0%	1.2E-42
1658	342-25-6	2,4'-difluorobenzophenone	218	75	1.3E-01	1.7E+01	3.5E+03	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.26	-9.07	-10.43	-2.17	0.13	0.0%	0.0%	2.2E-32
1659	6246-48-6	(2E)-3,7-dimethylocta-2,6-dien-1-amine	153	-5	1.8E+01	8.2E+03	2.9E+03	9.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.16	-8.94	-10.44	-2.81	1.30	0.0%	0.0%	6.0E-28
1660	138-59-0	(3R,4S,5R)-3,4,5-trihydroxycyclohex-1-enecarboxylic acid	174	133	6.7E-07	9.6E+04	4.6E-02	4.1	3.5E-06	5.9E-07	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-6.83	-8.10	-9.94	-1.07	0.75	0.0%	0.0%	4.5E-37
1661	55974-25-9	7-methoxy-4,4-dimethyl-1H-2-benzopyran-1,3(4H)-dione	220	89	2.2E-02	2.2E+02	1.9E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.3E+01	1.3E+00	4.7E+01	-8.89	-8.73	-10.38	-1.39	0.08	0.0%	0.0%	5.0E-38
1662	1696-20-4	4-acetylmorpholine	129	27	1.8E+01	2.3E+05	1.3E-01	-1.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.6E+01	1.3E+00	4.9E+01	-7.22	-8.46	-10.30	0.41	0.91	0.0%	0.0%	3.4E-53
1663	129-00-0	pyrene	202	120	4.6E-05	2.8E-02	8.5E+04	14.0	3.5E-06	2.2E-09	1.1E-08	conf	conf	5.8E+01	8.1E-01	2.8E+01	-8.11	-7.88	-8.83	-4.05	0.70	0.0%	0.0%	4.1E-12
1664	75-59-2	tetramethylammonium hydroxide	91	87	9.9E-03	6.3E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.5E+01	1.0E+00	3.7E+01	-7.17	-7.46	-9.10	-1.31	1.09	0.0%	0.0%	4.4E-29
1665	349-76-8	3'-(trifluoromethyl)acetophenone	188	6	5.1E+01	5.0E+02	4.4E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.88	-9.65	-10.97	-2.47	1.07	0.0%	0.0%	3.7E-34
1666	107-20-0	chloroacetaldehyde	78	-72	9.2E+03	5.7E+04	1.2E+00	14.0	3.5E-06	8.1E-07	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.66	-9.35	-10.81	-2.41	0.70	0.0%	0.0%	1.8E-33
1667	36888-99-0	5,5'-(1H-isoindole-1,3(2H)-diylidene)dibarbituric acid	367	350	7.5E-23	1.2E+04	1.2E-02	1.7	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.6E+01	1.3E+00	4.9E+01	-7.00	-8.09	-10.25	1.04	0.64	0.0%	0.0%	1.5E-33
1668	143-08-8	nonan-1-ol	144	-3	4.4E+00	1.2E+02	2.0E+03	14.0	3.5E-06	3.8E-06	1.1E-06	conf	conf	9.6E+01	1.3E+00	4.9E+01	-10.05	-9.88	-11.04	-1.96	0.33	0.0%	0.0%	8.4E-39
1669	5283-66-9	octyltrichlorosilane	248	8	9.4E+00	1.7E+02	2.8E+05	14.0	3.5E-06	1.3E-07	3.5E-07	conf	conf	6.4E+01	8.9E-01	3.1E+01	-9.63	-9.40	-10.60	-0.46	0.13	0.0%	0.0%	7.1E-48
1670	447-61-0	o-(trifluoromethyl)benzaldehyde	174	-6	9.0E+01	9.1E+02	4.7E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.93	-9.69	-10.95	-2.33	0.37	0.0%	0.0%	3.6E-35
1671	81-64-1	1,4-dihydroxyanthraquinone	240	181	9.5E-08	1.1E+03	8.7E+03	10.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.21	-9.47	-10.83	-3.35	0.24	0.0%	0.0%	6.0E-27
1672	760108-96-1	616-280-8	404	87	9.9E-03	2.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.4E+01	1.0E+00	3.7E+01	-7.14	-7.46	-9.12	-1.84	0.64	0.0%	0.0%	1.2E-25
1673	1083057-14-(	tert-butyl 3-(6-amino-3-methylpyridin-2-yl)benzoate	284	149	7.1E-05	1.0E+01	2.2E+04	5.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.96	-8.73	-10.38	-2.28	0.31	0.0%	0.0%	3.0E-31
1674	52567-96-1	3,6,7-trimethyloct-6-en-1-yn-3-ol	166	18	2.0E+00	1.1E+04	1.9E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.93	-8.75	-10.38	-1.75	0.55	0.0%	0.0%	3.4E-35
1675	1128026-41-	3,3-Dimethoxy-8,8,9,9-tetramethyl-2-oxa-7-thia-3,8-disiladecane	311	53	2.9E-01	3.3E+02	1.4E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.09	-8.86	-10.47	-1.46	0.64	0.0%	0.0%	2.9E-38
1676	93839-21-5	N-[4-(aminocarbonyl)phenyl]-4-nitrobenzamide	285	234	1.4E-09	4.4E+02	1.8E+01	14.0	3.5E-06	3.5E-06	3.5E-07	conf	conf	1.0E+02	1.4E+00	5.1E+01	-7.59	-8.81	-10.77	-2.08	0.64	0.0%	0.0%	1.1E-35
1677	146763-69-1	diethyl [4-(prop-2-yn-1-yloxy)benzylidene]propanedioate	302	64	3.1E-03	3.1E+01	1.7E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.90	-8.73	-10.39	-2.53	0.23	0.0%	0.0%	1.3E-29
1678	4180-23-8	(E)-anethole	148	-1	8.5E+00	1.4E+02	2.5E+03	14.0	3.5E-06	1.1E-07	3.5E-07	conf	conf	7.0E+01	9.8E-01	3.5E+01	-9.30	-9.03	-10.28	-2.15	0.12	0.0%	0.0%	1.7E-31
1679	7379-51-3	4-(methylthio)-3,5-xylenol	168	71	1.1E-01	1.3E+03	1.6E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.84	-8.72	-10.37	-2.32	0.31	0.0%	0.0%	6.9E-31
1680	90-31-3	2-(3-chlorophenyl)-2,4-dihydro-5-methyl-3H-pyrazol-3-one	209	124	1.8E-03	2.1E+04	1.6E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.78	-8.71	-10.36	-4.18	2.83	0.0%	0.0%	5.5E-19
1681	77-93-0	triethyl citrate	276	23	2.6E-02	3.8E+03	2.1E+00	9.9	3.5E-06	5.7E-07	1.1E-06	conf	conf	9.0E+01	1.3E+00	4.6E+01	-7.75	-8.13	-9.99	-0.49	1.05	0.0%	0.0%	3.1E-42
1682	5586-73-2	3-3-diphenylpropylamine	211	92	1.3E-02	5.3E+00	1.5E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.10	-8.88	-10.42	-2.67	0.61	0.0%	0.0%	9.1E-29
1683	3173-53-3	cyclohexyl isocyanate	125	-8	1.9E+02	1.3E+04	1.1E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.50	-9.27	-10.49	-1.33	0.64	0.0%	0.0%	2.1E-39
1684	25092-32-4	2-oxo-2-[(4aS,4bS,5aS,6aS,6bS,9aR,10aS,10bS)-4a,6a,8,8-tetramethyl-2-oxo-2,5a,6,6a,9a,10,10a,10b,11,12-decahydrc	457	216	2.4E-08	8.8E+00	1.1E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.65	-8.68	-10.33	-1.13	0.21	0.0%	0.0%	1.0E-39
1685	4023-34-1	cyclopropanecarbonyl chloride	105	-45	3.7E+03	1.6E+04	2.1E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.90	-9.65	-11.11	-1.24	0.64	0.0%	0.0%	2.1E-45
1686	531-18-0	1,3,5-triazine-2,4,6-triyltrinitrilohexamethanol	306	244	1.1E-12	4.3E+05	3.3E-06	2.6	3.5E-06	1.1E-07	3.5E-07	conf	conf	7.3E+01	1.0E+00	3.6E+01	-6.45	-7.45	-9.04	1.69	0.86	0.0%	0.0%	4.1E-25
1687	581076-60-0	611-622-2	368	236	9.5E-10	1.7E+01	1.3E+03	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.44	-8.53	-10.30	-2.06	0.56	0.0%	0.0%	2.9E-32
1688	1955-46-0	methyl 5-nitrohydrogen.isophthalate	225	147	2.7E-04	7.1E+02	3.4E+01	3.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.5E+01	1.3E+00	4.8E+01	-7.42	-8.36	-10.31	-0.76	0.79	0.0%	0.0%	1.0E-42
1689	1609-86-5	tert-butyl isocyanate	99	-45	1.8E+03	1.5E+04	1.4E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.92	-9.69	-10.86	-0.86	0.64	0.0%	0.0%	1.2E-46
1690	98-89-5	cyclohexanecarboxylic acid	128	44	7.6E+00	5.5E+03	2.3E+02	4.9	3.5E-06	9.3E-07	1.1E-06	conf	conf	9.3E+01	1.3E+00	4.8E+01	-8.13	-8.53	-10.29	-0.96	0.73	0.0%	0.0%	8.5E-41
1691	73097-51-5	N1-methyl-4-(methylsulfonyl)benzene-1,2-diamine	200	132	1.1E-03	1.4E+04	1.9E-01	1.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.4E+01	1.3E+00	4.8E+01	-7.22	-8.47	-10.32	-1.91	0.68	0.0%	0.0%	1.6E-33
1692	17462-58-7	sec-butyl chloroformate	137	-56	1.6E+03	1.7E+03	3.5E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-10.47	-10.20	-12.08	-1.69	0.44	0.0%	0.0%	3.4E-50
1693	3332-27-2	N,N-dimethyltetradecylamine N-oxide	257	183	1.5E-06	5.2E-02	4.6E+05	4.8	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.89	-8.70	-10.36	-2.72	0.92	0.0%	0.0%	4.5E-28
1694	63141-09-3	Ethanone, 1-(1-chlorocyclopropyl)-	119	-23	1.7E+03	1.2E+04	6.0E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.87	-9.64	-10.99	-1.45	1.27	0.0%	0.0%	1.3E-42
1695	93839-20-4	N-[4-(aminocarbonyl)phenyl]-4-methoxy-3-nitrobenzamide	315	245	2.5E-10	3.4E+02	2.2E+01	-0.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.4E+01	1.3E+00	4.8E+01	-7.21	-8.29	-10.25	-1.90	0.64	0.0%	0.0%	4.3E-33
1696	82530-64-1	617-343-2	199	16	2.9E+00	4.1E+02	7.1E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.34	-9.11	-10.47	-1.94	0.79	0.0%	0.0%	1.8E-34
1697	263355-39-1	(1E)-1-(methoxyimino)-1-(2,5,5-trimethyl-1,3-dioxan-2-yl)acetone	229	70	1.7E-01	2.2E+03	8.5E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.91	-8.76	-10.38	-1.85	0.78	0.0%	0.0%	1.7E-34
1698	77820-58-7	Methyl 2-amino-3-chlorobenzoate	186	75	1.5E-01	1.3E+03	8.1E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.69	-7.44	-9.05	-1.59	0.43	0.0%	0.0%	7.6E-27
1699	2478-10-6	4-hydroxybutyl acrylate	144	7	2.3E+00	5.4E+04	5.5E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.8E+01	1.4E+00	5.1E+01	-8.92	-9.03	-10.83	-1.78	0.12	0.0%	0.0%	1.6E-38
1700	368890-20-4	2-{[(4-chloro-3-methoxypyridin-2-yl)methyl]sulfanyl}-6-(difluoromethoxy)-1H-benzimidazole	372	226	4.5E-09	6.0E-01	1.1E+04	3.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.4E+01	1.3E+00	4.8E+01	-7.73	-8.46	-10.28	-3.42	0.29	0.0%	0.0%	5.8E-23
1701	22235-81-0	endo-(±)-8-aza-8-isopropylbicyclo[3.2.1]oct-3-yl (hydroxymethyl)phenylacetate	317	151	6.9E-07	3.9E+03	6.6E+02	10.1	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.58	-8.64	-10.31	-2.05	0.73	0.0%	0.0%	1.8E-32
1702	5417-35-6	4,7-dihydro-2-isopropyl-1,3-dioxepin	142	-30	2.0E+02	3.0E+03	6.2E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.80	-9.58	-10.78	-2.38	1.06	0.0%	0.0%	1.9E-33
1703	361442-00-4	(2S)-[(tert-butoxycarbonyl)amino](3-hydroxytricyclo[3.3.1.13,7]dec-1-yl)acetic acid	325	178	1.1E-07	6.5E-01	3.5E+02	3.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.4E+01	1.3E+00	4.8E+01	-7.67	-8.41	-10.33	-1.62	0.75	0.0%	0.0%	7.4E-36
1704	13188-60-8	dodecanedioic acid, compound with hexane-1,6-diamine (1:1)	347	87	9.9E-03	2.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.3E+01	1.0E+00	3.6E+01	-7.16	-7.47	-9.13	-1.84	0.64	0.0%	0.0%	1.1E-25
1705	15875-13-5	N,N,N',N',N'',N''-hexamethyl-1,3,5-triazine-1,3,5(2H,4H,6H)-tripropanamine	343	162	5.9E-05	5.2E+03	2.6E-02	9.9	3.5E-06	3.5E-06	3.5E-07	conf	conf	9.8E+01	1.4E+00	5.1E+01	-7.43	-8.54	-10.82	-1.67	0.78	0.0%	0.0%	2.4E-39
1706	110-80-5	2-ethoxyethanol	90	-44	4.1E+02	7.3E+05	3.8E-01	14.0	3.5E-06	1.0E-06	1.1E-06	conf	conf	9.3E+01	1.3E+00	4.8E+01	-8.60	-8.42	-10.21	0.89	0.12	0.0%	0.0%	5.4E-57
1707	58430-94-7	3,5,5-trimethylhexyl acetate	186	-14	5.1E+01	1.5E+01	1.3E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	7.8E+01	1.1E+00	3.9E+01	-10.77	-10.49	-12.69	-2.10	0.46	0.0%	0.0%	6.0E-52
1708	530-78-9	flufenamic acid	281	140	3.0E-04	3.6E+01	1.4E+05	4.2	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.3E+01	1.3E+00	4.8E+01	-7.90	-8.70	-10.36	-2.54	0.19	0.0%	0.0%	2.7E-29
1709	51336-94-8	2',4'-Difluoro-α-chloroacetophenone	191	31	7.6E+00	4.5E+02	2.1E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.51	-9.29	-10.53	-3.75	0.51	0.0%	0.0%	1.8E-22
1710	150928-21-5	604-759-4	807	327	5.0E-16	3.9E-02	6.9E+01	10.8	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.3E+01	1.3E+00	4.8E+01	-7.34	-8.45	-10.28	-2.07	1.03	0.0%	0.0%	4.5E-32
1711	255830-15-0	pentapotassium ({[(hydroxyphosphinato)methyl](phosphonatomethyl)nitroryl}methyl)phosphonate	128	-25	4.1E+03	2.6E+05	2.8E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.3E+01	1.3E+00	4.8E+01	-9.37	-9.19	-10.46	-0.31	0.64	0.0%	0.0%	5.9E-48
1712	89-25-8	3-methyl-1-phenyl-5-pyrazolone	174	113	4.6E-03	9.5E+04	3.6E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.67	-8.63	-10.35	-4.13	2.93	0.0%	0.0%	3.3E-19
1713	2517-43-3	3-methoxybutan-1-ol	104	-44	1.2E+02	5.3E+04	1.0E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.8E+01	1.4E+00	5.0E+01	-9.27	-9.14	-10.78	-0.26	0.51	0.0%	0.0%	2.2E-51
1714	543-49-7	heptan-2-ol	116	-39	1.1E+02	4.9E+03	1.7E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.55	-9.33	-10.50	-1.54	0.44	0.0%	0.0%	9.1E-38
1715	80012-43-7	1H-Dibenz[c,f]imidazo[1,5-a]azepin-3-amine, 9,13b-dihydro- | Epinastin | Epinastine	249	160	8.7E-05	3.7E+02	3.5E+02	9.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.71	-8.63	-10.36	-2.28	0.63	0.0%	0.0%	3.6E-31
1716	15520-10-2	2-methylpentane-1,5-diamine	116	13	1.3E+02	1.0E+06	1.9E+00	10.7	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.8E+01	1.4E+00	5.0E+01	-9.07	-8.96	-10.81	-1.00	0.77	0.0%	0.0%	6.5E-45
1717	500011-92-7	610-491-9	331	161	7.9E-05	2.3E+01	3.1E+02	0.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.66	-8.40	-10.34	-2.49	1.36	0.0%	0.0%	1.8E-29
1718	7384-80-7	2-methyl-3-phenylpropanol	150	17	4.3E-01	1.3E+03	3.0E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.87	-8.66	-10.36	-3.26	2.02	0.0%	0.0%	1.7E-24
1719	77-86-1	trometamol	121	81	3.0E-04	1.0E+06	2.8E-02	8.1	3.5E-06	3.5E-06	3.5E-06	conf	conf	9.8E+01	1.4E+00	5.0E+01	-7.67	-8.89	-10.79	0.34	0.90	0.0%	0.0%	3.1E-57
1720	102625-64-9	5-difluoromethoxy-2-[[(3,4-dimethoxy-2-pyridyl)methyl]thio]-1H-benzimidazole	367	229	3.2E-09	4.4E+00	9.5E+02	5.1	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.3E+01	1.3E+00	4.8E+01	-7.61	-8.45	-10.29	-3.00	0.65	0.0%	0.0%	1.2E-25
1721	79-44-7	dimethylcarbamoyl chloride	108	-16	2.4E+02	1.8E+05	1.9E-01	-0.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.3E+01	1.3E+00	4.8E+01	-7.10	-8.28	-10.28	-1.57	1.60	0.0%	0.0%	7.7E-36
1722	218768-11-7	(Z)-4-hydroxy-4-(6-methoxynaphthalen-2-yl)but-3-en-2-one	242	142	1.4E-06	3.6E+03	2.6E+02	8.6	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.26	-8.38	-10.28	-2.50	0.57	0.0%	0.0%	5.5E-29
1723	77326-36-4	2-amino-6-fluorobenzonitrile	136	56	1.4E+00	5.0E+03	2.3E+01	0.3	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.3E+01	1.3E+00	4.8E+01	-7.66	-8.55	-10.34	-2.03	0.73	0.0%	0.0%	9.3E-33
1724	133865-89-1	603-772-2	302	190	1.0E-06	8.4E+00	2.2E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-6.52	-7.36	-9.02	-2.00	0.61	0.0%	0.0%	5.2E-24
1725	121-60-8	N-acetylsulphanilyl chloride	234	166	4.5E-05	4.5E+03	1.1E+02	-1.8	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.3E+01	1.3E+00	4.8E+01	-7.40	-8.32	-10.26	-0.64	0.40	0.0%	0.0%	2.8E-43
1726	49701-24-8	4-amino-2,5-dimethoxy-N-methylbenzenesulphonamide	246	155	8.3E-05	2.6E+04	1.2E+00	1.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.3E+01	1.3E+00	4.8E+01	-7.01	-8.26	-10.26	-2.14	1.71	0.0%	0.0%	2.2E-31
1727	7087-68-5	ethyldiisopropylamine	129	-69	1.6E+03	1.3E+04	2.2E+02	11.0	3.5E-06	7.8E-08	3.5E-07	conf	conf	6.5E+01	9.1E-01	3.2E+01	-9.43	-9.15	-10.62	-1.05	0.70	0.0%	0.0%	8.3E-43
1728	86261-90-7	2-(2-oxoimidazolidin-1-yl)ethyl methacrylate	198	109	5.1E-03	2.4E+04	2.6E+00	-0.5	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.7E+01	1.3E+00	5.0E+01	-7.67	-9.00	-10.80	-0.47	0.36	0.0%	0.0%	1.3E-49
1729	27344-06-5	disodium 4,4'-bis[[4-anilino-6-[(2-carbamoylethyl)(2-hydroxyethyl)amino]-1,3,5,-triazin-2-yl]amino]stilbene-2,2'-disu	1015	87	9.9E-03	7.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.2E+01	1.0E+00	3.6E+01	-7.15	-7.47	-9.14	-0.66	0.65	0.0%	0.0%	4.4E-34
1730	24131-07-5	Methyl 2-cyano-2-phenylbutanoate	203	79	3.7E-02	1.9E+02	1.3E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.80	-8.60	-10.36	-2.72	0.90	0.0%	0.0%	5.3E-28
1731	959624-24-9	6-(hydroxymethyl)-4-phenyl-3,4-dihydro-2H-chromen-2-ol	256	155	1.8E-07	1.1E+02	1.2E+02	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.22	-8.32	-10.28	-2.00	0.59	0.0%	0.0%	1.3E-32
1732	13349-82-1	2-[2-(Piperazin-1-yl)ethoxy]ethanol	174	90	5.2E-03	1.0E+06	1.4E-02	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	9.2E+01	1.3E+00	4.6E+01	-6.46	-7.34	-8.99	-0.93	1.00	0.0%	0.0%	5.5E-31
1733	18559-94-9	salbutamol	239	146	1.2E-06	1.6E+04	4.4E+00	8.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.3E+01	1.3E+00	4.8E+01	-7.07	-8.22	-10.24	-2.60	0.96	0.0%	0.0%	4.4E-28
1734	4708-04-7	propylphosphonic dichloride	161	-35	1.9E+02	8.5E+03	7.2E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.50	-9.31	-10.55	-0.97	0.58	0.0%	0.0%	5.7E-43
1735	30433-91-1	thiophene-2-ethylamine	127	32	2.0E+01	1.1E+03	2.4E+01	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.20	-8.99	-10.42	-2.01	0.80	0.0%	0.0%	1.4E-33
1736	82543-15-5	3'H-Cycloprop[15,16]androsta-6,15-dien-17-one, 15,16-dihydro-3,5-dihydroxy-, (3β,5β,15α,16α)-	316	177	5.1E-08	8.6E+02	9.8E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.61	-8.65	-10.31	-2.27	0.73	0.0%	0.0%	7.7E-31
1737	393-52-2	2-fluorobenzoyl chloride	159	8	3.6E+01	5.2E+03	4.4E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.25	-9.05	-10.41	-1.79	0.89	0.0%	0.0%	4.1E-35
1738	139481-58-6	ethyl 2-ethoxy-1-{[2'-(1H-tetrazol-5-yl)biphenyl-4-yl]methyl}-1H-benzimidazole-7-carboxylate	469	322	1.2E-15	1.2E-03	1.7E+05	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	9.1E+01	1.3E+00	4.5E+01	-6.54	-7.43	-9.04	-2.89	0.96	0.0%	0.0%	7.0E-19
1739	641571-11-1	3-(4-methyl-1H-imidazol-1-yl)-5-(trifluoromethyl)aniline	241	137	3.9E-04	2.6E+02	2.6E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.83	-8.61	-10.36	-2.49	0.62	0.0%	0.0%	1.2E-29
1740	26447-85-8	Methyl hydroxy(di-2-thienyl)acetate	254	132	2.1E-05	4.4E+02	7.1E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.52	-8.51	-10.35	-1.29	0.95	0.0%	0.0%	1.3E-38
1741	99199-60-7	6-Fluorochromane-2-carboxylic acid	196	99	2.1E-02	3.4E+03	1.3E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.24	-8.69	-10.36	-0.94	0.33	0.0%	0.0%	1.2E-41
1742	161798-03-4	ethyl 2-[3-formyl-4-(2-methylpropoxy)phenyl]-4-methyl-1,3-thiazole-5-carboxylate	347	194	5.8E-07	5.1E-01	6.8E+04	1.8	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.85	-8.48	-10.33	-3.22	0.29	0.0%	0.0%	1.5E-24
1743	176972-62-6	methyl [(2S,3S)-4-chloro-3-hydroxy-1-phenylbutan-2-yl]carbamate	258	115	4.4E-05	6.3E+02	6.0E+01	10.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.50	-8.50	-10.35	-2.56	1.13	0.0%	0.0%	4.4E-29
1744	100-06-1	4'-methoxyacetophenone	150	25	1.8E+00	3.3E+03	5.6E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.93	-8.71	-10.37	-1.08	0.24	0.0%	0.0%	1.7E-40
1745	90315-82-5	ethyl (2R)-2-hydroxy-4-phenylbutanoate	208	67	3.3E-03	2.2E+03	5.9E+01	12.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.66	-8.50	-10.34	-1.89	0.80	0.0%	0.0%	7.0E-34
1746	1103234-56-	2,6-difluoro-3-[(propylsulfonyl)amino]benzoic acid	279	167	3.4E-05	4.4E+02	2.2E+01	1.8	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.36	-8.35	-10.32	-2.14	0.89	0.0%	0.0%	8.0E-32
1747	862574-88-7	1-(2,2-difluoro-1,3-benzodioxol-5-yl)cyclopropanecarboxylic acid	242	125	3.3E-03	7.5E+02	6.6E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.32	-8.82	-10.38	-2.27	1.18	0.0%	0.0%	2.2E-31
1748	5693-27-6	1H-2-Benzopyran-1,4(3H)-dione	162	86	1.5E-02	3.4E+03	4.6E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.81	-8.48	-10.33	-1.54	0.93	0.0%	0.0%	1.8E-36
1749	22038-86-4	(1R)-1-(4-Methoxyphenyl)ethanamine	151	34	7.6E+00	6.1E+03	3.7E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.86	-8.66	-10.33	-2.13	0.76	0.0%	0.0%	5.6E-32
1750	41851-59-6	(1S)-1-(4-methoxyphenyl)ethanamine	151	34	7.6E+00	6.1E+03	3.7E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.86	-8.66	-10.33	-2.13	0.76	0.0%	0.0%	5.6E-32
1751	88196-70-7	(1R)-1-(3-methoxyphenyl)ethanamine	151	34	7.6E+00	6.1E+03	3.7E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.86	-8.66	-10.33	-2.13	0.76	0.0%	0.0%	5.6E-32
1752	2743-38-6	dibenzoyl-L-tartaric acid monohydrate	358	208	3.4E-08	7.1E+03	7.8E+03	1.1	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.76	-8.60	-10.30	-1.52	0.85	0.0%	0.0%	2.1E-36
1753	99636-38-1	(2R)-1-Methoxy-2-propanamine	89	-52	5.4E+03	2.0E+05	3.2E-01	9.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.29	-9.03	-10.45	-1.74	1.47	0.0%	0.0%	7.7E-36
1754	99636-32-5	(S)-(+)-1-methoxy-2-propylamine	89	-52	5.4E+03	2.0E+05	3.2E-01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.29	-9.03	-10.46	-1.74	1.47	0.0%	0.0%	7.3E-36
1755	92-36-4	4-(6-methylbenzothiazol-2-yl)aniline	240	172	2.7E-06	8.9E+01	3.6E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.75	-8.74	-10.34	-3.17	0.37	0.0%	0.0%	6.5E-25
1756	152402-98-7	604-848-8	300	229	2.9E-09	1.7E+01	1.8E+03	12.1	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.48	-8.56	-10.30	-2.30	0.24	0.0%	0.0%	1.5E-30
1757	106410-46-2	4-[(5-{[(benzyloxy)carbonyl]amino}pentyl)(hydroxy)amino]-4-oxobutanoic acid	352	232	8.5E-12	2.6E+03	3.0E+01	4.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.25	-8.31	-10.26	-1.70	0.89	0.0%	0.0%	1.1E-34
1758	82796-69-8	(1S)-1-(3-methoxyphenyl)ethanamine	151	19	1.6E+01	6.1E+03	2.1E+01	9.2	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.91	-8.73	-10.33	-2.13	0.76	0.0%	0.0%	5.7E-32
1759	71839-12-8	Methyl 4-(butylamino)benzoate	207	73	1.0E-01	1.7E+02	2.1E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.01	-8.79	-10.42	-2.53	0.68	0.0%	0.0%	1.0E-29
1760	179688-27-8	Ethyl 2-amino-4,5-bis(2-methoxyethoxy)benzoate	313	152	3.6E-05	4.5E+02	7.1E+01	2.1	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.50	-8.38	-10.33	-1.24	0.51	0.0%	0.0%	7.7E-39
1761	3423-28-7	8-isopropyl-8-azabicyclo[3.2.1]octan-3-one	167	46	3.5E+00	1.3E+04	2.2E+01	9.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.70	-8.49	-10.32	-1.99	0.78	0.0%	0.0%	6.1E-33
1762	147118-40-9	methyl (3R,5S,6E)-7-{4-(4-fluorophenyl)-6-isopropyl-2-[methyl(methylsulfonyl)amino]pyrimidin-5-yl}-3,5-dihydroxyl	496	271	1.4E-15	1.1E+00	5.8E+02	1.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.57	-8.36	-10.27	-2.60	0.57	0.0%	0.0%	2.9E-28
1763	335153-21-4	608-880-3	281	179	5.5E-06	2.2E+02	5.6E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.82	-8.73	-10.36	-1.88	0.22	0.0%	0.0%	4.1E-34
1764	445-03-4	4-chloro-α,α,α-trifluoro-o-toluidine	196	32	1.3E+01	1.1E+03	4.8E+02	3.9	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.29	-8.66	-10.43	-2.25	0.53	0.0%	0.0%	7.8E-32
1765	110-76-9	2-ethoxyethylamine	89	-40	3.5E+03	2.1E+05	3.8E-01	9.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.17	-8.92	-10.38	-1.48	0.95	0.0%	0.0%	2.3E-37
1766	95-79-4	5-chloro-o-toluidine	142	42	6.1E+00	5.6E+02	1.9E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.36	-9.14	-10.43	-2.41	0.71	0.0%	0.0%	1.0E-30
1767	18480-53-0	3,4-Dichloro-5-isothiazolecarboxylic acid	198	113	1.6E-02	7.9E+02	1.4E+02	-0.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.58	-8.39	-10.32	-1.43	0.28	0.0%	0.0%	2.9E-37
1768	179688-26-7	605-866-9	343	171	1.1E-05	9.3E+01	1.7E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.37	-8.39	-10.34	-1.61	0.82	0.0%	0.0%	5.5E-36
1769	130-00-7	benz[cd]indol-2(1H)-one	169	143	1.1E-04	2.8E+02	1.3E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-6.54	-7.36	-9.01	-2.37	0.95	0.0%	0.0%	1.1E-21
1770	144163-97-3	4-Nitrophenyl 1,3-thiazol-5-ylmethyl carbonate	280	153	3.5E-05	1.1E+02	9.5E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.59	-8.54	-10.36	-1.76	0.80	0.0%	0.0%	5.9E-35
1771	141818-73-7	allyl (2S,4S)-4-(benzoylthio)-2-(dimethylcarbamoyl)pyrrolidine-1-carboxylate	362	202	1.9E-07	1.5E+02	9.3E+01	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-6.39	-7.33	-8.98	-1.95	0.60	0.0%	0.0%	4.9E-24
1772	112110-16-4	dimethyl 5-methylpyridine-2,3-dicarboxylate	209	27	1.0E+00	3.0E+02	5.1E+00	0.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.25	-8.34	-10.32	-1.75	0.76	0.0%	0.0%	8.9E-35
1773	13734-41-3	N-[(tert-butoxy)carbonyl]-L-valine	217	89	4.2E-02	3.8E+03	7.9E+01	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.20	-7.36	-9.01	-1.56	0.97	0.0%	0.0%	9.7E-27
1774	7785-70-8	(+)-pin-2(3)-ene	136	-14	5.4E+02	2.8E+01	1.9E+04	14.0	3.5E-06	9.7E-08	1.1E-07	conf	conf	5.6E+01	7.8E-01	2.7E+01	-10.54	-10.23	-12.59	-2.87	0.73	0.0%	0.0%	3.7E-44
1775	286-20-4	1,2-epoxycyclohexane	98	-52	1.5E+03	2.0E+04	4.6E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.0E+01	1.3E+00	4.6E+01	-9.73	-9.52	-10.74	-1.64	0.58	0.0%	0.0%	6.5E-39
1776	106006-84-2	Propanamide, N-[(6S)-2-amino-4,5,6,7-tetrahydro-6-benzothiazolyl]-	225	176	9.5E-06	5.3E+01	4.8E+01	5.1	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.71	-8.58	-10.36	-2.00	0.60	0.0%	0.0%	3.6E-33
1777	3423-25-4	endo-8-isopropyl-8-azabicyclo[3.2.1]octan-3-ol	169	44	3.4E-01	1.3E+04	1.4E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.44	-8.57	-10.35	-1.95	0.78	0.0%	0.0%	2.0E-33
1778	816431-72-8	617-251-2	354	229	2.8E-09	1.1E+01	5.5E+01	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-6.35	-7.31	-8.97	-1.89	1.17	0.0%	0.0%	2.5E-24
1779	2840-28-0	3-amino-4-chlorobenzoic acid	172	114	5.2E-04	3.6E+03	4.0E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	9.1E+01	1.3E+00	4.6E+01	-6.65	-7.44	-9.07	-2.01	0.68	0.0%	0.0%	3.1E-24
1780	99-34-3	3,5-dinitrobenzoic acid	212	148	4.1E-05	3.8E+03	3.2E+01	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.19	-8.25	-10.29	-0.99	0.81	0.0%	0.0%	1.3E-40
1781	120100-77-8	2-Chloro-4-(methylsulfonyl)-3-[(2,2,2-trifluoroethoxy)methyl]benzoic acid	347	175	9.9E-06	4.3E+01	2.7E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	9.1E+01	1.3E+00	4.6E+01	-6.64	-7.42	-9.07	-0.47	0.30	0.0%	0.0%	6.0E-35
1782	117-96-4	3,5-diacetamido-2,4,6-triiodobenzoic acid	614	285	4.8E-13	8.3E-01	2.3E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.23	-8.36	-10.27	-2.18	0.74	0.0%	0.0%	3.2E-31
1783	50977-10-1	3-(isotridecyloxy)propylamine	257	81	2.3E-02	3.6E-01	2.5E+05	9.9	3.5E-06	3.5E-07	1.1E-07	conf	conf	6.6E+01	9.2E-01	3.3E+01	-9.77	-9.54	-10.64	-3.56	0.52	0.0%	0.0%	2.4E-24
1784	28443-50-7	2-amino-5-chlorophenol	144	70	1.9E-01	4.4E+03	1.7E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.34	-8.41	-10.31	-2.48	0.48	0.0%	0.0%	2.3E-29
1785	95-85-2	2-amino-4-chlorophenol	144	70	3.4E-02	7.4E+03	1.7E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.70	-8.40	-10.32	-2.48	0.48	0.0%	0.0%	2.2E-29
1786	27006-83-3	5-Chloro-1,3-dimethyl-1H-pyrazole-4-carbonyl chloride	193	73	7.4E-01	1.0E+03	1.7E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.91	-7.64	-9.17	-3.32	1.01	0.0%	0.0%	3.4E-17
1787	80-20-6	3-amino-4-hydroxy-N-phenylbenzenesulphonamide	264	190	1.8E-07	5.6E+02	1.7E+01	3.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.47	-8.51	-10.30	-2.25	0.49	0.0%	0.0%	6.4E-31
1788	2736-23-4	2,4-dichloro-5-sulphamoylbenzoic acid	270	175	1.0E-05	3.2E+02	1.6E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.35	-8.38	-10.33	-1.78	1.12	0.0%	0.0%	1.2E-34
1789	13636-02-7	3-(dimethylamino)-1-(thiophen-2-yl)propan-1-ol	185	70	1.7E-02	2.4E+04	1.0E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	9.1E+01	1.3E+00	4.6E+01	-6.65	-7.40	-9.04	-1.79	0.78	0.0%	0.0%	1.9E-25
1790	617-89-0	furfurylamine	97	-8	6.6E+02	1.1E+05	2.8E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.07	-8.90	-10.32	-1.72	0.83	0.0%	0.0%	4.9E-35
1791	42142-52-9	α-[2-(methylamino)ethyl]benzyl alcohol	165	51	4.8E-02	9.0E+03	9.5E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.70	-8.35	-10.31	-1.90	0.80	0.0%	0.0%	1.6E-33
1792	598-72-1	2-bromopropionic acid	153	30	3.5E+01	1.0E+05	7.1E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.65	-8.45	-10.29	-0.28	0.44	0.0%	0.0%	9.0E-47
1793	4245-76-5	610-029-6	118	35	1.7E+01	3.7E+05	6.8E-02	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.40	-7.37	-9.01	-0.60	0.15	0.0%	0.0%	1.5E-33
1794	473799-16-5	S-allyl 5-amino-4-(2-methylphenyl)-3-oxo-2,3-dihydro-1H-pyrazole-1-carbothioate	289	216	2.1E-08	1.8E+01	4.9E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.16	-8.26	-10.28	-4.93	0.64	0.1%	0.0%	1.0E-14
1795	937203-35-5	3-(3,4-Dimethoxyphenyl)-2-hydrazinyl-2-methylpropanoic acid	254	161	6.9E-05	5.1E+01	3.0E+00	7.1	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.54	-8.47	-10.34	-2.85	3.02	0.0%	0.0%	4.6E-27
1796	696-23-1	2-methyl-4-nitroimidazole	127	107	1.8E-04	4.4E+03	2.6E+00	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.07	-8.12	-10.25	-2.01	0.80	0.0%	0.0%	2.9E-32
1797	60046-50-6	(4R,6R)-4-Hydroxy-2,2,6-trimethylcyclohexanone	156	52	1.9E-01	2.0E+04	7.6E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.08	-8.53	-10.34	-0.70	0.55	0.0%	0.0%	1.9E-43
1798	130-17-6	2-(4-aminophenyl)-6-methylbenzothiazole-7-sulphonic acid	320	238	2.5E-12	1.4E+03	2.6E+00	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	9.1E+01	1.3E+00	4.6E+01	-6.35	-7.33	-8.97	-1.87	0.24	0.0%	0.0%	1.7E-24
1799	142-30-3	2,5-dimethylhexyne-2,5-diol	142	45	9.4E-01	3.0E+17	6.5E+00	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	9.1E+01	1.3E+00	4.6E+01	-6.38	-7.34	-8.99	1.47	0.64	0.0%	0.0%	8.5E-25
1800	887-76-3	4,4'-azo-3-hydroxynaphthalene-1-sulphonate	250	274	3.4E-15	1.5E-02	7.8E-01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.17	-8.31	-10.26	-2.69	0.64	0.0%	0.0%	1.4E-27
1801	54527-65-0	2-(benzylmethylamino)ethyl acetoacetate	249	98	6.1E-03	1.2E+02	5.1E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.35	-8.32	-10.30	-1.76	0.85	0.0%	0.0%	1.5E-34
1802	1072-63-5	1-vinylimidazole	94	13	2.5E+01	4.6E+04	9.1E+00	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	8.2E+01	1.1E+00	4.2E+01	-8.16	-7.92	-9.67	-0.40	0.24	0.0%	0.0%	2.7E-40
1803	93-01-6	6-hydroxynaphthalene-2-sulphonic acid	224	173	4.1E-07	4.3E+03	3.4E-01	0.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-6.93	-8.23	-10.25	-1.22	0.36	0.0%	0.0%	2.3E-38
1804	84-87-7	4-hydroxynaphthalene-1-sulphonic acid	224	173	1.3E-07	4.0E+03	3.4E-01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-6.94	-8.09	-10.21	-1.16	0.32	0.0%	0.0%	1.5E-38
1805	89-36-1	4-(3-methyl-5-oxo-2-pyrazolin-1-yl)benzenesulphonic acid	254	197	4.3E-09	3.7E+03	2.5E-01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+01	1.3E+00	4.7E+01	-6.92	-8.08	-10.21	-3.72	3.12	0.0%	0.0%	9.2E-21

1806	265136-65-0	Ethyl 3-amino-4-[2-(phthalimido)ethoxy]crotonate	318	223	7.5E-09	2.2E+03	4.2E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.07	-8.22	-10.24	-2.25	0.64	0.0%	0.0%	0.0%	1.7E-30
1807	96240-10-7	689-404-1	142	124	2.3E-03	8.2E+04	9.1E-02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.23	-8.28	-10.29	-0.58	1.37	0.0%	0.0%	0.0%	4.8E-44
1808	98210-99-2	619-326-5	545	350	6.2E-23	4.4E-03	6.8E-02	14.0	3.5E-06	1.1E-06	3.5E-08	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-6.81	-7.96	-10.17	-1.22	0.64	0.0%	0.0%	0.0%	9.7E-38
1809	133047-57-1	3,10-Bis[(2-aminopropyl)amino]-6,13-dichloro[1,4]benzoxazino[2,3-b]phenoxazine-4,11-disulfonic acid	660	350	1.5E-25	4.8E-04	8.3E-02	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	conf	9.1E+01	1.3E+00	4.6E+01	-6.32	-7.30	-8.96	-2.25	0.64	0.0%	0.0%	0.0%	4.8E-22
1810	16415-12-6	hexadecyltrimethoxysilane	347	101	2.0E-03	1.6E-01	4.9E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	6.3E+01	8.8E-01	3.1E+01	-9.76	-9.81	-10.75	-0.51	1.76	0.0%	0.0%	0.0%	8.5E-49
1811	7529-16-0	616-206-4	111	63	7.2E-01	7.7E+04	2.8E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.71	-8.26	-10.28	-1.72	1.32	0.0%	0.0%	0.0%	9.9E-35
1812	51-34-3	hyoscine	303	151	2.6E-07	7.5E+03	2.5E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.03	-8.18	-10.24	-1.36	0.95	0.0%	0.0%	0.0%	3.5E-37
1813	88-23-3	3-amino-5-chloro-2-hydroxybenzenesulphonic acid	224	174	2.3E-07	5.6E+03	1.2E-02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-6.89	-8.04	-10.20	-1.85	0.66	0.0%	0.0%	0.0%	4.0E-33
1814	90-20-0	4-amino-5-hydroxynaphthalene-2,7-disulphonic acid	319	261	9.9E-15	6.5E+04	4.7E-03	-0.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.00	-8.37	-10.27	-1.07	1.15	0.0%	0.0%	0.0%	8.8E-40
1815	2963-69-1	608-385-2	320	195	6.9E-10	5.4E+02	2.0E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.24	-8.37	-10.27	-2.05	0.94	0.0%	0.0%	0.0%	3.4E-32
1816	172529-93-0	605-637-3	328	201	2.0E-07	1.3E+02	2.0E+00	12.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.12	-8.21	-10.28	-0.84	0.59	0.0%	0.0%	0.0%	9.0E-42
1817	1170-02-1	ethylenediamine-N,N'-bis(2-hydroxyphenyl)acetic acid)	360	324	1.2E-14	5.4E-01	3.3E-03	9.2	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-6.88	-8.03	-10.19	-1.85	0.58	0.0%	0.0%	0.0%	4.3E-33
1818	25157-64-6	607-578-9	282	350	2.9E-19	1.0E+06	2.3E-03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-6.88	-8.03	-10.19	-3.13	3.61	0.0%	0.0%	0.0%	2.9E-24
1819	1194-65-6	dichlobenil (reach)	53	53	7.8E-02	6.3E+01	6.6E+00	14.0	3.5E-06	3.2E-09	3.5E-08	conf	conf	conf	5.5E+01	7.7E-01	2.7E+01	-7.91	-7.63	-8.65	-2.03	0.58	0.0%	0.0%	0.0%	1.5E-21
1820	4684-28-0	[7(5)-[(1a,2β,4β,5a,7β)]]-3-oxa-9-azatricyclo[3.3.1.02,4]non-7-yl (hydroxymethyl)phenylacetate	289	158	5.7E-07	4.7E+03	1.5E+00	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.02	-8.16	-10.24	-1.26	1.05	0.0%	0.0%	0.0%	6.2E-38
1821	18063-03-1	2,6-difluorobenzamide	157	85	3.8E-02	1.3E+03	1.0E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.22	-8.40	-10.31	-0.74	0.29	0.0%	0.0%	0.0%	6.6E-43
1822	12135-20-6	2-((2-[(3-aminobenzoyl)amino]ethyl)sulfonyl)ethyl hydrogen sulphate	352	265	2.0E-14	1.3E+03	3.3E-05	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-6.99	-8.15	-10.23	-1.11	1.10	0.0%	0.0%	0.0%	4.5E-39
1823	6860-97-5	4-hydroxy-5-[(p-tolyl)sulphonyl]amino]naphthalene-2,7-disulphonic acid	474	334	6.5E-21	1.2E-01	5.9E-01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-6.95	-8.11	-10.22	-2.53	2.55	0.0%	0.0%	0.0%	2.6E-47
1824	143382-03-0	5-(methoxymethyl)pyridine-2,3-dicarboxylic acid	211	162	6.7E-05	4.6E+03	4.6E-01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.10	-8.17	-10.27	-0.51	0.64	0.0%	0.0%	0.0%	1.6E-44
1825	5926-26-1	Silane, (chloromethyl)trimethoxy-	171	-27	3.4E+02	3.9E+06	3.8E-01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.50	-8.38	-10.30	0.49	0.64	0.0%	0.0%	0.0%	7.0E-54
1826	598-55-0	methyl carbamate	75	-47	7.3E-01	4.5E+05	3.1E-01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.46	-8.36	-10.27	-0.98	1.27	0.0%	0.0%	0.0%	1.8E-40
1827	132-57-0	7-hydroxymethylthalene-1-sulphonic acid	224	173	1.2E-07	4.0E+03	3.4E-01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	conf	9.1E+01	1.3E+00	4.6E+01	-6.33	-7.31	-8.96	-1.14	0.31	0.0%	0.0%	0.0%	2.6E-29
1828	3577-63-7	5-sulphoanthranilic acid	217	187	2.2E-08	1.7E+05	1.6E-02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-6.88	-8.04	-10.20	-1.37	1.05	0.0%	0.0%	0.0%	9.7E-37
1829	7474-78-4	3,4-diaminobenzenesulphonic acid	188	161	6.6E-07	5.2E+04	1.0E-03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.00	-8.15	-10.23	-2.11	1.53	0.0%	0.0%	0.0%	2.1E-31
1830	74124-79-1	(diuscizinimide) carbaryle	256	240	5.8E-10	1.0E+06	1.7E-05	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-6.49	-8.15	-10.23	-1.13	1.84	0.0%	0.0%	0.0%	2.6E-39
1831	926-63-6	dimethyl(propyl)amine	87	-83	2.1E+04	1.4E+05	1.0E+01	10.1	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.4E+01	1.3E+00	4.8E+01	-10.17	-9.98	-11.30	-1.58	0.61	0.0%	0.0%	0.0%	4.2E-44
1832	4090-51-1	2,2'-oxybis[5,5-dimethyl-1,3,2-dioxaphosphorinane] 2,2'-disulphide	346	-20	3.6E-03	5.5E+00	3.3E+04	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	conf	7.3E+01	1.0E+00	3.7E+01	-8.64	-8.48	-10.03	-3.60	0.87	0.0%	0.0%	0.0%	2.1E-20
1833	63589-25-3	4-diazo-2,4-dihydro-7-nitro-3-oxonaphthalene-1-sulphonic acid	295	300	7.7E-17	7.2E+01	5.1E-01	-1.8	3.5E-06	3.5E-06	3.5E-07	conf	conf	conf	9.6E+01	1.3E+00	4.9E+01	-7.35	-8.70	-10.78	-0.60	0.64	0.0%	0.0%	0.0%	1.3E-48
1834	89-58-7	2-nitro-p-xylene	151	53	6.0E-00	1.2E+02	8.1E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	9.1E+01	1.3E+00	4.5E+01	-9.01	-8.70	-10.08	-1.83	0.45	0.0%	0.0%	0.0%	2.2E-32
1835	20193-20-8	N-ethylpropylamine	87	-67	1.1E+04	1.8E+05	2.0E+01	10.9	3.5E-06	1.1E-05	1.1E-06	conf	conf	conf	9.6E+01	1.3E+00	4.9E+01	-10.33	-10.23	-11.52	-0.80	0.92	0.0%	0.0%	0.0%	2.9E-53
1836	15793-73-4	4,4'-[[3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl]bis(azo)]bis[2,4-dihydro-5-methyl-2-(p-tolyl)-3H-pyrazol-3-one]	652	350	2.3E-19	1.1E-05	1.8E+11	0.7	3.5E-06	3.5E-07	3.5E-08	conf	conf	conf	8.0E+01	1.1E+00	4.0E+01	-7.97	-7.97	-8.97	-4.91	0.57	0.0%	0.0%	0.0%	3.5E-09
1837	89-87-2	4-nitro-m-xylene	151	53	4.3E-00	1.2E+02	8.1E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.83	-9.70	-11.00	-1.87	0.46	0.0%	0.0%	0.0%	3.8E-39
1838	107-94-8	3-chloropropionic acid	109	22	2.6E+02	1.2E+05	6.8E+00	4.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.5E+01	1.3E+00	4.9E+01	-7.95	-9.16	-10.89	-0.90	0.65	0.0%	0.0%	0.0%	1.8E-46
1839	91-22-5	quinoline	129	38	7.2E+00	3.5E+02	1.4E+02	5.0	3.5E-06	9.5E-08	3.5E-07	conf	conf	conf	6.8E+01	9.5E-01	3.4E+01	-7.92	-7.68	-9.13	-1.43	0.49	0.0%	0.0%	0.0%	2.0E-28
1840	122731-59-3	602-891-7	716	295	9.7E-14	1.7E-02	3.6E+01	1.7	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.0E+01	1.3E+00	4.6E+01	-7.69	-8.56	-10.30	-1.38	0.14	0.0%	0.0%	0.0%	1.7E-37
1841	924-88-9	diisopropyl succinate	202	-71	4.1E+01	2.4E+03	1.7E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.3E+01	1.3E+00	4.8E+01	-9.92	-9.76	-11.00	-1.68	0.88	0.0%	0.0%	0.0%	9.4E-41
1842	111-70-6	heptan-1-ol	116	-26	4.0E+01	1.5E+03	2.0E+02	14.0	3.5E-06	3.9E-06	3.5E-06	conf	conf	conf	9.3E+01	1.3E+00	4.8E+01	-10.01	-9.84	-11.02	-1.19	0.36	0.0%	0.0%	0.0%	4.5E-45
1843	66-25-1	hexanal	100	-55	1.3E+03	5.2E+03	6.3E+01	14.0	3.5E-06	3.9E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-10.35	-10.16	-11.49	-1.76	0.75	0.0%	0.0%	0.0%	2.8E-44
1844	454-31-9	ethyl difluoroacetate	124	-92	5.0E+03	1.3E+04	2.7E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-10.20	-9.98	-11.53	-1.01	1.99	0.0%	0.0%	0.0%	2.5E-51
1845	63968-64-9	(3R,5aS,6R,8aS,9R,12S,12aR)-3,6,9-trimethyloctahydro-3,12-epoxypyrano[4,3-j][1,2]benzodioxepin-10(3H)-one	282	133	2.9E-04	1.5E+02	7.1E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.54	-9.41	-10.90	-2.15	1.12	0.0%	0.0%	0.0%	4.8E-36
1846	3147-75-9	2-(2H-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)phenol	323	191	1.5E-07	5.1E-01	1.6E+06	-1.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	conf	8.0E+01	1.1E+00	4.1E+01	-7.47	-7.88	-9.69	-3.88	0.36	0.0%	0.0%	0.0%	5.4E-17
1847	535-13-7	ethyl 2-chloropropionate	137	-51	6.1E+02	5.0E+03	3.5E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	conf	9.1E+01	1.3E+00	4.5E+01	-9.27	-8.96	-10.50	-1.33	1.72	0.0%	0.0%	0.0%	2.6E-39
1848	4223-03-4	N-(1,1,3,3-tetramethylbutyl)acrylamide	183	84	8.8E-02	2.2E+02	7.4E+02	-0.4	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	8.8E+01	1.2E+00	4.5E+01	-7.90	-8.62	-10.37	-1.33	0.56	0.0%	0.0%	0.0%	1.7E-38
1849	563-80-4	3-methylbutanone	86	-79	7.3E+03	2.2E+04	4.7E+00	14.0	3.5E-06	5.5E-07	1.1E-06	conf	conf	conf	8.0E+01	1.1E+00	4.1E+01	-9.86	-9.59	-11.07	-0.84	0.34	0.0%	0.0%	0.0%	9.8E-49
1850	62-56-6	thiourea	76	26	7.8E+00	1.0E+06	4.9E-02	2.0	3.5E-06	2.7E-09	1.1E-06	conf	conf	conf	5.4E+01	7.6E-01	2.6E+01	-6.78	-7.40	-8.35	-1.49	1.43	0.0%	0.0%	0.0%	6.0E-23
1851	90474-13-8	diethyl 1,2-cyclopentanedicarboxylate	214	-34	4.6E+00	2.3E+04	4.0E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.68	-9.50	-10.95	-1.33	0.29	0.0%	0.0%	0.0%	1.1E-43
1852	118-48-9	4H-3,1-benzoxazine-2,4(1H)-dione	163	77	1.0E-01	3.4E+03	4.0E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.17	-9.39	-10.88	-1.30	0.35	0.0%	0.0%	0.0%	6.9E-43
1853	94695-50-8	Ethyl 3-oxo-3-(2,3,4,5-tetrafluorophenyl)propanoate	264	66	5.3E-01	1.1E+02	3.2E+02	14.0	3.5E-06	3.9E-06	3.5E-06	conf	conf	conf	9.3E+01	1.3E+00	4.8E+01	-10.01	-9.84	-11.02	-1.19	0.36	0.0%	0.0%	0.0%	4.5E-45
1854	97-53-0	eugenol	164	61	1.3E+00	2.5E+02	5.4E+02	10.0	3.5E-06	7.5E-07	1.1E-06	conf	conf	conf	8.5E+01	1.2E+00	4.3E+01	-9.50	-8.86	-10.28	-2.01	0.54	0.0%	0.0%	0.0%	1.5E-32
1855	116-16-5	hexachloroacetone	265	36	4.1E+01	1.8E+01	3.0E+02	14.0	3.5E-06	3.5E-08	3.5E-08	conf	conf	conf	5.4E+01	7.6E-01	2.6E+01	-10.10	-9.64	-11.88	-2.14	0.28	0.0%	0.0%	0.0%	2.4E-44
1856	70905-68-9	(1S,4R,6R)-1-[(3E)-5-hydroxy-3-methylpent-3-en-1-yn-1-yl]-2,2,6-trimethylcyclohexane-1,4-diol	252	149	7.0E-07	3.5E+02	2.3E+02	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.21	-9.42	-10.85	-2.33	0.77	0.0%	0.0%	0.0%	2.2E-34
1857	93839-71-5	4-[(E)-aminophenyl]methyl]amino]cyclohexyl acetate	262	134	2.1E-04	8.5E+02	2.2E+02	9.8	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.69	-9.36	-10.89	-1.69	1.08	0.0%	0.0%	0.0%	9.0E-40
1858	104632-26-0	Pramipexol	211	127	2.1E-03	5.8E+03	2.2E+02	14.0	3.5E-06	3.5E-06	3.5E-07	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.11	-9.18	-10.88	-2.11	5.08	0.0%	0.0%	0.0%	2.6E-36
1859	50892-62-1	8-chloro-5,10-dihydro-11H-dibenzo[b,e][1,4]diazepin-11-one	245	185	2.4E-06	4.6E+01	1.5E+03	2.4	3.5E-06	3.5E-06	3.5E-07	conf	conf	conf	9.3E+01	1.3E+00	4.8E+01	-8.16	-8.93	-10.85	-2.76	0.69	0.0%	0.0%	0.0%	3.8E-31
1860	112-15-2	2-(2-ethoxyethoxy)ethyl acetate	176	2	1.9E+01	6.6E+04	2.1E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.3E+01	1.3E+00	4.8E+01	-9.22	-9.05	-10.85	-0.56	0.32	0.0%	0.0%	0.0%	3.4E-49
1861	1229457-94-4	(4-(ado-1H-pyrazol-1-yl)piperidine	277	115	5.8E-03	1.3E+04	1.1E+02	14.0	3.5E-06	1.1E-05	1.1E-06	conf	conf	conf	9.4E+01	1.3E+00	4.8E+01	-8.81	-9.91	-11.40	-1.93	0.62	0.0%	0.0%	0.0%	5.4E-42
1862	74-97-5	bromochloromethane	129	-71	1.9E+04	1.3E+04	2.7E+01	14.0	3.5E-06	2.0E-08	1.1E-07	conf	conf	conf	5.4E+01	7.6E-01	2.6E+01	-9.91	-9.53	-11.62	-1.17	0.70	0.0%	0.0%	0.0%	1.3E-50
1863	50-21-5	lactic acid	90	23	3.8E+00	7.7E+05	2.2E-01	3.8	3.5E-06	4.7E-07	3.5E-07	conf	conf	conf	8.3E+01	1.1E+00	4.2E+01	-6.89	-7.97	-9.86	-0.44	0.46	0.0%	0.0%	0.0%	1.4E-41
1864	107-51-7	octamethylcyclotrisiloxane	237	-53	4.7E+02	6.2E-01	5.0E+06	14.0	3.5E-06	3.5E-09	3.5E-07	conf	conf	conf	5.3E+01	7.4E-01	2.6E+01	-6.78	-10.11	-12.65	-4.31	0.19	0.0%	0.0%	0.0%	5.4E-33
1865	18917-91-4	aluminium trilactate	294	87	9.9E-03	2.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	6.9E+01	9.6E-01	3.5E+01	-7.18	-7.49	-9.15	-2.55	1.28	0.0%	0.0%	0.0%	2.2E-21
1866	96-67-3	3-amino-2-hydroxy-5-nitrobenzenesulphonic acid	234	191	1.1E-08	2.8E+03	6.8E-03	-1.8	3.5E-06	3.5E-06	3.5E-07	conf	conf	conf	9.3E+01	1.3E+00	4.8E+01	-7.29	-8.65	-10.79	-0.49	0.97	0.0%	0.0%	0.0%	2.9E-49
1867	4435-53-4	3-methoxybutyl acetate	146	-38	3.7E+02	1.1E+04	1.0E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.91	-9.77	-11.05	-1.46	1.01	0.0%	0.0%	0.0%	5.4E-43
1868	924-50-5	methyl 3-methyl-2-butenoate	114	-66	2.1E+02	8.5E+03	4.9E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.76	-9.62	-10.89	-2.56	0.40	0.0%	0.0%	0.0%	6.1E-33
1869	611-07-4	5-chloro-2-nitrophenol	174	93	1.3E-01	7.8E+02	3.5E+02	14.0	3.5E-06	3.5E-06	3.5E-07	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.39	-9.25	-10.88	-2.13	0.23	0.0%	0.0%	0.0%	3.6E-36
1870	594-44-5	ethanesulphonyl chloride	129	4	1.7E+02	3.1E+04	5.8E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.65	-9.50	-10.87	-2.88	2.91	0.0%	0.0%	0.0%	1.6E-30
1871	5056-17-7	(E,E,E)-2,7-dimethyloctа-2,4,6-trienedial	164	7	1.4E+00	2.5E+03	5.5E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.51	-9.32	-10.90	-2.40	1.47	0.0%	0.0%	0.0%	1.8E-34
1872	203448-76-4	2-(4-methylpentan-2-yl)aniline	276	63	1.4E-01	1.4E+02	4.8E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.55	-9.37	-10.94	-2.47	0.31	0.0%	0.0%	0.0%	5.7E-34
1873	20208-39-3	(3-triethoxysilylpropyl propp-2-enoate	273	63	1.4E-01	1.4E+02	4.8E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.55	-9.37	-10.94	-2.47	0.30	0.0%	0.0%	0.0%	5.3E-34
1874	137-32-6	2-methylbutan-1-ol	88	-61	6.1E+02	3.7E+04	1.8E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	conf	9.1E+01	1.3E+00	4.6E+01	-8.69	-8.41	-9.65	-0.50	0.33	0.0%	0.0%	0.0%	2.3E-39
1875	13076-17-0	603-436-5	144	26	2.1E-02	1.5E+07	2.5E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.03	-9.21	-10.84	-0.25	0.50	0.0%	0.0%	0.0%	4.6E-52
1876	3120-74-9	4-(methylthio)-m-cresol	154	57	3.7E-01	3.4E+03	4.6E+02	9.5	3.5E-06	1.1E-05	3.5E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-10.09	-10.10	-11.40	-2.31	0.32	0.0%	0.0%	0.0%	7.5E-39
1877	915416-45-4	3',4',5'-trifluorobiphenyl-2-amine	223	94	2.2E-02	4.7E+01	2.8E+03	14.0	3.5E-06	3.5E-06	3.5E-07	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-9.60	-9.42	-10.93	-2.62	0.45	0.0%	0.0%	0.0%	8.0E-33
1878	4394-85-8	4-morpholinecarbaldehyde	115	25	6.5E-00	2.6E+08	4.8E-02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	8.8E+01	1.2E+00	4.5E+01	-7.09	-8.14	-10.27	0.81	0.65	0.0%	0.0%	0.0%	1.1E-56
1879	19719-28-9	2,4-dichloropenylacetic acid	205	98	2.3E-02	5.2E+02	5.2E+02	4.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.29	-9.21	-10.88	-1.68	0.23	0.0%	0.0%	0.0%	8.6E-40
1880	685-88-1	diethyl fluoromalonate	178	-94	4.2E+02	5.4E+03	5.8E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-10.05	-9.88	-11.30	-2.18	0.91	0.0%	0.0%	0.0%	4.5E-39
1881	97845-60-8	619-293-7	356	212	1.9E-08	3.8E+01	1.9E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-7.96	-9.15	-10.86	-1.85	0.93	0.0%	0.0%	0.0%	2.0E-38
1882	75028-24-9	(ZZ)-(5-amino-1,2,4-thiadiazol-3-yl)(ethoxyimino)acetic acid	216	161	8.5E-05	1.1E+04	9.1E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.15	-9.29	-10.87	-1.69	0.83	0.0%	0.0%	0.0%	1.2E-39
1883	52449-76-0	610-840-5	206	118	4.0E-03	7.6E+01	1.5E+01	14.0	3.5E-06	3.5E-06	1.1E-07	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.71	-8.71	-10.83	-2.32	0.59	0.0%	0.0%	0.0%	2.5E-34
1884	5537-71-3	m-(1-cyanoethyl)benzoic acid	175	110	3.7E-02	9.2E+02	7.2E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.50	-9.29	-10.88	-2.38	0.70	0.0%	0.0%	0.0%	3.4E-34
1885	144689-93-0	Ethyl 4-(2-hydroxypropan-2-yl)-2-propyl-1H-imidazole- 5-carboxylate	240	154	2.0E-07	8.3E+02	7.4E+01	2.9	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+01	1.3E+00	4.7E+01	-8.60	-9.10

1989	10109-95-2	2,5-dianiline terephthalic acid	348	242	4.0E-10	1.2E+02	3.0E+04	-0.5	3.5E-06	1.1E-06	1.1E-06	conf	conf	7.4E+01	1.0E+00	3.8E+01	-7.87	-8.70	-10.40	-2.95	0.65	0.0%	0.0%	0.0%	9.9E-27
1990	54-21-7	sodium salicylate	160	87	9.9E-03	1.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.8E+01	8.1E-01	2.9E+01	-7.27	-7.57	-9.22	0.13	0.50	0.0%	0.0%	0.0%	4.9E-41
1991	12286-66-7	calcium bis[4-[[1-[[(2-methylphenyl)amino]carbonyl]-2-oxopropyl]azo]-3-nitrobenzenesulphonate]	879	87	9.9E-03	6.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.8E+01	8.0E-01	2.9E+01	-7.24	-7.57	-9.23	-2.31	1.39	0.0%	0.0%	0.0%	2.2E-23
1992	29857-13-4	sodium 1,4-dioctyl sulphotrisuccinate	501	87	9.9E-03	3.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.7E+01	8.0E-01	2.9E+01	-7.21	-7.57	-9.23	-2.34	0.83	0.0%	0.0%	0.0%	5.5E-23
1993	97-74-5	tetramethylthiuram monosulphide	208	89	3.6E-02	1.9E+03	5.6E+00	14.0	3.5E-06	2.5E-08	3.5E-07	conf	conf	4.8E+01	6.7E-01	2.3E+01	-7.55	-7.50	-8.69	-2.80	0.80	0.0%	0.0%	0.0%	1.8E-17
1994	104-55-2	cinnamaldehyde	132	0	4.5E+00	3.9E+02	6.6E+01	14.0	3.5E-06	1.2E-06	1.1E-06	conf	conf	7.3E+01	1.0E+00	3.8E+01	-9.44	-9.24	-10.54	-1.90	0.84	0.0%	0.0%	0.0%	2.9E-35
1995	88-51-7	4-amino-6-chlorotoluene-3-sulphonic acid	222	150	2.1E-06	1.1E+03	1.3E-01	-1.2	3.5E-06	1.1E-06	1.1E-06	conf	conf	7.4E+01	1.0E+00	3.8E+01	-7.16	-8.52	-10.38	0.39	0.40	0.0%	0.0%	0.0%	1.1E-53
1996	80-46-6	p-[(1,1-dimethylpropyl)phenol	164	48	1.5E-01	7.1E+01	8.1E+03	10.0	3.5E-06	2.6E-09	1.1E-06	conf	conf	4.4E+01	6.2E-01	2.1E+01	-8.27	-8.06	-9.15	-2.58	0.84	0.0%	0.0%	0.0%	3.1E-21
1997	563-78-0	2,3-dimethylbut-1-ene	84	-116	3.3E+04	2.5E+02	1.3E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	5.2E+01	7.2E-01	2.5E+01	-10.85	-10.53	-13.40	-2.05	0.15	0.0%	0.0%	0.0%	2.2E-59
1998	131-17-9	diallyl phthalate	246	16	1.5E-01	9.3E+01	2.3E+03	14.0	3.5E-06	8.2E-07	3.5E-07	conf	conf	6.8E+01	9.5E-01	3.5E+01	-9.07	-8.84	-10.42	-2.34	0.72	0.0%	0.0%	0.0%	4.1E-31
1999	1561-92-8	sodium 2-methylprop-2-ene-1-sulphonate	158	87	9.9E-03	2.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.8E+01	7.9E-01	2.8E+01	-7.28	-7.58	-9.23	-1.84	0.64	0.0%	0.0%	0.0%	2.2E-26
2000	149-74-6	dichloro(methyl)(phenyl)silane	191	-6	3.5E+01	3.0E+02	6.9E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	5.9E+01	8.2E-01	3.0E+01	-9.80	-9.54	-10.91	-0.99	0.70	0.0%	0.0%	0.0%	6.6E-46
2001	118-82-1	2,2',6,6'-tetra-tert-butyl-4,4'-methylenediphenol	425	208	1.6E-09	5.4E-05	9.8E+08	11.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.6E+01	6.4E-01	2.2E+01	-8.94	-9.41	-9.61	-4.78	2.85	0.0%	0.0%	0.0%	2.5E-12
2002	78-95-5	chloroacetone	93	-59	2.2E+03	3.8E+04	1.0E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	6.4E+01	8.9E-01	3.3E+01	-9.37	-9.05	-10.43	-3.64	0.21	0.0%	0.0%	0.0%	1.4E-22
2003	2720-73-2	potassium O-pentyl dithiocarbonate	202	87	9.9E-03	1.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.6E+01	7.8E-01	2.8E+01	-7.28	-7.59	-9.24	-1.82	0.62	0.0%	0.0%	0.0%	2.7E-26
2004	1187-93-5	trifluoro(trifluoromethoxy)ethylene	166	-133	2.1E+05	4.2E+02	2.6E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	4.6E+01	6.4E-01	2.2E+01	-10.71	-10.25	-13.06	-1.64	1.12	0.0%	0.0%	0.0%	3.9E-60
2005	75-46-7	trifluoromethane	70	-171	2.3E+06	2.1E+03	3.8E+00	14.0	3.5E-06	3.5E-08	3.5E-08	conf	conf	4.3E+01	6.0E-01	2.1E+01	-10.75	-9.71	-12.45	-0.50	0.31	0.0%	0.0%	0.0%	1.2E-65
2006	19147-16-1	dipotassium adipate	222	87	9.9E-03	5.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.6E+01	7.8E-01	2.8E+01	-7.28	-7.59	-9.24	-1.07	0.38	0.0%	0.0%	0.0%	8.8E-32
2007	534-03-2	2-aminopropane-1,3-diol	91	26	2.2E+00	5.6E+05	2.8E-02	8.8	3.5E-06	3.5E-06	3.5E-06	conf	conf	7.5E+01	1.0E+00	3.9E+01	-8.19	-9.06	-10.93	-0.04	0.83	0.0%	0.0%	0.0%	6.6E-55
2008	21829-52-7	carbonic acid, compound with 2-aminoethanol (1:2)	184	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.6E+01	7.7E-01	2.8E+01	-7.29	-7.59	-9.24	-1.28	0.59	0.0%	0.0%	0.0%	3.2E-30
2009	4292-10-8	[carboxymethyl]dimethyl-3-[[1-oxododecyl]amino]propylammonium hydroxide	343	283	6.4E-13	1.7E-02	4.9E+02	-1.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.1E+01	9.9E-01	3.6E+01	-7.66	-8.47	-10.38	-2.43	0.44	0.0%	0.0%	0.0%	3.3E-30
2010	6915-15-7	malic acid	134	133	3.9E-04	3.4E+05	2.1E+02	3.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	7.4E+01	1.0E+00	3.8E+01	-7.61	-9.04	-10.92	-0.49	0.25	0.0%	0.0%	0.0%	1.5E-50
2011	76-03-9	trichloroacetic acid	163	27	2.6E+01	1.6E+05	2.8E+01	0.6	3.5E-06	5.8E-08	3.5E-07	conf	conf	5.0E+01	6.9E-01	2.5E+01	-7.07	-7.61	-8.99	-0.35	1.16	0.0%	0.0%	0.0%	2.5E-35
2012	24544-04-5	2,6-diisopropylaniline	177	51	2.5E+00	1.3E+01	9.8E+03	4.0	3.5E-06	6.3E-09	1.1E-07	conf	conf	4.3E+01	6.0E-01	2.1E+01	-7.88	-7.57	-8.53	-2.59	0.45	0.0%	0.0%	0.0%	1.1E-17
2013	29091-09-6	2,4-dichloro-1,3-dinitro-5-(trifluoromethyl)benzene	305	122	5.0E+03	1.0E+07	7.6E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	6.5E+01	9.1E-01	3.3E+01	-9.12	-8.91	-10.57	-3.05	0.99	0.0%	0.0%	0.0%	3.2E-27
2014	3159-62-4	calcium(2+) 12-hydroxyoctadecanoate	639	87	9.9E-03	4.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+01	7.6E-01	2.7E+01	-7.27	-7.59	-9.25	-0.26	1.14	0.0%	0.0%	0.0%	4.6E-38
2015	542-28-9	δ-valerolactone	100	-32	1.8E+01	3.4E+04	1.5E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	7.4E+01	1.0E+00	3.8E+01	-9.30	-9.14	-10.92	-1.61	0.93	0.0%	0.0%	0.0%	1.1E-40
2016	3699-54-5	1-(2-hydroxyethyl)imidazolidin-2-one	130	93	1.1E-03	5.4E+05	3.2E-02	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	7.4E+01	1.0E+00	3.8E+01	-7.91	-9.05	-10.94	0.46	0.61	0.0%	0.0%	0.0%	1.3E-60
2017	5332-73-0	3-methoxypropylamine	89	-40	2.3E+03	3.2E+05	3.8E-01	9.9	3.5E-06	3.5E-06	1.1E-06	conf	conf	7.3E+01	1.0E+00	3.8E+01	-9.49	-9.36	-10.91	-1.29	0.32	0.0%	0.0%	0.0%	2.4E-43
2018	32588-76-4	N,N'-ethylenebis(3,4,5,6-tetrabromophthalimide)	952	350	1.8E-21	1.5E-08	6.3E+09	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.2E+01	5.8E-01	2.0E+01	-10.83	-10.83	-10.83	-4.83	0.58	0.0%	0.0%	0.0%	5.2E-18
2019	85959-68-8	diammonium [N,N-bis[2-[bis(carboxymethyl)amino]ethyl]glycinato(5-)]ferrate(2-)	480	87	9.9E-03	3.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.4E+01	7.5E-01	2.7E+01	-7.28	-7.60	-9.26	-0.66	1.09	0.0%	0.0%	0.0%	5.1E-35
2020	505-52-2	tridecanedioic acid	244	150	2.1E-04	3.4E+02	4.7E+01	4.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.9E+01	8.1E-01	3.5E+01	-7.98	-8.64	-10.47	-2.87	0.54	0.0%	0.0%	0.0%	5.6E-28
2021	41200-97-9	1,5-dichloro-2-(1-methylethoxy)-4-nitrobenzene	250	102	1.9E-02	8.4E+00	1.2E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	6.3E+01	8.7E-01	3.2E+01	-9.34	-9.14	-10.64	-2.76	0.48	0.0%	0.0%	0.0%	1.1E-29
2022	25134-21-8	1,2,3,6-tetrahydromethyl-3,6-methanophthalic anhydride	178	39	1.9E+00	4.2E+03	2.0E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	7.1E+01	9.8E-01	3.6E+01	-9.69	-9.51	-11.03	-0.82	0.74	0.0%	0.0%	0.0%	1.8E-48
2023	110-59-8	valeronitrile	83	-46	8.0E+01	1.5E+04	2.1E+02	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	6.1E+01	8.4E-01	3.1E+01	-8.61	-9.15	-10.40	-1.06	0.32	0.0%	0.0%	0.0%	5.8E-41
2024	565-62-8	3-methylpent-3-en-2-one	98	-64	2.5E+03	1.3E+04	2.3E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	6.6E+01	9.2E-01	3.4E+01	-10.11	-9.87	-11.19	-1.04	0.48	0.0%	0.0%	0.0%	6.4E-48
2025	51263-08-2	sodium hydrogen [6R-(6α,7β)]-3-[acetoxymethyl]-7-[[5-amino-5-carboxylato-1-oxopentyl]amino]-8-oxo-5-thia-1-aza	221	87	9.9E-03	1.5E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.3E+01	7.4E-01	2.6E+01	-6.74	-7.58	-9.24	-1.84	0.64	0.0%	0.0%	0.0%	2.0E-26
2026	89-79-2	isopulegol	154	-5	6.6E-01	1.4E+03	2.5E+03	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.6E+01	6.3E-01	2.3E+01	-8.15	-7.87	-9.42	-1.38	0.26	0.0%	0.0%	0.0%	7.8E-31
2027	26496-99-1	bis(2,4-dichlorophenyl) carbonate	352	137	4.0E-05	6.7E-02	6.0E+05	14.0	3.5E-06	1.1E-07	1.1E-08	conf	conf	6.4E+01	6.1E-01	2.2E+01	-8.66	-8.52	-9.75	-3.97	0.44	0.0%	0.0%	0.0%	7.5E-17
2028	1117-86-8	octane-1,2-diol	146	24	2.2E-01	4.0E+03	4.7E+01	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	7.0E+01	9.7E-01	3.6E+01	-9.42	-9.51	-10.99	-1.46	0.70	0.0%	0.0%	0.0%	1.4E-42
2029	75-85-4	2-methylbutan-2-ol	88	-61	2.4E+03	1.1E+05	1.7E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	4.6E+01	6.4E-01	2.3E+01	-9.11	-8.83	-10.07	0.22	0.70	0.0%	0.0%	0.0%	3.2E-49
2030	652-67-5	1,4,3,6-dianhydro-D-glucitol	146	61	4.1E-02	4.9E+04	1.2E-01	13.7	3.5E-06	1.1E-06	1.1E-06	conf	conf	6.7E+01	9.3E-01	3.4E+01	-7.47	-8.43	-10.43	0.10	1.38	0.0%	0.0%	0.0%	1.6E-51
2031	6574-99-8	3,4-dichlorobenzonitrile	172	53	1.8E+00	6.3E+01	6.8E+02	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	5.0E+01	7.0E-01	2.5E+01	-9.16	-8.90	-10.17	-2.53	0.53	0.0%	0.0%	0.0%	5.1E-28
2032	140-93-2	proxan-sodium	158	87	9.9E-03	1.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.2E+01	7.2E-01	2.6E+01	-7.32	-7.62	-9.27	-1.84	0.91	0.0%	0.0%	0.0%	1.3E-26
2033	2280-49-1	N-phenyl-N-[(trichloromethyl)thio]benzenesulphonamide	383	186	1.2E-06	1.7E-01	3.3E+04	14.0	3.5E-06	3.5E-06	3.5E-07	conf	conf	6.0E+01	8.3E-01	3.0E+01	-9.08	-9.69	-11.09	-0.30	0.35	0.0%	0.0%	0.0%	6.3E-54
2034	624-03-3	ethane-1,2-diyl palmitate	539	165	2.6E-07	1.2E-08	1.4E+14	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.9E+01	5.5E-01	1.9E+01	-10.93	-10.93	-10.93	-1.64	1.15	0.0%	0.0%	0.0%	1.9E-40
2035	4559-86-8	tetrabutylurea	284	100	2.6E-03	1.6E+00	4.9E+05	0.1	3.5E-06	3.5E-07	1.1E-07	conf	conf	4.7E+01	6.6E-01	2.4E+01	-7.84	-8.13	-9.97	-2.88	0.20	0.0%	0.0%	0.0%	2.2E-24
2036	6712-98-7	1-(N,N-bis-[2-hydroxyethyl]amino)propan-2-ol	163	82	7.0E-04	8.1E+05	8.7E-03	7.8	3.5E-06	3.5E-06	3.5E-06	conf	conf	6.9E+01	9.5E-01	3.5E+01	-7.85	-9.05	-10.96	-0.55	0.12	0.0%	0.0%	0.0%	2.4E-50
2037	6610-29-3	4-methylthiosemicarbazide	105	30	3.8E-01	1.0E+06	6.2E-02	1.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	6.6E+01	9.1E-01	3.4E+01	-7.35	-8.62	-10.47	-1.73	0.45	0.0%	0.0%	0.0%	4.6E-36
2038	105-53-3	diethyl malonate	160	-83	4.8E+01	4.1E+04	7.9E+00	13.0	3.5E-06	1.0E-06	1.1E-06	conf	conf	6.5E+01	9.0E-01	3.3E+01	-9.03	-8.82	-10.46	-0.98	0.75	0.0%	0.0%	0.0%	4.7E-42
2039	56677-60-2	tetradecyl chloroformate	277	65	4.3E-02	1.4E-02	3.3E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.3E+01	5.9E-01	2.1E+01	-10.77	-10.58	-12.43	-2.69	1.18	0.0%	0.0%	0.0%	2.8E-44
2040	135-57-9	N,N'-dithiodi-o-phenylenedibenzamide	457	316	2.1E-15	1.3E-02	3.8E+04	1.1	3.5E-06	1.1E-06	1.1E-06	conf	conf	6.5E+01	9.0E-01	3.3E+01	-7.93	-8.77	-10.46	-4.22	0.36	0.0%	0.0%	0.0%	2.5E-19
2041	76-22-2	bornan-2-one	152	28	1.4E+00	1.0E+03	1.1E+03	14.0	3.5E-06	4.8E-07	1.1E-06	conf	conf	5.9E+01	8.2E-01	3.0E+01	-8.85	-8.62	-10.19	-1.25	0.92	0.0%	0.0%	0.0%	1.1E-37
2042	28281-49-4	1-(1,3-benzodioxol-5-yl)propan-1-one	178	69	2.9E-01	1.9E+03	1.7E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	6.4E+01	8.9E-01	3.3E+01	-8.95	-8.76	-10.51	-1.79	0.64	0.0%	0.0%	0.0%	6.3E-36
2043	123-04-6	3-(chloromethyl)heptane	149	-47	1.9E+02	1.4E+00	2.8E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	4.1E+01	5.7E-01	2.0E+01	-10.82	-10.48	-13.22	-2.35	0.65	0.0%	0.0%	0.0%	1.2E-54
2044	27213-90-7	sodium diisobutylnaphthalenesulphonate	346	61	4.1E-02	2.4E+03	1.2E+01	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.0E+01	7.0E-01	2.5E+01	-7.32	-7.63	-9.29	-0.92	0.16	0.0%	0.0%	0.0%	2.5E-33
2045	55566-30-8	tetrakis(hydroxymethyl)phosphonium sulphate(2:1)	406	87	9.9E-03	2.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.0E+01	7.0E-01	2.5E+01	-7.32	-7.63	-9.29	-1.46	0.57	0.0%	0.0%	0.0%	2.5E-29
2046	41198-08-7	O-(4-bromo-2-chlorophenyl) O-ethyl S-propyl phosphorothioate	374	86	1.0E-03	4.1E-01	6.6E+04	14.0	3.5E-06	3.9E-09	3.5E-07	conf	conf	3.9E+01	5.4E-01	1.9E+01	-8.57	-8.41	-9.53	-4.45	1.09	0.0%	0.0%	0.0%	1.9E-13
2047	100-40-3	4-vinylcyclohexene	108	-62	1.8E+03	5.9E+05	5.4E+03	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.5E+01	6.3E-01	2.2E+01	-10.38	-9.51	-12.24	-1.91	0.20	0.0%	0.0%	0.0%	1.3E-49
2048	52334-81-3	2-chloro-5-(trifluoromethyl)pyridine	182	3	3.6E+02	5.4E+02	2.6E+02	-1.7	3.5E-06	3.5E-07	1.1E-07	conf	conf	5.8E+01	8.0E-01	2.9E+01	-7.28	-7.96	-9.84	-3.13	0.68	0.0%	0.0%	0.0%	4.8E-22
2049	2162-74-5	bis(2,6-diisopropylphenyl)carbodiimide	363	141	1.9E-05	5.8E-04	5.2E+08	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	3.9E+01	5.4E-01	1.9E+01	-9.20	-9.37	-9.76	-3.67	1.18	0.0%	0.0%	0.0%	1.6E-18
2050	112-44-7	undecanal	170	3	8.1E+00	1.3E+01	1.8E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	4.7E+01	6.6E-01	2.3E+01	-10.18	-9.91	-11.52	-2.42	0.27	0.0%	0.0%	0.0%	6.3E-39
2051	780-69-8	triethoxyphenylsilane	240	52	1.7E-01	6.4E+01	1.0E+02	14.0	3.5E-06	2.6E-07	1.1E-07	conf	conf	5.5E+01	7.6E-01	2.8E+01	-8.85	-8.62	-10.00	-0.99	0.67	0.0%	0.0%	0.0%	2.E-38
2052	102-81-8	2-dibutylaminoethanol	173	29	1.7E+00	2.4E+03	1.0E+02	9.9	3.5E-06	1.1E-06	1.1E-06	conf	conf	6.3E+01	8.7E-01	3.2E+01	-9.14	-8.92	-10.56	-1.26	0.63	0.0%	0.0%	0.0%	1.3E-40
2053	29911-27-1	1-(1-methyl-2-propoxyethoxy)propan-2-ol	176	7	4.7E+00	4.8E+03	4.4E+00	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	5.7E+01	7.9E-01	2.9E+01	-8.50	-8.26	-9.92	-0.88	0.57	0.0%	0.0%	0.0%	1.7E-38
2054	120570-77-6	601-722-4	162	-60	1.2E-06	1.2E-06	1.1E-01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	6.6E+01	9.2E-01	3.4E+01	-7.93	-8.91	-10.97	-0.86	0.30	0.0%	0.0%	0.0%	1.3E-47
2055	144-83-2	sulfapyridine	249	176	5.5E-06	2.5E+03	3.4E+00	3.1	3.5E-06	4.3E-09	1.1E-06	conf	conf	3.8E+01	5.3E-01	1.8E+01	-7.07	-7.56	-8.52	-1.68	1.03	0.0%	0.0%	0.0%	7.6E-23
2056	1809-19-4	dibutyl phosphonate	194	17	3.2E+00	6.8E+04	6.5E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	6.2E+01	8.7E-01	3.2E+01	-8.76	-8.69	-10.51	-0.77	0.91	0.0%	0.0%	0.0%	2.8E-44
2057	1704-62-7	2-[2-(dimethylamino)ethoxy]ethanol	133	2	9.3E+00	1.0E+06	6.2E-02	8.7	3.5E-06	1.1E-06	1.1E-06	conf	conf	6.2E+01	8.6E-01	3.2E+01	-7.95	-8.44	-10.46	-0.52	0.38	0.0%	0.0%	0.0%	4.5E-46
2058	2385-77-5	(R)-3,7-dimethyloct-6-enal	154	-28	3.4E+01	7.9E+02	3.4E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	5.7E+01	8.0E-01	2.9E+01	-10.18	-9.93	-11.15	-1.91	0.23	0.0%	0.0%	0.0%	5.0E-40
2059	3457-61-2	tert-butyl α,α-dimethylbenzyl peroxide	208	35	3.0E+00	5.6E+01	4.6E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	4.8E+01	6.7E-01	2.4E+01	-9.80	-9.56	-10.72	-2.77	0.74	0.0%	0.0%	0.0%	3.6E-30
2060	70516-41-5	2'-anilino-6'-[ethyl(3-methylbutyl)amino]-3'-methylspiro[isobenzofuran-1(3H),9'-[9H]xanthene]-3-one	519	289	2.4E-13	4.6E-06	5.2E+08	3.8	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.6E+01	7.8E-01	2.9E+01	-8.33	-8.98	-10.53	-0.70	0.96	0.0%	0.0%	0.0%	4.5E-45
2061	1643-19-2	tetrabutylammonium bromide	322	87	9.9E-03	2.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.8E+01	6.7E-01	2.4E+01	-7.34	-7.65	-9.31	-0.58	0.66	0.0%	0.0%	0.0%	5.5E-36
2062	118-75-2	tetrachloro-p-benzoquinone	246	102	3.0E-04	6.3E+02	1.7E+02	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	4.7E+01	6.5E-01	2.3E+01	-6.98	-7.70	-9.29	-2.70	0.53	0.0%	0.0%	0.0%	2.4E-21
2063	150-84-5	citronellyl acetate	198	-7	7.0E+00	5.2E+01	3.6E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	5.4E+01	7.5E-01	2.7E+01	-10.64	-10.43	-11.66	-2.15	0.20	0.0%	0.0%	0.0%	2.2E-42
2064	3006-86-8	cyclohexylidenebis(tert-butyl) peroxide	260	66	1.9E-01	2.1E+01	1.9E+06	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	4.1E+01	5.7E-01	2.0E+01	-9.32	-9.76	-10.72	-2.57	1.04	0.0%	0.0%	0.0%	1.2E-31
2065	26159-31-9	(±)-2-(6-methoxy-2-naphthyl)propionic acid	230	138	1.7E-04	2.8E+02	1.3E+03	4.4	3.5E-06	8.0E-09	3.5E-07	conf	conf	3.7E+01	5.2E-01	1.8E+01	-7.41	-7.58	-8.60	-0.83	0.10	0.0%	0.0%	0.0%	5.9E-29
2066	6711-48-4	N'-[3-(dimethylamino)propyl]-N,N-dimethylpropane-1,3-diamine	187	37	4.7E+00	1.6E+05	1.6E+00	11.7	3.5E-06	1.1E-06	1.1E-06	conf	conf	6.1E+01	8.4E-01	3.1E+01	-8.54	-8.60	-10.50	-1.58	0.41	0.0%	0.0%	0.0%	1.6E-37
2067	2786-76-7	4-[[4-(aminocarbonyl)phenyl]azo]-N-[2-ethoxyphenyl]-3-hydroxynaphthalene-2-carboxamide	454	327	1.9E-17	1.5E-01	1.1E+06	-0.9	3.5E-06	3.5E-07	3.5E-08	conf	conf	5.4E+01	7.5E-01	2.7E+01	-7.60	-7.90	-9.79	-0.96	1.04	0.0%	0.0%	0.0%	9.4E-37
2068	4724-48-5	octylphosphonic acid	194	76	1.1E-04	1.6E+03	2.8E+02	2.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	6.0E+01	8.4E-01	3.1E+01	-7.28	-8.58	-10.50	-1.37	0.39	0.0%	0.0%	0.0%	3.5E-39
2069	3547-33-9	2-(octylthio)ethanol	190	39	4.2E-02	2.6E+01	2.4E+03	14.0	3.5E-06	1.2E-07	1.1E-06	conf	conf	4.5E+01	6.3E-01	2.3E+01	-8.50	-8.27	-9.68	-2.90	0.41	0.0%	0.0%	0.0%	1.6E-22
2070	68855-18-5	Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol	216	57	1.4E-02	2.3E+02	1.7E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	6.0

2172	1120-71-4	1,3-propanesultone	122	26	3.2E+01	1.4E+05	5.2E-01	14.0	3.5E-06	1.1E-05	3.5E-06	conf	conf	4.9E+01	6.9E-01	2.5E+01	-10.08	-9.97	-11.65	-0.76	0.67	0.0%	0.0%	8.3E-55
2173	111-49-9	perhydroazepine	99	-14	9.3E+02	6.6E+04	4.8E+01	11.0	3.5E-06	3.1E-09	3.5E-07	conf	conf	2.8E+01	3.9E-01	1.4E+01	-8.99	-8.71	-9.86	-1.03	0.70	0.0%	0.0%	8.5E-37
2174	5922-69-0	N-[3-(dimethylamino)propyl]formamide	130	68	5.9E-01	1.0E+06	1.1E-01	9.4	3.5E-06	3.5E-06	3.5E-06	conf	conf	4.8E+01	6.7E-01	2.5E+01	-8.25	-9.30	-11.14	-2.07	0.53	0.0%	0.0%	1.0E-38
2175	107-93-7	trans-crotonic acid	86	2	3.3E+01	1.2E+05	7.1E+01	14.0	3.5E-06	4.2E-06	1.1E-06	conf	conf	4.8E+01	6.7E-01	2.5E+01	-9.63	-9.49	-11.20	-0.75	0.79	0.0%	0.0%	1.1E-50
2176	34396-03-7	trimethoxy(2,4,4-trimethylpentyl)silane	234	7	2.2E+01	1.1E+02	3.8E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	3.7E+01	5.2E-01	1.9E+01	-10.06	-9.79	-11.39	-1.06	0.83	0.0%	0.0%	1.4E-49
2177	367-25-9	2,4-difluoroaniline	129	4	2.1E+02	2.5E+03	3.0E+01	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.6E+01	6.4E-01	2.4E+01	-7.70	-8.68	-10.62	-2.30	0.47	0.0%	0.0%	6.8E-33
2178	90-82-4	pseudoephedrine	165	41	1.4E+00	1.4E+04	4.8E+00	9.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.6E+01	6.4E-01	2.4E+01	-8.76	-8.63	-10.59	-0.87	0.55	0.0%	0.0%	4.3E-44
2179	111-21-7	2,2'-[ethane-1,2-diylbis(oxy)]bisethyl diacetate	234	-16	5.5E-01	5.1E+04	7.2E-01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.8E+01	6.7E-01	2.5E+01	-8.75	-9.16	-11.15	-0.66	0.23	0.0%	0.0%	4.8E-51
2180	1889-67-4	1,1'-[1,1,2,2-tetramethylethylene]dibenzene	238	74	4.2E-02	6.1E-02	3.0E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.1E+01	4.4E-01	1.5E+01	-10.78	-10.60	-11.99	0.22	0.24	0.0%	0.0%	1.8E-68
2181	3031-66-1	hex-3-yne-2,5-diol	114	34	2.3E+00	1.5E+17	7.9E-01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.6E+01	6.4E-01	2.4E+01	-7.47	-8.61	-10.56	-0.96	1.00	0.0%	0.0%	3.7E-43
2182	28770-01-6	608-245-0	159	45	2.7E-01	1.9E+05	1.1E+02	8.3	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.8E+01	6.7E-01	2.5E+01	-7.90	-8.70	-10.62	-1.68	0.85	0.0%	0.0%	1.1E-37
2183	76918-62-2	sodium N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxynaphthalene-2-carboxamidate	342	87	9.9E-03	2.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.6E+01	5.0E-01	1.8E+01	-7.47	-7.78	-9.44	-1.84	0.64	0.0%	0.0%	9.1E-28
2184	39072-70-3	N,N''-hexane-1,6-diylbis[N'-benzylurea]	383	250	1.2E-10	2.5E+00	6.2E+03	0.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.3E+01	5.9E-01	2.2E+01	-8.04	-8.74	-10.61	-2.88	0.55	0.0%	0.0%	1.1E-28
2185	42355-78-2	tetrasodium 2,2'-ethene-1,2-diylbis[5-[[4-[diethylamino]-6-[[4-sulfonatophenyl]amino]-1,3,5-triazin-2-yl]amino]benzenesulfonate]	1101	87	9.9E-03	7.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.5E+01	4.9E-01	1.8E+01	-7.45	-7.78	-9.45	-6.00	0.64	0.0%	0.0%	6.6E-28
2186	123-75-1	pyrrolidine	71	-36	9.9E+03	6.3E+05	5.0E+00	10.9	3.5E-06	1.1E-05	1.1E-06	conf	conf	4.8E+01	6.7E-01	2.5E+01	-10.30	-10.22	-11.61	-1.09	0.44	0.0%	0.0%	2.5E-51
2187	97-78-9	N-lauroylsarcosine	271	149	5.1E-05	8.9E+00	1.3E+04	3.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.5E+01	6.3E-01	2.3E+01	-8.19	-8.80	-10.66	-1.25	0.26	0.0%	0.0%	1.9E-41
2188	93-04-9	methyl 2-naphthyl ether	158	38	3.6E-01	7.9E+01	1.8E+03	14.0	3.5E-06	1.1E-08	3.5E-07	conf	conf	2.8E+01	3.9E-01	1.4E+01	-8.64	-8.37	-9.51	-2.23	0.33	0.0%	0.0%	1.3E-25
2189	17766-26-6	1,3,5-triazine-2,4,6(1H,3H,5H)-trithione, trisodium salt	243	87	9.9E-01	1.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.3E+01	4.9E-01	1.8E+01	-7.48	-7.79	-9.44	-0.73	0.62	0.0%	0.0%	7.8E-36
2190	33626-25-4	800-188-1	138	-25	2.9E+02	5.4E+00	2.2E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.8E+01	4.0E-01	1.4E+01	-10.95	-10.62	-13.24	-2.43	0.23	0.0%	0.0%	3.9E-54
2191	6362-80-7	1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene	236	67	3.0E-02	1.8E-01	3.2E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.1E+01	4.3E-01	1.5E+01	-10.60	-10.46	-11.54	-3.74	0.19	0.0%	0.0%	3.8E-29
2192	108-16-7	1-(dimethylamino)propan-2-ol	103	-41	6.7E+02	8.2E+05	3.0E-01	8.8	3.5E-06	3.5E-06	3.5E-06	conf	conf	4.7E+01	6.5E-01	2.4E+01	-9.64	-9.49	-11.13	-1.01	0.14	0.0%	0.0%	1.1E-47
2193	104-38-1	2,2'-p-phenylenediacetonitrile	198	103	8.4E-05	2.1E+05	4.1E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.5E+01	6.2E-01	2.3E+01	-7.45	-8.56	-10.58	0.19	0.43	0.0%	0.0%	9.6E-54
2194	2212-11-5	606-938-2	155	-45	9.9E+02	1.0E+05	6.9E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.4E+01	6.2E-01	2.3E+01	-9.62	-9.43	-10.75	-1.84	0.64	0.0%	0.0%	2.0E-37
2195	930-02-9	1-(vinyloxy)octadecane	297	75	4.2E-02	1.9E-04	5.9E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.7E+01	3.8E-01	1.3E+01	-9.84	-9.97	-11.63	-5.84	0.47	0.0%	0.0%	6.5E-17
2196	86-73-7	fluorene	166	64	4.4E-02	4.1E+00	1.2E+04	14.0	3.5E-06	8.9E-08	3.5E-08	conf	conf	3.1E+01	4.4E-01	1.5E+01	-8.79	-9.97	-2.62	0.78	0.0%	0.0%	0.0%	4.2E-26
2197	88-18-6	2-tert-butylphenol	150	37	7.1E+00	1.3E+03	2.6E+03	10.8	3.5E-06	2.2E-09	1.1E-06	conf	conf	2.7E+01	3.7E-01	1.3E+01	-8.77	-8.50	-9.65	-2.44	0.84	0.0%	0.0%	3.3E-25
2198	20749-68-2	8,9,10,11-tetrachloro-12H-phthaloperin-12-one	408	231	2.3E-09	3.7E-04	6.2E+05	7.2	3.5E-06	1.1E-08	3.5E-09	conf	conf	2.7E+01	3.7E-01	1.3E+01	-7.87	-8.18	-9.09	0.17	1.10	0.0%	0.0%	3.0E-40
2199	462-94-2	pentamethylenediamine	102	13	1.3E+02	1.0E+06	7.1E-01	10.7	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.4E+01	6.1E-01	2.3E+01	-8.83	-8.72	-10.61	-0.82	1.06	0.0%	0.0%	5.9E-45
2200	1746-23-2	p-tert-butylstyrene	160	0	3.0E+01	5.9E+00	6.3E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.8E+01	4.0E-01	1.4E+01	-10.80	-10.52	-12.56	-2.61	0.21	0.0%	0.0%	3.7E-46
2201	78-16-0	2-ethyl-2-[[(1-oxohepty)loxy]methyl]propane-1,3-diyl bisheptanoate	471	130	2.4E-06	3.0E-03	1.5E+09	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.7E+01	3.8E-01	1.4E+01	-8.01	-9.14	-10.82	-4.53	0.54	0.0%	0.0%	1.2E-19
2202	54112-23-1	N,N'-(methylenedi-p-phenylene)bis[hexahydro-2-oxo-1H-azepine-1-carboxamide]	477	350	8.8E-18	1.1E+00	3.0E+04	0.4	3.5E-06	1.1E-06	1.1E-07	conf	conf	3.3E+01	5.3E-01	2.0E+01	-8.07	-8.61	-10.63	-2.73	0.57	0.0%	0.0%	8.6E-30
2203	57-88-5	cholesterol	387	162	2.4E-05	1.4E-03	5.5E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.7E+01	3.8E-01	1.3E+01	-9.68	-9.99	-5.26	0.48	0.0%	0.0%	0.0%	7.4E-12
2204	2123-24-2	hexahydro-2H-azepin-2-one, sodium salt	135	87	9.9E-03	9.3E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.4E+01	4.7E-01	1.7E+01	-7.51	-7.81	-9.45	0.18	0.42	0.0%	0.0%	2.1E-43
2205	760-93-0	methacrylic anhydride	154	-65	1.2E+03	4.0E+03	1.7E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.4E+01	6.1E-01	2.2E+01	-10.63	-10.41	-12.02	-0.93	0.62	0.0%	0.0%	7.5E-57
2206	470-82-6	cineole	154	8	2.1E+02	7.2E+00	1.3E+04	14.0	3.5E-06	4.4E-09	1.1E-06	conf	conf	2.6E+01	3.6E-01	1.3E+01	-10.83	-10.44	-12.93	-1.03	0.70	0.0%	0.0%	4.4E-65
2207	75-57-0	tetramethylammonium chloride	110	87	9.9E-03	7.6E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.4E+01	4.7E-01	1.7E+01	-7.51	-7.81	-9.45	-1.07	1.17	0.0%	0.0%	2.3E-33
2208	13472-08-7	2,2'-azobis[2-methylbutyronitrile]	192	64	1.2E-01	1.4E+02	7.2E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	3.6E+01	5.1E-01	1.8E+01	-8.86	-8.63	-10.22	-0.94	0.54	0.0%	0.0%	4.9E-28
2209	104-66-5	1,2-diphenoxyethane	214	71	2.2E-02	2.8E+01	6.5E+03	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	3.7E+01	5.1E-01	1.8E+01	-8.88	-8.66	-10.25	-2.94	0.25	0.0%	0.0%	7.6E-26
2210	132900-75-5	2-methylbenzene-1,4-diyl bis[4-[4-(acryloyloxy)butoxy]benzoate]	617	288	1.7E-13	1.0E-04	1.7E+08	14.0	3.5E-06	3.5E-07	6.6E-10	conf	conf	2.7E+01	3.8E-01	1.3E+01	-8.83	-8.70	-9.32	-4.40	0.82	0.0%	0.0%	1.0E-12
2211	2031-67-6	triethoxy(methyl)silane	178	-23	7.7E+02	1.7E+03	6.3E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	3.9E+01	5.5E-01	2.0E+01	-10.40	-10.12	-11.91	0.25	1.08	0.0%	0.0%	6.6E-68
2212	133-66-4	disodium 4,4'-bis[(4,6-dianilino-1,3,5-triazin-2-yl)amino]stilbene-2,2'-disulphonate	937	87	9.9E-03	6.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.3E+01	4.6E-01	1.7E+01	-7.48	-7.81	-9.47	-0.37	0.25	0.0%	0.0%	5.8E-39
2213	4246-51-9	3,3'-oxybis(ethyleneoxy)bis(propylamine)	220	93	9.2E-02	1.0E+06	3.5E-02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.3E+01	6.0E-01	2.2E+01	-7.39	-8.44	-10.59	-0.75	0.55	0.0%	0.0%	3.5E-45
2214	107-11-9	allylamine	57	-73	3.4E+04	1.0E+06	1.6E+00	10.0	3.5E-06	4.2E-07	1.1E-06	conf	conf	3.9E+01	5.4E-01	2.0E+01	-9.60	-9.37	-10.49	-1.59	0.54	0.0%	0.0%	2.3E-37
2215	2691-41-0	octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine	296	183	3.2E-06	1.0E+06	6.6E+00	14.0	3.5E-06	1.0E-07	1.1E-07	conf	conf	3.2E+01	4.5E-01	1.6E+01	-6.85	-7.77	-9.34	-1.52	0.10	0.0%	0.0%	3.1E-29
2216	54914-37-3	1,3,3-trimethyl-N-(2-methylpropylidene)-5-[(2-methylpropylidene)amino]cyclohexanemethylamine	278	41	8.7E-02	1.7E+00	1.4E+07	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	2.7E+01	3.8E-01	1.3E+01	-9.71	-9.48	-10.45	-1.22	0.47	0.0%	0.0%	5.2E-40
2217	84-51-5	2-ethylanthraquinone	236	147	9.8E-06	1.2E-01	2.4E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.7E+01	5.1E-01	1.9E+01	-8.60	-9.40	-10.87	-3.45	0.22	0.0%	0.0%	1.6E-26
2218	5726-19-2	2-methylcyclohexyl acetate	156	-18	6.5E+01	1.8E+03	1.1E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.2E+01	5.9E-01	2.2E+01	-10.42	-10.24	-11.40	-1.52	0.27	0.0%	0.0%	1.4E-45
2219	6022-22-6	disodium 4,4'-diamino-9,9',10,10'-tetrahydro-9,9',10,10'-tetraoxo[1,1'-bianthracene]-3,3'-disulphonate	649	87	9.9E-03	4.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.3E+01	4.6E-01	1.6E+01	-7.49	-7.81	-9.48	-1.84	0.64	0.0%	0.0%	4.9E-28
2220	455-14-1	α,α,α-trifluoro-p-toluidine	161	10	5.5E-01	4.4E+03	1.1E+02	2.6	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.2E+01	5.8E-01	2.2E+01	-7.95	-8.97	-10.76	-2.23	0.63	0.0%	0.0%	1.8E-34
2221	104-23-4	4'-aminoazobenzene-4-sulphonic acid	277	197	1.9E-09	5.2E+02	1.1E+00	0.4	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.2E+01	5.8E-01	2.1E+01	-7.53	-8.80	-10.63	-1.44	0.33	0.0%	0.0%	1.3E-39
2222	5578-42-7	dichlorocyclohexylmethylsilane	197	-21	1.8E+02	4.7E+00	3.2E+04	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.6E+01	3.7E-01	1.3E+01	-10.97	-10.68	-13.27	-1.51	0.36	0.0%	0.0%	1.2E-63
2223	27503-81-7	2-phenyl-3H-benzimidazole-5-sulphonic acid	274	243	1.8E-13	1.2E+00	6.0E-01	-0.4	3.5E-06	2.2E-09	3.5E-08	conf	conf	2.5E+01	3.5E-01	1.2E+01	-9.73	-7.57	-8.52	-2.21	0.96	0.0%	0.0%	1.0E-19
2224	27076-30-8	3-[(2-hydroxyethyl)amino]propionamide	132	112	5.3E-04	1.0E+05	2.2E-03	8.8	3.5E-06	3.5E-06	3.5E-06	conf	conf	4.4E+01	6.1E-01	2.2E+01	-8.10	-9.25	-11.17	-0.64	1.10	0.0%	0.0%	1.9E-51
2225	7787-93-1	dichloro(3-chloropropyl)methylsilane	192	-31	3.8E+02	8.1E+02	3.0E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	2.8E+01	3.9E-01	1.4E+01	-10.11	-9.81	-11.63	-0.75	0.61	0.0%	0.0%	8.8E-55
2226	93-70-9	2'-chloroacetoacetanilide	212	135	9.4E-04	3.9E+03	1.2E+01	10.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.1E+01	5.8E-01	2.1E+01	-7.71	-8.71	-10.67	-1.12	0.39	0.0%	0.0%	1.0E-42
2227	59719-67-4	bis[2-[2-(1-methylethyl)-3-oxazolidinyl]ethyl] hexan-1,2-diylbiscarbamate	487	215	5.8E-08	3.4E+01	8.3E+02	6.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.3E+01	6.0E-01	2.2E+01	-7.96	-8.94	-10.66	-1.87	1.46	0.0%	0.0%	1.8E-36
2228	23386-52-9	sodium 1,4-dicyclohexyl sulphonatosuccinate	384	87	9.9E-03	2.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.2E+01	4.4E-01	1.6E+01	-7.52	-7.83	-9.49	-0.30	0.64	0.0%	0.0%	1.3E-39
2229	144-15-0	tris(2-ethylhexyl) 2-(acetyloxy)propane-1,2,3-tricarboxylate	571	185	1.4E-08	3.2E-05	9.1E+09	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.4E+01	3.4E-01	1.2E+01	-9.14	-9.28	-9.41	-4.78	0.70	0.0%	0.0%	1.8E-11
2230	26741-53-7	3,9-bis(2,4-di-tert-butylphenoxy)-2,4,8,10-tetraoxa-3,9-diphosphaspiro[5.5]undecane	605	257	3.9E-11	1.6E-06	7.9E+10	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.4E+01	3.4E-01	1.2E+01	-9.15	-9.13	-9.26	-1.63	0.90	0.0%	0.0%	5.3E-28
2231	762-12-9	bisdecanoyl peroxide	343	14	5.9E-03	1.3E-02	2.4E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.5E+01	3.5E-01	1.2E+01	-9.91	-10.07	-11.08	-5.03	0.67	0.0%	0.0%	2.7E-18
2232	141-17-3	bis(2-(2-butoxyethoxy)ethyl) adipate	435	117	1.1E-04	2.0E+00	1.7E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.9E+01	5.4E-01	2.0E+01	-9.23	-9.10	-10.77	-1.40	0.90	0.0%	0.0%	3.5E-41
2233	112-82-3	1-bromohexadecane	305	66	7.6E-02	4.0E-04	3.5E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.5E+01	3.4E-01	1.2E+01	-9.99	-10.12	-11.91	-4.81	0.64	0.0%	0.0%	1.8E-24
2234	586-62-9	p-mentha-1,4(8)-diene	136	-30	1.3E+02	1.8E+01	7.6E+04	14.0	3.5E-06	5.6E-07	3.5E-07	conf	conf	2.7E+01	3.7E-01	1.3E+01	-10.95	-10.67	-12.79	-2.63	0.70	0.0%	0.0%	5.4E-48
2235	62S8-06-6	sodium 1-amino-4-bromo-9,10-dioxoanthracene-2-sulphonate	404	87	9.9E-03	2.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.1E+01	4.3E-01	1.6E+01	-7.52	-7.84	-9.49	-1.84	0.64	0.0%	0.0%	3.7E-28
2236	104-92-7	4-bromoanisole	187	11	2.3E+01	3.2E+02	9.1E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	3.4E+01	4.7E-01	1.7E+01	-9.93	-9.67	-10.96	-1.71	0.12	0.0%	0.0%	3.4E-40
2237	16029-98-4	iodotrimethylsilane	200	-66	8.7E+03	6.9E+02	9.8E+02	14.0	3.5E-06	3.5E-09	3.5E-06	conf	conf	2.4E+01	3.3E-01	1.2E+01	-10.44	-9.80	-12.27	-1.17	0.27	0.0%	0.0%	6.4E-57
2238	3121-61-7	2-methoxyethyl acrylate	130	-40	6.0E+02	4.5E+04	2.8E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.2E+01	5.8E-01	2.1E+01	-9.97	-9.85	-11.24	-2.21	0.15	0.0%	0.0%	2.1E-38
2239	2372-45-4	sodium butanolate	96	87	9.9E-03	6.6E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.1E+01	4.3E-01	1.5E+01	-7.55	-7.85	-9.49	-1.84	0.64	0.0%	0.0%	4.0E-28
2240	124-12-9	octanenitrile	125	-11	3.7E+01	9.3E+01	6.5E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.6E+01	5.1E-01	1.8E+01	-9.81	-9.64	-11.22	-2.32	0.69	0.0%	0.0%	2.7E-37
2241	109-65-9	1-bromobutane	137	-66	5.5E+03	6.6E+02	4.5E+02	14.0	3.5E-06	3.5E-08	3.5E-07	conf	conf	2.4E+01	3.3E-01	1.2E+01	-10.75	-10.43	-12.68	-1.44	0.64	0.0%	0.0%	2.4E-58
2242	24461-61-8	methyl (R)-aminophenylacetate	165	45	2.0E+00	1.2E+05	3.5E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.1E+01	5.8E-01	2.1E+01	-9.03	-9.36	-11.21	-1.37	0.98	0.0%	0.0%	3.7E-45
2243	2923-16-2	potassium trifluoroacetate	152	87	9.9E-03	1.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.1E+01	4.3E-01	1.5E+01	-7.55	-7.85	-9.50	-0.25	1.50	0.0%	0.0%	4.1E-40
2244	67-51-6	3,5-dimethylpyrazole	96	28	2.8E+00	7.9E+03	1.4E+01	4.2	3.5E-06	3.5E-07	1.1E-07	conf	conf	3.5E+01	4.9E-01	1.8E+01	-7.19	-8.17	-10.04	-2.58	0.35	0.0%	0.0%	8.3E-27
2245	26479-35-6	potassium carbamoylcarbamate	142	87	9.9E-03	9.8E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.1E+01	4.3E-01	1.5E+01	-7.55	-7.85	-9.50	-0.83	0.25	0.0%	0.0%	1.6E-35
2246	122731-58-2	602-890-1	284	233	1.9E-12	1.5E+04	1.9E-01	3.1	3.5E-06	3.5E-06	3.5E-07	conf	conf	4.1E+01	5.7E-01	2.1E+01	-7.69	-9.05	-11.15	-1.29	0.64	0.0%	0.0%	2.4E-45
2247	5026-74-4	p-[2,3-epoxypropoxy]-N,N-bis[2,3-epoxypropyl]aniline	277	128	7.6E-04	1.6E+03	7.4E+00	3.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.9E+01	5.4E-01	2.0E+01	-7.65	-8.71	-10.70	-1.95	0.34	0.0%	0.0%	2.7E-36
2248	3445-11-2	1-(2-hydroxyethyl)pyrrolidin-2-one	129	75	2.5E-02	2.4E+05	8.3E-02	-0.7	3.5E-06	3.5E-06	3.5E-06	conf	conf	4.1E+01	5.7E-01	2.1E+01	-8.06	-9.54	-11.18	-1.03	1.61	0.0%	0.0%	6.9E-48
2249	16039-53-5	zinc dilactate	244	87	9.9E-03	1.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.0E+01	4.2E-01	1.5E+01	-7.55	-7.86	-9.51	-2.20	0.67	0.0%	0.0%	8.5E-26
2250	94-71-3	2-ethoxyphenol	138	36	8.4E-00	1.5E+04	6.8E+01	10.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.0E+01	5.5E-01	2.0E+01	-9.88	-9.70	-11.25	-1.76	0.25	0.0%	0.0%	3.3E-42
2251	2705-87-5	allyl 3-cyclohexylpropionate	196	17	2.9E+00	9.4E+01	3.0E+04	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	3.3E+01	4.6E-01	1.7E+01	-9.98	-11.14	-12.91	-2.91	0.50	0.0%	0.0%	3.0E-32
2252	3069-29-2	N-[3-(dimethoxymethylsilyl)propyl]ethylenediamine	206	55	1.6E+00	7.5E+04	3.8E-01	9.7	3.5E-06	3.5E-06	3.5E-06	conf	conf	4.0E+01	5.5E-01	2.1E+01	-9.24	-9.45	-11.24	-1.38	0.96	0.0%	0.0%	2.4E-45
2253	2226-96-2	4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl	173	102	2.0E-04	1.8E+06	3.6E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	3.8E+01	5.3E-01	2.0E+01	-7.69	-8.81	-10.67	-0.52	0.49	0.0%	0.0%	6.9E-48
2254	1003-03-8	cyclopentylamine	85	-38	2.5E+03	4.2E+04	1.4E+01	10.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.7E+01	5.2E-01	1.9E+01	-10.08	-9.86	-11.12	-1.08	0.24	0.0%	0.0%	6.5E-47
2255	106-25-2	nerol	154	-11	2.1E+00	3.4E+02	3.0E+03	14.0	3.5E-06	5.8E-07	1.1E-06	conf	conf	3.4E+01	4.8E-01	1.7E+01	-9.46	-9

2355	1067-25-0	trimethoxypropylsilane	164	-35	6.8E+02	5.1E+03	2.0E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.9E+01	4.0E-01	1.5E+01	-10.34	-10.09	-11.57	-2.43	0.61	0.0%	0.0%	2.7E-39
2356	114-07-8	erythromycin	734	350	2.8E-23	2.2E+00	3.0E+02	9.0	3.5E-06	2.7E-07	3.5E-07	conf	conf	2.5E+01	3.5E-01	1.3E+01	-7.66	-8.45	-10.11	-1.81	1.35	0.0%	0.0%	9.8E-33
2357	4156-21-2	sodium p-[(4,6-dichloro-1,3,5-triazin-2-yl)amino]benzenesulphonate	343	87	9.9E-03	2.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.2E-01	1.1E+01	-7.66	-7.97	-9.63	-0.18	0.29	0.0%	0.0%	7.7E-42
2358	118969-29-2	601-577-7	342	87	9.9E-03	2.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.2E-01	1.1E+01	-7.66	-7.97	-9.63	-1.84	0.64	0.0%	0.0%	4.3E-29
2359	91-16-7	veratrole	138	-6	3.6E+01	2.7E+03	4.4E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.9E+01	4.0E-01	1.5E+01	-9.88	-9.68	-10.94	-1.54	0.75	0.0%	0.0%	2.1E-41
2360	2568-90-3	1,1'-[methylenebis(oxy)]dibutane	160	-21	1.8E+02	5.8E+02	5.6E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.7E+01	3.7E-01	1.4E+01	-10.58	-10.33	-11.86	-1.51	0.36	0.0%	0.0%	8.7E-50
2361	629-40-3	suberonitrile	136	43	8.2E-01	1.1E+03	2.1E+01	0	3.5E-06	1.1E-08	3.5E-07	conf	conf	1.8E+01	2.5E-01	8.8E+00	-7.42	-7.88	-8.93	-0.47	0.33	0.0%	0.0%	6.2E-34
2362	698-90-8	cyclohexylurea	142	71	3.1E-01	2.0E+04	1.5E+01	0.1	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.9E+01	4.0E-01	1.5E+01	-8.11	-9.05	-10.84	-1.67	1.29	0.0%	0.0%	1.7E-39
2363	706-14-9	decan-4-olide	170	20	6.8E-01	2.0E+02	3.7E+02	14.0	3.5E-06	4.8E-07	1.1E-07	conf	conf	2.6E+01	3.7E-01	1.3E+01	-9.21	-8.99	-10.49	-1.81	0.43	0.0%	0.0%	1.3E-35
2364	13515-40-7	2-[[4-chloro-2-nitrophenyl]azo]-N-(2-methoxyphenyl)-3-oxobutyramide	391	239	6.2E-10	1.9E+00	3.5E+03	-0.1	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.5E+01	3.5E-01	1.3E+01	-7.90	-8.45	-10.22	-1.57	0.90	0.0%	0.0%	2.4E-35
2365	75980-60-8	diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide	348	90	5.9E-06	2.7E-01	7.4E+02	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.9E+01	4.0E-01	1.5E+01	-8.59	-8.69	-10.36	-2.39	0.13	0.0%	0.0%	2.6E-30
2366	629-15-2	ethylene diformate	118	-102	1.7E+02	2.6E+05	2.0E-01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	3.0E+01	4.2E-01	1.6E+01	-9.60	-9.47	-11.29	-0.96	0.44	0.0%	0.0%	1.2E-49
2367	99-82-1	1-isopropyl-4-methylcyclohexane	140	-53	2.5E+02	2.9E-01	8.3E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.8E+01	2.5E-01	8.8E+00	-11.23	-10.90	-13.72	-3.10	0.79	0.0%	0.0%	2.5E-52
2368	7526-26-3	diphenyl methylphosphonate	248	85	9.9E-03	2.4E+01	8.9E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.5E+01	3.5E-01	1.3E+01	-8.70	-10.37	-2.10	0.45	0.0%	0.0%	0.0%	1.9E-32
2369	105-05-5	1,4-diethylbenzene	134	-17	1.2E+02	3.6E+01	1.7E+04	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.8E+01	2.7E-01	9.5E+00	-10.84	-10.55	-12.52	-2.38	0.44	0.0%	0.0%	7.2E-48
2370	29923-31-7	sodium hydrogen N-(1-oxododecyl)-L-glutamate	351	87	9.9E-03	2.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+01	3.1E-01	1.1E+01	-7.67	-7.98	-9.64	-0.84	0.60	0.0%	0.0%	1.6E-36
2371	13393-93-6	tetradecahydro-7-isopropyl-1,4a-dimethylphenanthren-1-methanol	293	117	4.5E-05	2.1E-01	2.5E+06	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.9E+01	2.7E-01	9.4E+00	-9.32	-9.57	-10.61	-0.58	0.22	0.0%	0.0%	7.6E-47
2372	52-51-7	bronopol	200	91	2.7E-04	1.7E+05	2.3E-01	14.0	3.5E-06	1.6E-08	3.5E-07	conf	conf	1.8E+01	2.5E-01	8.8E+00	-7.58	-7.95	-9.06	-2.68	1.04	0.0%	0.0%	1.7E-20
2373	624-89-5	ethyl methyl sulphide	76	-95	2.0E+04	8.6E+03	2.6E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.1E+01	2.9E-01	1.0E+01	-10.61	-10.27	-12.25	-1.99	0.89	0.0%	0.0%	5.5E-49
2374	81782-77-6	4-methyl-3-decen-5-ol	170	-3	7.9E-01	2.1E+02	1.1E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.6E+01	3.6E-01	1.3E+01	-9.77	-9.56	-10.99	-2.87	0.32	0.0%	0.0%	1.9E-31
2375	3779-63-3	(2,4,6-trioxotriazine-1,3,5(2H,4H,6H)-triyl)tris(hexamethylene) isocyanate	505	307	1.3E-14	2.8E-03	6.5E+09	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.7E+01	2.4E-01	8.3E+00	-9.30	-9.47	-9.60	-0.58	0.52	0.0%	0.0%	2.7E-38
2376	7320-37-8	tetradecyloxirane	240	51	2.6E-01	1.5E-02	5.8E+06	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+01	2.6E-01	9.4E+00	-8.59	-9.33	-11.15	-4.00	0.37	0.0%	0.0%	8.6E-25
2377	13501-76-3	(3-chloropropyl)diethoxymethylsilane	210	2	1.5E+01	1.3E+02	2.2E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.6E+01	3.7E-01	1.3E+01	-10.49	-10.25	-11.56	-0.41	0.16	0.0%	0.0%	2.0E-57
2378	57843-53-5	N,N,N',N'-tetrakis(2-hydroxypropyl)adipamide	377	238	2.2E-13	6.4E+03	7.1E-03	-0.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.8E+01	3.9E-01	1.5E+01	-7.52	-8.89	-10.79	-0.56	0.47	0.0%	0.0%	1.1E-48
2379	79-81-2	retinyl palmitate	525	222	1.6E-07	1.1E-08	3.8E+15	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.7E+01	2.4E-01	8.1E+00	-10.97	-10.97	-10.97	-0.66	1.68	0.0%	0.0%	2.4E-49
2380	507-20-0	2-chloro-2-methylpropane	93	-100	1.9E+04	1.1E+03	2.8E+02	0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.8E+01	2.5E-01	9.3E+00	-8.12	-8.64	-10.41	-1.44	0.28	0.0%	0.0%	6.2E-38
2381	2624-17-1	sodium 1,3,5-triazinane-2,4,6-trione	151	87	9.9E-03	1.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+01	3.0E-01	1.1E+01	-7.70	-8.00	-9.64	0.52	0.45	0.0%	0.0%	4.3E-48
2382	26351-32-6	(D)-3-(9-octadecenylamino)propiononitrile	321	148	1.2E-05	1.5E-04	3.0E+07	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.8E+01	2.6E-01	9.4E+00	-8.18	-9.31	-11.09	-4.61	0.20	0.0%	0.0%	1.0E-20
2383	98-10-2	benzenesulphonamide	157	79	2.0E-02	5.1E+03	2.3E+00	10.1	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.5E+01	3.5E-01	1.3E+01	-7.60	-8.24	-10.15	-1.45	1.38	0.0%	0.0%	8.4E-36
2384	100-18-5	1,4-diisopropylbenzene	162	-16	2.9E+01	1.2E+00	7.9E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.7E+01	2.4E-01	8.5E+00	-11.15	-10.85	-13.28	-3.08	0.37	0.0%	0.0%	2.2E-48
2385	2458-08-4	3α,7α-dihydroxy-12-oxo-5β-cholan-24-oic acid	407	232	2.3E-12	3.0E+01	5.1E+03	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	2.7E+01	3.8E-01	1.4E+01	-6.85	-7.82	-9.48	-0.63	0.22	0.0%	0.0%	6.8E-37
2386	4747-21-1	N-methylisopropylamine	73	-92	3.8E+04	3.5E+05	5.9E+00	11.1	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.9E+01	4.0E-01	1.5E+01	-12.16	-10.41	-11.68	-1.31	0.44	0.0%	0.0%	6.0E-50
2387	7597-60-6	6-amino-5-formamido-1,3-dimethyluracil	198	195	5.1E-07	7.5E+04	4.4E-02	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	2.7E+01	3.8E-01	1.4E+01	-6.84	-7.82	-9.48	-3.58	0.64	0.0%	0.0%	1.8E-17
2388	2896-70-0	2,2,6,6-tetramethyl-4-oxopiperidinooxy	171	104	4.9E-04	5.3E+04	1.1E+00	3.9	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.7E+01	3.8E-01	1.4E+01	-7.88	-9.03	-10.86	-0.71	0.21	0.0%	0.0%	5.5E-48
2389	930-28-9	chlorocyclopentane	105	-68	2.7E+03	3.7E+02	7.4E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.8E+01	2.5E-01	8.9E+00	-10.94	-10.63	-12.81	-1.36	0.29	0.0%	0.0%	2.0E-60
2390	88-66-4	1-chloro-2-(dichloromethyl)benzene	195	16	8.2E+00	1.5E+01	4.2E+03	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	1.8E+01	2.5E-01	8.9E+00	-10.33	-10.04	-11.79	-1.11	0.64	0.0%	0.0%	8.1E-53
2391	14073-97-3	L-menthan-3-one	154	-2	4.9E+01	7.4E+02	7.4E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.6E+01	3.6E-01	1.3E+01	-10.40	-10.16	-11.33	-1.24	0.22	0.0%	0.0%	2.1E-47
2392	112-96-9	octadecyl isocyanate	296	110	2.6E-01	5.8E-04	1.4E+09	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.6E+01	2.3E-01	7.9E+00	-9.94	-10.04	-11.52	-5.47	1.07	0.0%	0.0%	3.0E-18
2393	169115-74-6	Carbamic acid, (2-hydroxypropyl-, compd. with 1-amino-2-propanol (1:1)	194	87	9.9E-03	1.3E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	2.9E-01	1.1E+01	-7.15	-7.98	-9.64	-0.67	0.30	0.0%	0.0%	6.4E-38
2394	2814-77-9	1-[(2-chloro-4-nitrophenyl)azo]-2-naphthol	328	204	2.1E-08	2.3E+00	3.5E+06	8.7	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.8E+01	2.5E-01	8.7E+00	-9.04	-9.63	-10.53	-3.10	0.94	0.0%	0.0%	1.3E-26
2395	13560-89-9	1,6,7,8,9,14,15,16,17,17,18,18-dodecachloropentacyclo[12.2.1.16,9.02,13.05,10]octadeca-7,15-diene	654	206	9.4E-08	4.8E-06	1.9E+11	14.0	3.5E-06	3.5E-08	1.1E-08	conf	conf	1.6E+01	2.2E-01	7.7E+00	-9.31	-9.18	-9.21	-6.43	0.97	0.0%	0.0%	3.0E-26
2396	2978-58-7	1,1-dimethylprop-3-ynylamine	83	-26	1.2E+04	6.0E+05	2.8E+00	8.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.8E+01	3.9E-01	1.4E+01	-10.18	-10.05	-11.37	-1.81	1.10	0.0%	0.0%	8.4E-43
2397	72361-35-4	triisotridecyl benzene-1,2,4-tricarboxylate	757	313	5.3E-15	9.2E-14	9.1E+18	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.6E+01	2.2E-01	7.7E+00	-16.03	-16.03	-16.03	-1.73	0.33	0.0%	0.0%	4.0E-93
2398	2602-34-8	[3-(2,3-epoxypropoxy)propyl]trichloro(vinyl)silane	278	78	7.7E-02	6.8E+02	3.6E+00	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.4E+01	3.3E-01	1.2E+01	-8.65	-8.43	-10.25	-0.61	0.12	0.0%	0.0%	2.1E-43
2399	127-39-9	sodium 1,2-dibisobutoxycarbonylethanesulphonate	332	87	9.9E-03	2.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	2.9E-01	1.0E+01	-7.70	-8.02	-9.67	0.06	0.64	0.0%	0.0%	3.1E-44
2400	84170-74-1	(2,2-Dioctyl-1,3-propanediyl)bis[oxy-3,1-propanediyl] bisacrylate	328	20	2.2E-02	2.8E+01	8.1E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.7E+01	3.8E-01	1.4E+01	-10.20	-10.02	-11.52	-2.07	0.52	0.0%	0.0%	8.6E-42
2401	16088-62-3	(S)-1,2-epoxypropane	58	-100	7.1E+04	5.8E+04	2.3E+00	14.0	3.5E-06	6.1E-07	3.5E-07	conf	conf	2.3E+01	3.2E-01	1.2E+01	-10.52	-10.13	-12.02	-1.14	0.38	0.0%	0.0%	1.1E-54
2402	58567-11-6	(ethoxymethoxy)cyclododecane	242	25	3.1E-01	2.3E+00	3.2E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.0E+01	2.8E-01	1.0E+01	-10.77	-10.55	-11.71	-2.26	0.86	0.0%	0.0%	8.5E-42
2403	68134-22-5	N-[2,3-dihydro-2-oxo-1H-benzimidazol-5-yl]-3-oxo-2-[[2-(trifluoromethyl)phenyl]azo]butyramide	405	251	9.8E-11	7.6E+00	1.5E+03	1.8	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.6E+01	3.7E-01	1.4E+01	-8.18	-8.52	-10.82	-1.83	1.01	0.0%	0.0%	5.4E-38
2404	52636-67-6	morpholinium sulphamate	184	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	2.9E-01	1.0E+01	-7.72	-8.02	-9.67	-0.50	0.64	0.0%	0.0%	1.6E-39
2405	762240-92-6	616-309-4	229	87	9.9E-03	1.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	2.9E-01	1.0E+01	-7.71	-8.02	-9.67	-1.84	0.64	0.0%	0.0%	2.1E-29
2406	21282-97-3	2-[(2-methyl-1-oxoallyl)oxy]ethyl acetoacetate	214	-23	2.8E+00	7.1E+03	1.7E+00	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	2.7E+01	3.8E-01	1.4E+01	-8.13	-8.05	-9.63	-0.83	0.42	0.0%	0.0%	1.4E-36
2407	3923-79-3	4,5-dihydroxy-1,3-dimethylimidazolidin-2-one	146	86	1.8E-03	9.9E+05	1.0E-03	-1.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.6E+01	3.7E-01	1.4E+01	-7.42	-8.69	-10.77	-1.05	2.71	0.0%	0.0%	3.8E-44
2408	41484-35-9	thiodiethylene bis[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate]	643	289	1.0E-15	3.9E-07	2.3E+10	11.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.6E+01	2.2E-01	7.6E+00	-9.41	-9.41	-9.53	-5.96	2.58	0.0%	0.0%	1.7E-07
2409	78-73-9	choline hydrogen carbonate	165	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+01	2.8E-01	1.0E+01	-7.72	-8.02	-9.67	-0.30	0.64	0.0%	0.0%	3.6E-41
2410	428-59-1	trifluoro(trifluoromethoxy)benzene	166	-89	1.5E+05	7.5E+01	5.2E+03	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.7E+01	2.3E-01	8.2E+00	-11.16	-10.80	-13.63	-2.04	0.64	0.0%	0.0%	8.1E-62
2411	141-62-8	decamethyltetrasiloxane	311	-36	6.5E+01	2.4E-02	1.4E+08	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	1.6E+01	2.2E-01	7.6E+00	-10.32	-10.05	-11.77	-4.62	0.41	0.0%	0.0%	8.1E-25
2412	76199-85-4	2-cyano-2-[2,3-dihydro-3-(tetrahydro-2,4,6-trioxo-5(2H)-pyrimidinylidene)-1H-isoindol-1-ylidene]-N-methylacetamide	337	350	7.9E-18	2.6E+03	7.9E-02	1.8	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.6E+01	3.6E-01	1.3E+01	-7.45	-8.75	-10.79	-2.00	0.64	0.0%	0.0%	1.9E-36
2413	96-17-3	2-methylbutyraldehyde	86	-79	1.4E+03	2.0E+04	1.7E+01	0	3.5E-06	7.4E-07	3.5E-06	conf	conf	2.1E+01	2.9E-01	1.0E+01	-7.39	-8.02	-9.67	0.06	0.52	0.0%	0.0%	2.0E-37
2414	6600-31-3	3,9-dicyclohex-3-enyl-2,4,8,10-tetraoxaspiro[5.5]undecane	320	142	2.3E-04	3.2E+01	2.3E+04	0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.3E+01	3.2E-01	1.2E+01	-8.52	-9.25	-10.97	-1.39	1.26	0.0%	0.0%	5.9E-43
2415	111-75-1	2-butylaminoethanol	117	0	1.0E+01	4.2E+05	2.1E+00	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	2.7E+01	3.8E-01	1.4E+01	-9.44	-9.73	-11.39	-1.17	0.74	0.0%	0.0%	1.4E-48
2416	56-18-8	3,3'-iminodi(propylamine)	131	41	1.1E+01	1.0E+06	7.1E-02	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	2.7E+01	3.8E-01	1.4E+01	-7.61	-7.88	-9.53	-0.74	0.54	0.0%	0.0%	1.8E-36
2417	855425-38-6	1-(2-Ethylhexyl)cyclohexanecarbonitrile	193	48	4.1E-01	2.4E+00	9.1E+04	0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.9E+01	2.7E-01	9.8E+00	-8.11	-8.52	-10.36	-2.96	0.28	0.0%	0.0%	2.0E-26
2418	1129-42-6	6-methyl-2-oxoperhydropyrimidin-4-ylurea	172	155	1.9E-04	3.3E+05	1.5E-02	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	2.7E+01	3.8E-01	1.4E+01	-8.25	-9.44	-11.36	-0.70	1.71	0.0%	0.0%	1.0E-52
2419	24863-70-5	1-Cyclopentene-1-acetic acid, 3-oxo-2-pentyl-, methyl ester	224	86	2.8E-02	1.3E+02	2.0E+03	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.2E+01	3.1E-01	1.1E+01	-8.98	-8.76	-10.41	-1.68	0.27	0.0%	0.0%	4.7E-36
2420	127-06-0	acetone oxime	73	-70	1.6E+02	5.6E+04	1.6E+01	12.5	3.5E-06	2.8E-07	1.1E-06	conf	conf	2.2E+01	3.1E-01	1.1E+01	-9.06	-8.81	-10.25	-0.61	0.65	0.0%	0.0%	1.8E-43
2421	5810-11-7	2-chloro-N,N-dimethyl-3-oxobutyramide	164	47	2.4E+00	2.5E+06	8.5E-01	6.2	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.3E+01	3.2E-01	1.2E+01	-7.43	-8.39	-10.25	-2.91	0.38	0.0%	0.0%	5.4E-26
2422	14814-09-6	3-(trietho xysilyl)propanethiol	238	37	1.0E+00	3.3E+02	5.4E+01	10.2	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.3E+01	3.2E-01	1.2E+01	-9.21	-8.98	-10.45	-4.84	0.79	0.0%	0.0%	3.7E-43
2423	66669-53-2	tetrasodium hydrogen 2-phosphonobutane-1,2,4-tricarboxylate	358	87	9.9E-03	2.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+01	2.8E-01	1.0E+01	-7.72	-8.03	-9.69	0.06	0.89	0.0%	0.0%	2.4E-44
2424	993-13-5	methylphosphonic acid	96	7	4.4E-02	4.6E+06	1.0E-01	14.0	3.5E-06	1.1E-07	1.1E-07	conf	conf	2.0E+01	2.9E-01	1.0E+01	-7.16	-8.04	-9.63	-1.01	0.99	0.0%	0.0%	3.9E-35
2425	764-99-8	1,1'-[oxybis(ethyleneoxy)]diethylene	158	-18	7.6E+01	8.3E+03	1.7E+00	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.3E+01	3.2E-01	1.2E+01	-9.41	-9.16	-10.53	-0.53	0.31	0.0%	0.0%	1.2E-46
2426	29171-20-8	3,7-dimethyloct-6-en-1-yn-3-ol	152	15	4.6E+00	5.2E+02	5.6E+02	13.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.5E+01	3.5E-01	1.3E+01	-9.85	-9.65	-10.97	-1.38	0.10	0.0%	0.0%	4.4E-43
2427	9011-11-4	618-465-9	222	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+01	2.8E-01	9.9E+00	-7.73	-8.04	-9.69	-1.84	0.64	0.0%	0.0%	1.7E-29
2428	79-16-3	N-methylacetamide	73	20	3.2E+01	2.3E+06	2.0E-01	14.0	3.5E-06	3.5E-07	1.1E-06	conf	conf	2.3E+01	3.2E-01	1.2E+01	-8.06	-8.43	-10.25	0.25	0.21	0.0%	0.0%	4.2E-51
2429	56-45-1	L-serine	105	218	4.0E-06	1.9E+05	3.5E-04	2.1	3.5E-06	3.5E-06	3.5E-06	conf	conf	2.7E+01	3.7E-01	1.4E+01	-8.16	-9.64	-11.36	-0.27	1.21	0.0%	0.0%	8.1E-57
2430	41026-17-9	2,2-dimethylpropane-1,3-diyl cyclohex-4-ene-1,2-dicarboxylate	408	119	1.1E-08	5.7E+02	4.5E+03	4.1	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.5E+01	3.5E-01	1.3E+01	-8.26	-9.01	-10.85	-1.52	0.83	0.0%	0.0%	4.4E-41
2431	4051-63-2	4,4'-diamino[1,1'-bianthracene]-9,9',10,10'-tetraone	444	317	2.6E-15	7.2E-02	6.8E+06	0.5	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.5E+01	3.5E-01	1.3E+01	-8.33	-9.24	-10.88	-3.20	0.21	0.0%	0.0%	2.5E-28
2432	3437-84-1	bisisobutyryl peroxide	174	-94	3.1E+02	2.8E+03	2.2E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	2.5E+01	3.5E-01	1.3E+01	-10.84	-10.65	-11.94	-0.67	0.33	0.0%	0.0%	1.3E-58
2433	51181-50-1	sodium [N-[2-[bis(carboxymethyl)amino]ethyl]-N-(2-hydroxyethyl)glycinato(4-)]ferrate(1-)	353	87	9.9E-03	2.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.9E+01	2.7E-01	9.7E+00	-7.73	-8.04	-9.70	-0.94	0.69	0.0%	0.0%	3.0E-36
2434	97-39-2	1,3-di-o-tolylguanidine	239	142	6.9E-05	5.5E+00	8.8E+03	10.1	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.3E+01	3.2E-01	1.2E+01	-9.01	-9.33	-10.98	-2.03	0.22	0.0%	0.0%	9.4E-38
2435	593-45-3	octadecane	255	31	1.9E-01	2.9E-04	1.5E+09	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.5E+01	2.1E-01	7.3E+00	-9.97	-10.06	-11.52	-6.04	0.76	0.0%	0.0%	7.3E-44
2436	2489-05-6	silver docosanoate	447	87	9.9E-03	3.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.9E+01	2.7E-01	9.7E+00	-7.73	-8.05	-9.70	-4.43	1.12	0.0%	0.0%	2.4E-14
2437	74441-05-7	N-[4-[aminocarbonyl]phenyl]-4-[[1-[[[2,3-dihydro-2-oxo-1H-benzimidazol-5-yl]amino]carbonyl]-2-oxopropyl]azo]benzamide	499	350	4.5E-20	1.9E+01	4.6E+09	2.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.6E+01	3.6E-01	1.3E+01	-9.11	-9.09	-10.86	-1.83	1.01	0.0%	0.0%	2.2E-38

2538	60111-54-8	3,3-bis[(dimethylvinylsilyl)oxy]-1,1,5,5-tetramethyl-1,5-divinyltrisiloxane	433	12	6.8E-01	1.2E-07	1.1E+11	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E+01	1.5E-01	5.4E+00	-9.98	-9.90	-10.84	-5.30	3.06	0.0%	0.0%	0.0%	1.2E-15
2539	765-30-0	cyclopropylamine	57	-61	3.8E+04	1.0E+06	1.4E+00	9.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.9E+01	2.7E-01	9.9E+00	-10.42	-10.28	-11.56	-1.76	0.93	0.0%	0.0%	0.0%	7.8E-45
2540	5580-57-4	3,3'-[[2-chloro-5-methyl-p-phenylene]bis[imino(1-acetyl-2-oxoethylene)azo]]bis[4-chloro-N-(3-chloro-o-tolyl)benza	937	350	1.7E-28	6.7E-10	4.5E+07	4.9	3.5E-06	3.5E-08	1.1E-08	conf	conf	1.2E+01	1.6E-01	5.7E+00	-12.17	-12.17	-12.17	-0.63	0.23	0.0%	0.0%	0.0%	2.3E-61
2541	63469-23-8	1,1'-[[3-(dimethylamino)propyl]imino]bispropan-2-ol	218	84	9.5E-04	1.9E+05	3.3E-01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.9E+01	2.7E-01	9.9E+00	-8.38	-9.50	-11.53	-1.37	0.89	0.0%	0.0%	0.0%	4.6E-48
2542	67801-15-4	3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-one	206	44	1.9E+00	3.0E+00	2.6E+04	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.5E+01	2.1E-01	7.5E+00	-11.03	-10.76	-12.36	-2.37	0.50	0.0%	0.0%	0.0%	1.7E-46
2543	920-66-1	1,1,1,3,3,3-hexafluoropropan-2-ol	168	-96	2.1E+04	7.5E+03	1.3E+01	8.8	3.5E-06	1.4E-07	1.1E-06	conf	conf	1.2E+01	1.6E-01	5.7E+00	-10.90	-10.57	-12.74	-1.08	0.19	0.0%	0.0%	0.0%	1.4E-62
2544	3749-87-9	methyl 3-α,7-α-diacetoxy-12-α-hydroxy-5-β-cholan-24-oate	507	202	1.3E-10	5.7E-01	2.6E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.4E+01	2.0E-01	7.2E+00	-8.81	-9.86	-11.14	-0.63	0.22	0.0%	0.0%	0.0%	2.9E-51
2545	898566-17-1	2-(4-fluorophenyl)-5-(5-iodo-2-methylbenzyl)thiophene	408	174	2.6E-06	9.4E-03	5.6E+07	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+01	1.6E-01	5.8E+00	-9.66	-10.26	-10.74	-4.29	0.22	0.0%	0.0%	0.0%	1.4E-20
2546	21890-09-5	2-methyl-2,3,4,5,6,7,8,9,10,11,12,13-dodecahydro-1H-cyclopentacyclododecene	220	46	3.3E-01	1.2E-02	1.3E+07	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+01	1.6E-01	5.6E+00	-11.25	-11.13	-13.48	-3.89	0.39	0.0%	0.0%	0.0%	4.9E-43
2547	18127-01-0	3-(4-tert-butylphenyl)propionaldehyde	190	46	6.7E-01	1.4E+02	8.7E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.5E+01	2.1E-01	7.7E+00	-9.57	-9.32	-10.68	-2.67	0.18	0.0%	0.0%	0.0%	1.4E-30
2548	109-76-2	trimethylenediamine	74	-11	3.8E+02	1.0E+06	7.4E+00	2.9	3.5E-06	4.0E-07	1.1E-06	conf	conf	1.2E+01	2.3E-01	8.4E+00	-7.91	-8.83	-10.54	-0.54	0.67	0.0%	0.0%	0.0%	1.5E-46
2549	38083-17-9	climbazole	293	153	2.8E-05	5.7E+01	5.8E+03	7.0	3.5E-06	1.2E-08	3.5E-07	conf	conf	1.1E+01	1.6E-01	5.5E+00	-8.03	-8.29	-9.34	-3.12	0.69	0.0%	0.0%	0.0%	3.4E-19
2550	27871-49-4	methyl (S)-(-)-lactate	104	-40	2.4E+02	3.4E+05	2.1E-01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	1.9E+01	2.6E-01	9.3E+00	-8.53	-8.24	-9.79	-0.06	0.47	0.0%	0.0%	0.0%	2.7E-44
2551	18328-90-0	N-ethylmethacrylamine	99	-65	3.4E+03	7.1E+04	5.1E+01	10.2	3.5E-06	1.1E-05	1.1E-06	conf	conf	1.9E+01	2.6E-01	9.7E+00	-11.05	-10.95	-12.20	-2.98	0.64	0.0%	0.0%	0.0%	6.4E-40
2552	16529-56-9	2-methyl-3-butenenitrile	81	-59	1.1E+03	4.1E+03	3.6E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.4E+01	2.2E-01	7.9E+00	-10.32	-10.05	-11.42	-2.60	0.15	0.0%	0.0%	0.0%	1.1E-36
2553	14338-82-0	dibutyl methylenedithiodi(acetate)	308	4	1.3E-02	2.0E+01	6.8E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.7E+01	2.4E-01	8.8E+00	-10.43	-10.26	-11.71	-1.70	0.45	0.0%	0.0%	0.0%	1.1E-46
2554	574-93-6	2H,3H-phthalocyanine	515	350	5.0E-19	4.9E-06	4.9E+07	0	3.5E-06	1.1E-07	1.1E-08	conf	conf	1.1E+01	1.5E-01	5.5E+00	-8.31	-8.31	-9.83	-0.60	0.64	0.0%	0.0%	0.0%	5.5E-40
2555	71902-23-3	6-[(1-oxooctyl)oxy]methyl]hexanoic acid	271	182	3.6E-06	5.6E-04	7.8E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.6E+01	2.3E-01	8.4E+00	-8.54	-9.53	-11.09	-1.04	0.97	0.0%	0.0%	0.0%	8.9E-24
2556	98-55-5	p-menth-1-en-8-ol	154	12	2.6E+00	3.8E+03	2.1E+03	14.0	3.5E-06	6.4E-07	3.5E-07	conf	conf	1.6E+01	2.3E-01	8.4E+00	-9.47	-9.24	-10.87	-1.27	0.24	0.0%	0.0%	0.0%	4.5E-43
2557	123-68-2	allyl hexanoate	156	-22	9.6E+01	5.0E+02	1.5E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.7E+01	2.4E-01	8.9E+00	-11.13	-10.91	-12.22	-3.23	0.52	0.0%	0.0%	0.0%	4.7E-38
2558	79-07-2	2-chloroacetamide	94	42	1.4E+00	9.2E+04	2.6E-01	-2.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.6E+01	2.2E-01	8.1E+00	-7.37	-8.53	-10.37	-1.94	0.26	0.0%	0.0%	0.0%	1.1E-33
2559	83-56-7	naphthalene-1,5-diol	160	110	1.7E-05	1.1E+03	5.6E+02	14.0	3.5E-06	3.5E-06	3.5E-07	conf	conf	1.8E+01	2.6E-01	9.5E+00	-8.65	-9.82	-11.55	-2.50	0.34	0.0%	0.0%	0.0%	5.6E-38
2560	13001-46-2	potassium O-isobutyl dithiocarbonate	188	87	9.9E-03	1.3E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+01	1.9E-01	6.8E+00	-7.33	-8.16	-9.82	-1.41	0.69	0.0%	0.0%	0.0%	1.5E-33
2561	2920-38-9	p-phenylbenzonitrile	179	86	1.3E-02	1.9E+01	2.0E+03	14.0	3.5E-06	3.5E-07	3.5E-08	conf	conf	1.5E+01	2.1E-01	7.7E+00	-9.06	-8.82	-10.50	-2.14	0.12	0.0%	0.0%	0.0%	3.7E-33
2562	70-54-2	DL-lysine	146	299	1.6E-07	1.3E+05	1.0E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.7E+01	2.6E-01	9.5E+00	-8.11	-9.32	-11.49	-1.72	1.01	0.0%	0.0%	0.0%	6.8E-41
2563	7691-02-3	N-(dimethylvinylsilyl)-1,1-dimethyl-1-vinylsilylamine	185	-36	5.3E-02	1.2E+02	2.1E+03	9.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.3E+01	1.8E-01	6.5E+00	-11.22	-10.92	-13.20	-0.70	0.46	0.0%	0.0%	0.0%	1.3E-71
2564	3089-17-6	2,9-dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione	381	254	6.0E-13	5.1E-03	9.3E+04	-0.6	3.5E-06	1.1E-07	3.5E-08	conf	conf	1.3E+01	1.9E-01	6.7E+00	-7.90	-8.17	-9.76	-0.82	0.72	0.0%	0.0%	0.0%	1.1E-37
2565	2162-73-4	2,4,6-triisopropyl-m-phenylene diisocyanate	288	83	1.9E-02	6.4E-01	3.6E+07	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.1E+01	1.5E-01	5.3E+00	-9.22	-10.28	-10.98	-0.50	1.16	0.0%	0.0%	0.0%	5.9E-51
2566	4151-51-3	tris(p-isocyanatophenyl) thiophosphate	465	90	2.7E-06	2.7E-02	1.9E+08	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.1E+01	1.5E-01	5.3E+00	-9.56	-10.23	-10.46	-3.47	0.21	0.0%	0.0%	0.0%	8.9E-24
2567	503-74-2	isovaleric acid	102	4	1.5E+02	4.6E+04	3.1E+01	4.9	3.5E-06	3.5E-07	1.1E-06	conf	conf	1.5E+01	2.2E-01	7.8E+00	-8.65	-8.79	-10.51	-1.02	0.66	0.0%	0.0%	0.0%	3.4E-42
2568	2605-79-0	N,N-dimethyldecylamine N-oxide	201	153	4.6E-05	1.0E+01	4.9E+03	4.8	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.5E+01	2.1E-01	7.8E+00	-8.15	-8.62	-10.45	-2.65	0.95	0.0%	0.0%	0.0%	3.8E-29
2569	682-01-9	tetraproyl orthosilicate	264	49	1.4E+00	1.7E+01	1.6E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.5E+01	2.1E-01	7.8E+00	-10.53	-12.35	-12.35	-0.81	0.93	0.0%	0.0%	0.0%	1.2E-61
2570	3266-23-7	2,3-epoxybutane	72	-91	3.2E+04	8.8E+04	6.2E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.7E+01	2.3E-01	8.4E+00	-10.76	-10.50	-11.94	-0.74	0.32	0.0%	0.0%	0.0%	7.6E-58
2571	91-97-4	3,3'-dimethylbiphenyl-4,4'-diyl diisocyanate	264	116	2.9E-03	7.7E+01	1.1E+06	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	1.2E+01	1.7E-01	6.2E+00	-10.03	-10.04	-11.30	-2.40	0.50	0.0%	0.0%	0.0%	2.4E-37
2572	103-26-4	methyl cinnamate	162	10	1.7E+00	3.7E+02	2.3E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.6E+01	2.4E-01	9.0E+00	-10.64	-10.23	-11.63	-2.13	0.41	0.0%	0.0%	0.0%	2.9E-42
2573	544-76-3	hexadecane	226	23	9.3E-01	5.0E-04	1.6E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+01	1.5E-01	5.1E+00	-10.59	-10.67	-12.70	-5.26	0.49	0.0%	0.0%	0.0%	9.8E-27
2574	2033-24-1	2,2-dimethyl-1,3-dioxane-4,6-dione	144	27	4.4E-02	6.7E+04	6.2E+04	5.1	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.7E+01	2.4E-01	8.9E+00	-8.98	-10.11	-11.56	-1.36	1.12	0.0%	0.0%	0.0%	1.9E-48
2575	78181-99-4	[2-[[2-cyano-3-[4-(diethylamino)phenyl]-1-oxoallyl]oxy]ethyl]]3-[[2-cyano-3-[4-(diethylamino)phenyl]-1-oxoallyl]oxy	636	87	9.9E-04	4.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+01	1.8E-01	6.6E+00	-7.89	-8.21	-9.87	-1.69	0.07	0.0%	0.0%	0.0%	7.1E-32
2576	4065-45-6	sulfobenzone	308	211	1.8E-09	3.2E+02	5.6E+00	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	1.1E+01	1.6E-01	5.7E+00	-7.26	-8.23	-9.88	0.61	0.69	0.0%	0.0%	0.0%	4.6E-51
2577	93-92-5	1-phenylethyl acetate	164	0	1.5E+01	1.1E+03	3.2E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.7E+01	2.3E-01	8.5E+00	-10.13	-9.93	-11.20	-1.53	0.46	0.0%	0.0%	0.0%	1.0E-43
2578	717-74-8	1,3,5-trisoropoylbenzene	204	13	6.9E+00	6.9E-01	2.3E+06	0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.0E+01	1.5E-01	5.2E+00	-8.37	-8.86	-10.70	-3.86	0.20	0.0%	0.0%	0.0%	8.2E-23
2579	121-30-2	4-amino-6-chlorobenzene-1,3-disulphonamide	286	200	5.3E-08	4.7E+03	3.1E-01	7.8	3.5E-06	3.5E-06	3.5E-07	conf	conf	1.8E+01	2.4E-01	9.0E+00	-8.07	-9.28	-11.50	-1.12	1.15	0.0%	0.0%	0.0%	4.5E-50
2580	7704-67-8	erythromycin thiocyanate	793	87	9.9E-03	5.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+01	1.8E-01	6.5E+00	-7.89	-8.22	-9.88	-0.68	0.64	0.0%	0.0%	0.0%	8.8E-40
2581	120-57-0	piperonal	150	56	1.4E+00	6.2E+03	5.9E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.7E+01	2.3E-01	8.5E+00	-9.63	-9.43	-11.11	-1.89	0.68	0.0%	0.0%	0.0%	6.3E-40
2582	56718-70-8	[[p-[2-methoxyethyl]phenoxy]methyl]oxirane	280	18	1.8E-01	1.3E+03	7.8E+01	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+01	2.3E-01	8.2E+00	-8.44	-8.16	-9.78	-1.43	0.26	0.0%	0.0%	0.0%	3.7E-33
2583	3576-88-3	2,2'-iminobis[4,6-diamino-1,3,5-triazine]	235	210	5.2E-08	1.9E+04	2.4E+00	5.3	3.5E-06	1.1E-07	1.1E-07	conf	conf	1.3E+01	1.8E-01	6.4E+00	-7.23	-8.20	-9.79	-1.46	0.11	0.0%	0.0%	0.0%	2.9E-42
2584	76-16-4	perfluoroethane	138	-156	2.0E+06	5.2E+01	1.4E+02	14.0	3.5E-06	3.5E-08	3.5E-08	conf	conf	9.9E+00	1.4E-01	4.8E+00	-11.35	-10.80	-13.55	-1.28	0.18	0.0%	0.0%	0.0%	4.6E-69
2585	126-97-6	(2-hydroxyethyl)ammonium mercaptoacetate	153	87	9.9E-03	1.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+01	2.4E-01	8.9E+00	-8.98	-10.11	-11.56	-1.36	1.12	0.0%	0.0%	0.0%	1.0E-37
2586	36788-39-3	7-[2-(2-hydroxyethoxy)ethoxy]methyl]ethoxy]tetramethyl-3,6,8,11-tetraoxa-7-phosphatridecane-1,13-diol	430	208	4.5E-11	6.1E+02	3.8E-02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.3E+01	1.8E-01	6.6E+00	-7.89	-8.71	-9.75	-10.95	-0.07	1.15	0.0%	0.0%	0.0%	9.7E-55
2587	1941-30-6	tetrapropylammonium bromide	266	87	9.9E-03	1.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+01	1.8E-01	6.4E+00	-7.92	-8.23	-9.88	-0.56	0.64	0.0%	0.0%	0.0%	8.8E-41
2588	65212-76-2	disodium 4,5-dichloro-2-[[4,5-dihydro-3-methyl-5-oxo-1-(3-sulphonatophenyl)-1H-pyrazol-4-yl]azo]benzenesulphon	551	87	9.9E-03	3.8E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+01	1.8E-01	6.4E+00	-7.34	-8.19	-9.86	-0.17	0.64	0.0%	0.0%	0.0%	6.7E-44
2589	287930-71-6	5-[5-chloro-3-[4-(methylsulfonyl)phenyl]pyridin-2-yl]-2-methylpyridinium 4-methylbenzenesulfonate	531	87	9.9E-03	3.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+01	1.8E-01	6.4E+00	-7.91	-8.22	-9.88	-1.84	0.64	0.0%	0.0%	0.0%	6.7E-31
2590	554-68-7	triethylammonium chloride	138	87	9.9E-03	9.5E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+01	1.8E-01	6.4E+00	-7.93	-8.23	-9.88	-1.84	0.64	0.0%	0.0%	0.0%	7.8E-31
2591	33704-61-9	1,2,3,5,6,7-hexahydro-1,1,2,3,3-pentamethyl-4H-inden-4-one	206	71	5.4E-01	6.2E+01	3.1E+04	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.4E+01	2.0E-01	7.2E+00	-10.28	-10.08	-11.36	-2.35	0.35	0.0%	0.0%	0.0%	3.2E-38
2592	79-37-8	oxalyl dichloride	127	-16	2.5E+04	1.7E+04	1.5E-02	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	1.1E+01	1.5E-01	5.2E+00	-10.50	-10.04	-12.31	-0.94	0.63	0.0%	0.0%	0.0%	1.1E-59
2593	74-88-4	iodomethane	142	-95	5.4E+04	1.3E+04	3.9E+01	0	3.5E-06	4.3E-08	3.5E-09	conf	conf	1.0E+01	1.4E-01	4.9E+00	-7.17	-8.17	-9.51	-2.85	0.19	0.0%	0.0%	0.0%	9.4E-22
2594	1999-85-5	α,α,α',α'-tetramethyl-m-xylene-α,α'-diol	194	78	4.2E-03	8.8E+02	2.0E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.6E+01	2.2E-01	8.2E+00	-8.76	-9.35	-11.11	-0.53	0.73	0.0%	0.0%	0.0%	6.6E-52
2595	61597-98-6	612-179-8	228	48	1.3E-02	3.2E+01	2.2E+03	12.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.6E+01	2.3E-01	8.3E+00	-10.40	-10.24	-11.69	-1.75	0.69	0.0%	0.0%	0.0%	4.5E-46
2596	921-03-9	1,1,3-trichloroacetone	161	-13	1.9E+02	1.1E+03	2.8E+00	14.0	3.5E-06	1.1E-07	3.5E-07	conf	conf	1.6E+01	2.3E-01	8.2E+00	-8.44	-8.16	-9.78	-1.43	0.26	0.0%	0.0%	0.0%	1.5E-29
2597	110-73-6	2-ethylaminoethanol	89	-24	5.9E+01	1.0E+06	2.2E-01	10.0	3.5E-06	5.0E-07	3.5E-06	conf	conf	1.3E+01	1.8E-01	6.4E+00	-7.23	-8.20	-9.79	-1.46	0.11	0.0%	0.0%	0.0%	2.0E-46
2598	94200-74-5	sodium 2-butyloctyl sulphate	288	87	9.9E-03	2.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+01	1.8E-01	6.3E+00	-7.92	-8.23	-9.89	-1.81	0.65	0.0%	0.0%	0.0%	4.0E-31
2599	79-24-3	nitroethane	75	-39	2.7E+03	3.7E+04	2.8E+00	8.8	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.7E+01	2.2E-01	8.6E+00	-10.66	-10.51	-11.77	-0.69	1.02	0.0%	0.0%	0.0%	1.2E-56
2600	2781-00-2	di-tert-butyl α,α,α',α'-tetramethyl-(p-phenylenedimethylene) diperoxide	338	113	2.3E-03	5.4E-02	2.2E+07	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.0E+01	1.4E-01	4.9E+00	-10.42	-10.41	-11.22	-3.01	1.02	0.0%	0.0%	0.0%	5.4E-32
2601	112-60-7	3,6,9-trioxaundecane-1,11-diol	194	83	1.5E-03	1.7E+07	9.5E-03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.6E+01	2.2E-01	8.3E+00	-7.78	-8.93	-10.99	0.43	1.19	0.0%	0.0%	0.0%	3.6E-60
2602	1493-13-6	trifluoromethanesulphonic acid	150	24	7.3E+01	2.7E+04	3.2E-01	-2.8	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.7E+01	2.3E-01	8.7E+00	-8.67	-9.99	-11.61	-0.91	0.72	0.0%	0.0%	0.0%	5.7E-53
2603	840-65-3	dimethyl naphthalene-2,6-dicarboxylate	244	25	3.2E-02	3.2E+01	6.9E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.6E+01	2.2E-01	8.0E+00	-7.76	-9.54	-11.18	-2.28	0.57	0.0%	0.0%	0.0%	1.2E-37
2604	1897-52-5	2,6-difluorobenzonitrile	139	3	9.4E+01	6.4E+02	8.7E+01	0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.4E+01	1.9E-01	7.0E+00	-7.72	-8.59	-10.46	-1.71	0.60	0.0%	0.0%	0.0%	3.5E-36
2605	109-63-7	diethyl ether--boron trifluoride	142	87	9.9E-03	9.8E+02	3.0E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.3E+01	1.7E-01	6.4E+00	-9.19	-9.59	-11.22	-1.16	0.78	0.0%	0.0%	0.0%	3.3E-47
2606	6607-34-7	2,3,7,8-tetrahydro-2,5,8-benzotrioxacyclooundecine-1,9-dione	236	124	3.6E-05	2.2E+03	1.9E+01	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.6E+01	2.2E-01	8.2E+00	-7.97	-9.06	-11.02	-1.71	0.84	0.0%	0.0%	0.0%	1.1E-40
2607	136890-12-5	603-981-9	355	166	1.0E-08	3.8E-02	7.1E+06	14.0	3.5E-06	6.6E-10	1.1E-06	conf	conf	1.1E+01	1.5E-01	5.3E+00	-8.89	-8.89	-10.12	-4.84	0.69	0.0%	0.0%	0.0%	2.4E-14
2608	17636-10-1	sodium 3-mercaptopropanesulphonate	178	87	9.9E-03	1.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+01	1.7E-01	6.2E+00	-7.94	-8.24	-9.89	1.98	0.64	0.0%	0.0%	0.0%	6.2E-31
2609	106-21-8	3,7-dimethyloctan-1-ol	158	-14	4.7E+00	4.6E+01	4.4E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.5E+01	2.0E-01	7.5E+00	-10.74	-10.49	-11.67	-1.92	0.45	0.0%	0.0%	0.0%	2.0E-44
2610	80-10-4	dichloro(diphenyl)silane	253	67	8.1E-02	1.1E+01	1.1E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.3E+01	1.8E-01	6.5E+00	-10.31	-10.14	-11.40	-1.82	0.45	0.0%	0.0%	0.0%	6.5E-43
2611	24293-43-4	bis(2-ethylhexyl) 2,2'-thiobisacetate	375	20	2.0E-03	1.3E-01	5.4E+06	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.0E+01	1.4E-01	5.0E+00	-10.31	-10.27	-11.18	-3.44	0.44	0.0%	0.0%	0.0%	9.8E-29
2612	141-98-0	O-isopropyl ethylthiocarbamate	147	13	4.9E+01	1.7E+03	8.5E+01	12.0	3.5E-06	4.0E-09	1.1E-06	conf	conf	9.6E+00	1.3E-01	4.6E+00	-9.72	-9.44	-10.70	-1.37	0.22	0.0%	0.0%	0.0%	7.8E-41
2613	82985-35-1	bis(trimethoxysilylpropyl)amine	342	98	1.0E-02	4.4E+03	6.0E-02	9.8	3.5E-06	3.5E-06	3.5E-07	conf	conf	1.7E+01	2.3E-01	8.5E+00	-9.57	-9.33	-11.60	-1.44	0.61	0.0%	0.0%	0.0%	5.4E-48
2614	18297-63-7	1,3-bis(trimethylsilyl)urea	204	61	1.0E+00	4.1E+01	1.5E+02	0.1	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.5E+01	2.1E-01	7.9E+00	-8.37	-9.17	-11.10	-2.80	0.41	0.0%	0.0%	0.0%	9.4E-33
2615	71832-85-4	calcium bis[4-[[1-[[(2-chloropheny)amino]carbonyl]-2-oxopropyl]azo]-3-nitrobenzenesulphonate]	920	87	9.9E-03	6.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+01	1.7E-01	6.1E+00	-7.92	-8.24	-9.91	-2.31	1.39	0.0%	0.0%	0.0%	9.0E-28
2616	87-33-2	isosorbide dinitrate	236	82	8.0E-02	4.5E+04	5.8E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.6E+01	2.2E-01	8.0E+00	-8.28	-9.08	-11.08	-0.37	1.59	0.0%	0.0%	0.0%	3.6E-53
2617	116-53-0	2-methylbutyric acid	102	4	1.5E+02	3.7E+04	3.1E+01	4.9	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.6E+01	2.3E-01	8.3E+00	-8.54	-9.98	-11.63	-1.19	0.10	0.0%	0.0%	0.0%	1.2E-50
2618	7237-83-4	tris(oxiranylmethyl) benzene-1,2,4-tricarboxylate	378	162	5.2E-06	1.3E+03	1.3E+00	14.0	3

2721	65405-77-8	(Z)-3-hexenyl salicylate	220	100	2.6E-03	2.0E+00	6.9E+04	9.8	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E+01	1.6E-01	5.7E+00	-10.07	-9.93	-11.38	-2.81	0.47	0.0%	0.0%	0.0%	1.0E-34
2722	112-64-1	myristoyl chloride	247	58	4.9E-01	6.4E-02	2.6E+05	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-8.78	-9.59	-11.45	-4.59	0.20	0.0%	0.0%	0.0%	5.4E-23
2723	15217-42-2	sodium 1H-benzotriazolide	141	87	9.9E-03	9.7E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+01	1.5E-01	5.2E+00	-8.02	-8.32	-9.96	-1.06	0.39	0.0%	0.0%	0.0%	2.3E-37
2724	105-67-9	2,4-xylenol	122	25	1.9E-01	1.7E+03	4.1E+02	10.0	3.5E-06	4.5E-07	3.5E-07	conf	conf	1.2E+01	1.7E-01	6.2E+00	-9.79	-9.55	-10.86	-2.20	0.84	0.0%	0.0%	0.0%	1.1E-35
2725	67330-25-0	614-050-1	337	130	3.0E-04	2.7E-01	8.3E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+00	1.3E-01	4.5E+00	-10.15	-10.49	-11.36	-3.24	0.26	0.0%	0.0%	0.0%	2.0E-31
2726	128-42-7	4,4'-dinitrostilbene-2,2'-disulphonic acid	430	295	1.3E-17	6.2E+02	1.1E+00	-0.6	3.5E-06	1.1E-06	1.1E-07	conf	conf	1.3E+01	1.9E-01	6.9E+00	-7.71	-8.92	-11.05	-0.50	1.12	0.0%	0.0%	0.0%	1.3E-51
2727	5384-21-4	4,4'-methylenedi-2,6-xylenol	256	162	2.6E-06	6.3E+00	1.7E+05	10.6	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.9E+00	1.4E-01	4.9E+00	-8.65	-9.38	-10.78	-3.10	0.18	0.0%	0.0%	0.0%	2.6E-28
2728	219715-41-0	2-methoxy-4-(trifluoromethyl)pyridine-3-sulfonyl chloride	276	109	1.6E-02	6.8E+02	1.8E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.2E+01	1.6E-01	5.8E+00	-9.00	-8.93	-10.65	-2.05	1.72	0.0%	0.0%	0.0%	5.2E-35
2729	14078-41-2	3,3'-di-tert-butyl-5,5'-dimethoxybiphenyl-2,2'-diol	358	199	7.7E-09	1.3E-01	6.0E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+00	1.3E-01	4.5E+00	-9.77	-10.41	-11.24	-0.58	0.25	0.0%	0.0%	0.0%	1.3E-52
2730	675-62-7	dichloromethyl(3,3,3-trifluoropropyl)silane	211	-59	4.5E+03	9.4E+01	2.9E+03	14.0	3.5E-06	3.5E-08	1.1E-08	conf	conf	7.9E+00	1.1E-01	3.8E+00	-11.31	-10.61	-13.27	-1.36	0.42	0.0%	0.0%	0.0%	3.3E-65
2731	114798-26-4	Losartan	423	300	1.3E-16	2.8E-03	1.6E+05	14.0	3.5E-06	1.1E-07	1.1E-08	conf	conf	1.1E+01	1.6E-01	5.0E+00	-7.61	-8.48	-10.01	0.20	0.45	0.0%	0.0%	0.0%	2.0E-48
2732	163802-53-7	3-(trimethoxysilyl)propyl (2E,4E)-hexa-2,4-dienoate	274	62	8.2E-02	1.7E+02	2.5E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.4E+01	1.9E-01	7.0E+00	-10.30	-10.11	-11.75	-2.41	0.29	0.0%	0.0%	0.0%	6.6E-41
2733	69-53-4	ampicillin	349	325	3.8E-11	3.5E+03	2.8E+01	7.0	3.5E-06	5.5E-08	3.5E-07	conf	conf	9.1E+00	1.3E-01	4.5E+00	-7.65	-8.34	-9.69	-1.16	2.09	0.0%	0.0%	0.0%	1.7E-34
2734	3407-42-9	3-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexan-1-ol	236	88	1.6E-03	2.1E+01	3.2E+05	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	1.1E+01	1.4E-01	4.9E+00	-8.75	-8.52	-10.08	-1.74	0.33	0.0%	0.0%	0.0%	4.7E-33
2735	2431-50-7	2,3,4-trichlorobut-1-ene	159	-52	2.6E+02	7.3E+03	2.9E+03	0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.1E+00	1.3E-01	4.6E+00	-7.66	-8.39	-9.99	-1.93	1.08	0.0%	0.0%	0.0%	2.5E-31
2736	125971-57-5	BIBEA	293	189	5.6E-07	1.1E+01	1.8E+04	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	1.3E+01	1.8E-01	6.3E+00	-7.28	-8.17	-9.83	-2.57	0.31	0.0%	0.0%	0.0%	1.7E-25
2737	25013-16-5	tert-butyl-4-methoxyphenol	360	87	9.9E-03	2.5E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+01	1.4E-01	5.0E+00	-7.46	-8.30	-9.96	-2.50	0.84	0.0%	0.0%	0.0%	8.3E-27
2738	26591-72-0	3-methyl-1-vinyl-1H-imidazolium methyl sulphate	222	87	9.9E-03	1.5E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+01	1.4E-01	5.0E+00	-7.46	-8.30	-9.96	-0.11	1.66	0.0%	0.0%	0.0%	3.0E-45
2739	93-17-4	3,4-dimethoxyphenylacetonitrile	177	75	1.3E-01	2.4E+03	1.6E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	1.3E+01	1.8E-01	6.4E+00	-8.44	-8.29	-9.91	-0.75	0.19	0.0%	0.0%	0.0%	2.2E-39
2740	100-64-1	cyclohexanone oxime	113	-9	1.5E+00	4.4E+04	8.1E+00	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	1.1E+01	1.5E-01	5.5E+00	-8.29	-8.33	-9.96	-1.12	0.54	0.0%	0.0%	0.0%	7.5E-37
2741	93918-85-5	3-(dodecylthio)butyrozinitile	270	89	2.3E-03	2.9E-02	1.8E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+00	1.3E-01	4.5E+00	-11.02	-10.88	-11.91	-4.16	0.02	0.0%	0.0%	0.0%	9.2E-29
2742	135043-68-4	trisodium 6,6',6''-(1,3,5-triazine-2,4,6-triyltriimino)trihexanoate	535	87	9.9E-03	3.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.9E+00	1.4E-01	5.0E+00	-8.33	-9.99	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	1.1E-31
2743	124-19-6	nonanal	142	-19	7.5E+01	1.5E+02	1.9E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	1.0E+01	1.4E-01	5.0E+00	-10.74	-10.47	-12.11	-2.65	0.18	0.0%	0.0%	0.0%	7.2E-42
2744	33201-02-2	1-(1,1-dimethylethoxy)-2-methylpropane	130	-68	4.4E+03	1.4E+02	6.8E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.1E+00	1.3E-01	4.5E+00	-11.52	-11.21	-13.89	-1.69	0.22	0.0%	0.0%	0.0%	2.7E-68
2745	2890-61-1	608-291-1	161	9	9.1E+01	6.2E+01	1.8E+04	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.1E+00	1.3E-01	4.5E+00	-10.97	-10.68	-12.61	-2.09	0.38	0.0%	0.0%	0.0%	1.0E-57
2746	142-29-0	cyclopentene	68	-93	5.1E+04	8.9E+02	3.0E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+00	1.3E-01	4.5E+00	-11.56	-11.17	-13.90	-1.53	0.65	0.0%	0.0%	0.0%	3.3E-70
2747	18531-99-2	606-050-5	286	211	9.7E-10	3.8E+01	1.4E+05	9.2	3.5E-06	1.1E-07	1.1E-08	conf	conf	8.6E+00	1.2E-01	4.2E+00	-8.12	-8.82	-10.22	-3.55	0.30	0.0%	0.0%	0.0%	7.9E-22
2748	3218-36-8	p-phenylbenzaldehyde	182	73	2.5E-02	1.3E+01	3.0E+03	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.1E+01	1.5E-01	5.5E+00	-9.36	-9.13	-10.69	-2.66	0.36	0.0%	0.0%	0.0%	2.4E-31
2749	161599-46-8	Cytidine, 5'-deoxy-5-fluoro-, 2',3'-diacetate	329	151	3.6E-05	5.0E+02	4.3E-01	2.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.3E+01	1.8E-01	6.8E+00	-8.54	-9.89	-11.73	-1.11	1.72	0.0%	0.0%	0.0%	2.8E-52
2750	63157-72-2	tris[4-(diethylamino)phenyl]methylium acetate	516	87	9.9E-03	3.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.8E+00	1.4E-01	4.9E+00	-8.02	-8.34	-10.00	-4.10	0.58	0.0%	0.0%	0.0%	1.7E-17
2751	998-30-1	triethoxysilane	163	-45	1.1E+03	1.2E+04	1.8E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.2E+01	1.7E-01	6.2E+00	-10.65	-10.42	-11.84	-2.33	0.66	0.0%	0.0%	0.0%	2.7E-42
2752	3069-40-7	trimethoxycyclosilane	234	22	4.8E-00	1.0E+02	5.9E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+01	1.7E-01	6.1E+00	-10.64	-10.66	-11.66	-2.63	1.66	0.0%	0.0%	0.0%	2.2E-38
2753	746595-79-9	616-123-3	102	26	6.4E+01	8.8E+06	1.2E-01	6.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+01	1.7E-01	6.4E+00	-8.13	-9.07	-11.13	-4.08	3.16	0.0%	0.0%	0.0%	3.4E-24
2754	94-70-2	o-phenetidine	137	40	9.1E+00	4.7E+03	4.5E+01	4.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+01	1.7E-01	6.4E+00	-8.64	-9.33	-11.22	-2.18	0.69	0.0%	0.0%	0.0%	1.7E-38
2755	83-32-9	acenaphthene	154	54	1.7E-01	5.5E+00	1.4E+04	14.0	3.5E-06	1.2E-08	1.1E-08	conf	conf	7.7E+00	1.1E-01	3.7E+00	-9.88	-9.61	-10.78	-3.04	0.44	0.0%	0.0%	0.0%	9.9E-29
2756	30674-80-7	2-isocyanatoethyl methacrylate	155	10	4.7E+01	1.1E+04	5.2E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.3E+01	1.8E-01	6.5E+00	-9.66	-9.92	-11.74	-1.24	1.09	0.0%	0.0%	0.0%	1.8E-57
2757	2941-64-2	ethyl chlorothiolformate	125	-31	5.4E+02	2.8E+03	3.0E+00	14.0	3.5E-06	1.1E-07	3.5E-07	conf	conf	9.1E+00	1.3E-01	4.5E+00	-10.34	-10.04	-11.63	-2.11	1.08	0.0%	0.0%	0.0%	2.1E-42
2758	63302-43-2	613-198-4	206	89	2.7E-02	5.2E+01	9.1E+02	6.3	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.2E+01	1.7E-01	6.3E+00	-9.71	-9.62	-11.29	-2.63	0.37	0.0%	0.0%	0.0%	1.7E-35
2759	66063-15-8	4-chloro-N-cyclopentylbenzylamine	210	71	1.3E-01	7.6E+02	9.1E+03	14.0	3.5E-06	1.3E-07	3.5E-08	conf	conf	9.1E+00	1.3E-01	4.5E+00	-9.93	-8.68	-10.16	-2.14	0.72	0.0%	0.0%	0.0%	1.1E-30
2760	542-54-6	chlorocyclohexane	119	-57	7.7E+02	6.1E+02	2.3E+03	14.0	3.5E-06	1.4E-08	3.5E-07	conf	conf	7.5E+00	1.0E-01	3.6E+00	-10.81	-10.53	-12.36	-1.56	0.25	0.0%	0.0%	0.0%	5.2E-54
2761	67989-88-2	diammonium [N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4-)-N,N',O,O',ON,ON']cuprate(2-)	388	87	9.9E-03	2.7E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.6E+00	1.3E-01	4.8E+00	-7.48	-8.32	-9.98	-0.54	0.72	0.0%	0.0%	0.0%	8.8E-42
2762	58353-68-7	disodium (Z)-4-(9-octadecenylamino)-4-oxo-2(or 3)-sulphonatobutyrate	492	87	9.9E-03	3.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.5E+00	1.3E-01	4.8E+00	-8.04	-8.35	-10.01	-0.96	0.36	0.0%	0.0%	0.0%	1.6E-38
2763	108-12-3	isovaleryl chloride	121	-54	3.2E+03	3.7E+03	8.5E+00	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	1.1E+01	1.5E-01	5.4E+00	-10.51	-10.10	-12.13	-1.66	0.78	0.0%	0.0%	0.0%	6.2E-51
2764	112-03-8	trimethyloctadecylammonium chloride	348	87	9.9E-03	2.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.5E+00	1.3E-01	4.7E+00	-8.04	-8.36	-10.01	-4.29	0.24	0.0%	0.0%	0.0%	1.5E-16
2765	88-75-5	2-nitrophenol	139	71	6.4E+00	1.0E+04	8.1E+01	7.5	3.5E-06	2.7E-08	3.5E-07	conf	conf	7.9E+00	1.1E-01	3.9E+00	-8.76	-8.49	-9.61	-1.57	0.84	0.0%	0.0%	0.0%	7.4E-31
2766	75302-98-6	616-210-1	472	230	2.6E-09	6.4E-02	6.0E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+00	1.3E-01	4.5E+00	-9.75	-10.16	-11.34	-3.61	0.74	0.0%	0.0%	0.0%	1.2E-28
2767	92-55-7	5-nitrofurfurylidene di(acetate)	243	67	4.8E-02	2.5E+03	5.5E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.3E+01	1.8E-01	6.5E+00	-9.66	-9.92	-11.74	-1.24	1.09	0.0%	0.0%	0.0%	3.6E-51
2768	871544-06-8	lithium 2-methoxy-4-(trifluoromethyl)pyridine-3-thiolate	128	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.4E+00	1.3E-01	4.7E+00	-8.05	-8.36	-10.01	-10.04	-11.63	-2.11	1.08	0.0%	0.0%	2.1E-42
2769	1189-08-8	1-methylethylene dimethacrylate	226	-57	5.0E+00	8.7E+02	1.3E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.2E+01	1.7E-01	6.3E+00	-10.72	-10.54	-11.86	-1.49	0.52	0.0%	0.0%	0.0%	6.0E-50
2770	111360-16-8	2-hexyldecyl methanesulfonate	92	-59	3.2E+03	4.6E+02	3.5E+02	0	3.5E-06	9.3E-07	1.1E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-8.24	-9.23	-11.22	-1.78	0.35	0.0%	0.0%	0.0%	9.4E-42
2771	211515-46-7	1-(2-ethylbutyl)cyclohexanecarbonyl chloride	231	53	1.0E+00	6.7E-02	4.3E+04	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	7.6E+00	1.1E-01	3.7E+00	-11.06	-10.23	-12.87	-3.28	0.07	0.0%	0.0%	0.0%	5.1E-43
2772	2741-57-3	1-(dichloromethyl)-2-(trichloromethyl)benzene	278	69	1.9E-01	2.8E+00	7.6E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+00	1.3E-01	4.5E+00	-10.61	-10.36	-11.58	-3.08	0.72	0.0%	0.0%	0.0%	1.1E-34
2773	112-36-7	bis(2-ethoxyethyl) ether	162	-15	1.2E+02	4.6E+05	3.2E+00	14.0	3.5E-06	9.8E-07	3.5E-07	conf	conf	1.2E+01	1.7E-01	6.1E+00	-9.41	-9.21	-11.09	0.43	0.58	0.0%	0.0%	0.0%	3.4E-61
2774	6925-69-5	1H-phthaloperin-12-one	270	196	4.6E-07	4.5E+00	1.6E+03	14.0	3.5E-06	3.5E-07	3.5E-08	conf	conf	1.1E+01	1.5E-01	5.3E+00	-7.95	-8.82	-10.63	-0.82	0.14	0.0%	0.0%	0.0%	7.0E-45
2775	216699-04-6	Pentanediolic acid, compd. with (15,4R)-4-[2-amino-6-(cyclopropylamino)-9H-purin-9-yl]-2-cyclopentene-1-methanol	418	87	9.9E-03	2.9E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.4E+00	1.3E-01	4.7E+00	-8.04	-8.36	-10.02	-0.70	0.25	0.0%	0.0%	0.0%	9.5E-41
2776	281-23-2	tricyclo[3.3.1.13,7]decane	136	-19	9.9E+00	3.5E+00	8.7E+03	14.0	3.5E-06	3.7E-09	3.5E-07	conf	conf	7.2E+00	1.0E-01	3.5E+00	-8.56	-8.29	-9.26	-3.55	0.70	0.0%	0.0%	0.0%	1.6E-16
2777	361366-16-7	609-206-0	359	109	3.6E-04	7.7E-01	4.3E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+00	1.3E-01	4.5E+00	-10.18	-10.18	-11.49	-2.90	0.37	0.0%	0.0%	0.0%	5.8E-35
2778	3088-31-1	sodium 2-(2-dodecyloxyethoxy)ethyl sulphate	376	87	9.9E-03	2.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.3E+00	1.3E-01	4.7E+00	-8.05	-8.36	-10.02	-1.16	0.54	0.0%	0.0%	0.0%	4.9E-37
2779	109-13-7	tert-butyl peroxyisobutyrate	160	-31	1.7E+02	7.3E+02	2.2E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.9E+00	1.4E-01	5.3E+00	-10.39	-9.98	-11.97	-1.73	0.72	0.0%	0.0%	0.0%	6.6E-49
2780	7226-23-5	tetrahydro-1,3-dimethyl-1H-pyrimidin-2-one	128	28	1.5E+01	6.9E+04	1.5E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+01	1.7E-01	6.1E+00	-9.37	-9.19	-11.15	-1.31	1.43	0.0%	0.0%	0.0%	3.7E-45
2781	6330-25-2	2-cyano-N-methylacetamide	98	73	2.4E-01	1.5E+05	3.6E-01	12.2	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.2E+01	1.7E-01	6.1E+00	-8.13	-9.05	-11.14	-1.44	1.35	0.0%	0.0%	0.0%	5.0E-44
2782	54464-54-9	1-(1,6-dimethyl-3-(4-methylpent-3-enyl)-3-cyclohexen-1-yl)ethan-1-one	234	66	1.8E-01	4.3E+00	3.4E+05	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.1E+00	1.3E-01	4.5E+00	-10.91	-10.74	-11.82	-2.68	0.12	0.0%	0.0%	0.0%	2.5E-39
2783	29878-91-9	1,1'-biisophthal-8,8'-dicarboxylic acid	342	255	7.1E-11	1.0E-01	7.4E+05	14.0	3.5E-06	1.1E-07	1.1E-08	conf	conf	9.1E+00	1.3E-01	4.4E+00	-8.53	-9.09	-10.30	-3.59	0.68	0.0%	0.0%	0.0%	4.6E-22
2784	2896-97-1	N-(2-benzoyl-4-chlorophenyl)cyclopropanecarboxamide	300	198	3.5E-07	2.5E+01	2.8E+04	-1.1	3.5E-06	1.1E-07	1.1E-07	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.12	-8.42	-9.99	-3.10	0.50	0.0%	0.0%	0.0%	4.0E-23
2785	141573-96-8	619-511-0	195	43	9.1E+00	2.2E+03	2.5E+00	0	3.5E-06	1.1E-08	3.5E-08	conf	conf	9.1E+00	1.3E-01	4.6E+00	-7.48	-8.34	-9.94	-3.42	1.49	0.0%	0.0%	0.0%	6.1E-21
2786	213265-81-7	606-738-5	259	119	1.9E-02	1.9E+01	4.5E+02	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	9.1E+00	1.3E-01	4.5E+00	-8.85	-8.58	-10.09	-2.28	0.08	0.0%	0.0%	0.0%	2.1E-29
2787	599-61-1	3,3'-sulphonyldianiline	248	183	4.1E-06	2.1E+03	5.9E+00	3.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.2E+01	1.7E-01	6.1E+00	-8.32	-9.41	-11.22	-2.00	0.81	0.0%	0.0%	0.0%	6.8E-40
2788	7360-38-5	propane-1,2,3-trisl 2-ethylhexanoate	471	73	2.4E-05	1.1E-02	9.5E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.3E+00	1.0E-01	3.5E+00	-9.72	-10.09	-10.28	-4.09	0.09	0.0%	0.0%	0.0%	4.7E-19
2789	57-09-0	cetrimonium bromide	364	87	9.9E-03	2.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.2E+00	1.3E-01	4.6E+00	-8.05	-8.37	-10.02	-3.90	0.80	0.0%	0.0%	0.0%	1.1E-18
2790	5927-18-4	trimethyl phosphonoacetate	182	9	7.1E+00	1.0E+05	5.8E-01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.2E+01	1.7E-01	6.4E+00	-9.80	-9.76	-11.72	-3.00	3.27	0.0%	0.0%	0.0%	5.4E-36
2791	361366-15-6	609-205-5	318	94	1.2E-03	2.5E+00	3.2E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+00	1.3E-01	4.6E+00	-10.17	-10.14	-11.48	-2.77	0.43	0.0%	0.0%	0.0%	7.5E-36
2792	1441670-89-1	tert-butyl (6S)-6-[4-(7-bromo-9,9-difluoro-9H-fluoren-2-yl)-1H-imidazol-2-yl]-5-azaspiro[2.4]heptane-5-carboxylate	542	268	7.3E-12	5.8E-06	1.3E+08	5.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E+00	1.3E-01	4.6E+00	-9.08	-9.93	-11.30	-3.31	0.72	0.0%	0.0%	0.0%	1.6E-30
2793	1499193-67-7	2-[(1R,3S,4S)-2-azabicyclo[2.2.1]hept-3-yl]-5-(7-[2-[(6S)-5-azaspiro[2.4]hept-6-yl]-1H-imidazol-4-yl]-9,9-difluoro-9H-f	721	87	9.9E-03	5.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.05	-8.37	-10.03	-1.84	0.64	0.0%	0.0%	0.0%	5.7E-32
2794	7347-25-3	sodium taurinate	147	87	9.9E-03	1.0E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-7.51	-8.34	-10.00	-1.84	0.64	0.0%	0.0%	0.0%	1.0E-31
2795	1176987-11-1	Dibenzo[b,f][1,4]thiazepin-11-amine hydrochloride (1:1)	263	87	9.9E-03	1.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.06	-8.37	-10.03	-1.84	0.64	0.0%	0.0%	0.0%	6.3E-32
2796	1798-50-1	α,α-diphenylpiperidine-4-methanol hydrochloride	304	87	9.9E-03	2.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.3E+00	1.3E-01	4.6E+00	-8.06	-8.37	-10.03	-0.83	0.64	0.0%	0.0%	0.0%	8.8E-40
2797	1874-83-5	cyclohexane-1,3-dione, monosodium salt	134	87	9.9E-03	9.3E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.08	-8.38	-10.02	-1.84	0.64	0.0%	0.0%	0.0%	6.9E-32
2798	84332-87-6	diammonium propylenebis(dithiocarbamate)	260	87	9.9E-03	1.8E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-7.50	-8.34	-10.00	-3.44	0.64	0.0%	0.0%	0.0%	3.6E-21
2799	930086-71-8	2-(2-14-(dibenzo[b,f][1,4]thiazepin-11-yl)piperazin-1-yl)ethoxy)ethanol hydrochloride (1:1)	420	87	9.9E-03	2.9E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.06	-8.37	-10.03	-1.84	0.64	0.0%	0.0%	0.0%	6.0E-32
2800	151604-82-9	disodium [7-amino-4-(hydroxy-kO)-3-[[2-[(2-hydroxy-kO)-5-sulphophenyl]diazenyl-kN1]-4,5-dimethoxyphenyl]diazen	709	87	9.9E-03	4.9E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-7.48	-8.33	-10.01	-1.84	0.64	0.0%	0.0%	0.0%	8.8E-32
2801	160332-89-8	N,N'-diisopropylethane-1,2-diaminium bis[2R,3Z,5R]-3-(2-hydroxyethylidene)-7-oxo-4-oxa-1-azabicyclo[3.2.0]hepta	543	87	9.9E-03	3.7E+03	3.0

2904	1035-69-4	Androsta-4,9(11)-diene-3,17-dione	284	151	2.3E-04	1.4E+01	4.7E+02	0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-8.35	-8.89	-10.70	-1.64	0.17	0.0%	0.0%	1.3E-38
2905	104372-31-8	(4aR,7S,8aR)-9,9-dimethyltetrahydro-4a,7-methanooxazirenо[3,2-i][2,1]benzothiazole 3,3-dioxide	229	121	1.4E-02	6.5E+03	4.5E+02	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+00	1.3E-01	4.6E+00	-8.40	-8.94	-10.72	-1.51	1.27	0.0%	0.0%	8.5E-40
2906	1638-86-4	diethyl phenylphosphonite	198	26	1.9E+00	1.7E+02	1.5E+02	0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-8.01	-8.75	-10.63	-1.74	0.19	0.0%	0.0%	2.8E-37
2907	4073-98-7	4,4'-methylenebis(2,6-xylidine)	254	163	2.0E-05	6.8E+00	2.3E+02	0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+00	1.3E-01	4.6E+00	-8.43	-8.80	-10.65	-2.10	1.63	0.0%	0.0%	1.3E-34
2908	3886-69-9	D-α-methylbenzylamine	121	0	7.2E+01	3.7E+03	3.1E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	9.1E+00	1.3E-01	4.6E+00	-9.77	-9.50	-10.76	-1.75	0.34	0.0%	0.0%	3.1E-38
2909	2627-86-3	L-α-methylbenzylamine	121	0	7.2E+01	3.7E+03	3.1E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	9.1E+00	1.3E-01	4.6E+00	-9.77	-9.50	-10.76	-1.73	0.21	0.0%	0.0%	2.1E-38
2910	27472-21-5	(3,4-diethoxyphenyl)acetonitrile	205	95	1.4E-02	1.6E+02	1.5E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.62	-8.40	-10.03	-3.13	0.32	0.0%	0.0%	3.3E-23
2911	7575-23-7	pentaerythritol tetrakis(3-mercaptopropionate)	489	198	6.4E-09	2.1E+01	3.9E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.1E+01	1.5E-01	5.4E+00	-9.06	-10.29	-11.77	-3.21	0.62	0.0%	0.0%	1.1E-34
2912	201214-53-1	methyl 4-acetamido-5-iodo-2-methoxybenzoate	349	177	6.1E-06	1.6E+02	1.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-7.49	-8.35	-10.01	-1.89	1.09	0.0%	0.0%	1.8E-31
2913	7319-16-6	615-927-1	72	-101	3.4E+04	2.1E+04	6.8E+00	0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+00	1.3E-01	4.7E+00	-8.36	-9.59	-11.35	-2.76	1.69	0.0%	0.0%	5.8E-35
2914	3071-32-7	1-phenylethyl hydroperoxide	138	21	7.1E+01	8.2E+03	5.0E+02	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+00	1.3E-01	4.6E+00	-9.17	-10.73	-12.59	-2.59	0.88	0.0%	0.0%	1.3E-31
2915	877179-04-9	3',4'-dichloro-5-fluorobiphenyl-2-amine	256	123	9.7E-04	1.7E+00	2.1E+04	3.0	3.5E-06	3.5E-07	3.5E-08	conf	conf	9.2E+00	1.3E-01	4.6E+00	-8.16	-8.72	-10.64	-3.28	0.32	0.0%	0.0%	3.6E-26
2916	1182822-31-4	5-Amino-2,4-di-tert-butylphenyl methyl carbonate	279	108	9.4E-04	1.3E+01	2.2E+04	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	9.1E+00	1.3E-01	4.5E+00	-8.64	-8.40	-10.03	-2.45	0.32	0.0%	0.0%	1.3E-27
2917	84713-17-7	2,2,4,(or 2,4,4)-trimethylhexanedinitrile	150	39	3.1E+00	2.0E+04	4.4E+02	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.61	-8.46	-10.07	-0.85	0.39	0.0%	0.0%	6.0E-40
2918	37750-29-1	609-474-9	236	125	7.6E-04	9.0E+00	2.5E+04	3.3	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+00	1.3E-01	4.6E+00	-8.41	-8.82	-10.67	-2.74	0.55	0.0%	0.0%	5.1E-30
2919	42872-29-7	3-(1-cyanoethyl)benzoyl chloride	194	82	4.6E-02	3.1E+02	2.6E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-9.16	-8.94	-10.70	-2.69	0.71	0.0%	0.0%	1.2E-30
2920	39811-17-1	5-phenyl-o-anisidine	199	110	2.5E-03	5.0E+01	8.3E+02	0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-8.21	-8.77	-10.64	-2.30	0.50	0.0%	0.0%	5.2E-33
2921	222408-90-4	606-964-4	346	208	4.5E-10	1.4E+02	5.4E+04	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.2E+00	1.3E-01	4.6E+00	-8.09	-8.92	-10.67	-2.75	0.64	0.0%	0.0%	5.4E-30
2922	81-83-4	naphthalene-1,8-dicarboximide	197	210	5.1E-08	2.0E+02	9.8E+01	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-7.34	-8.31	-9.97	-2.11	1.03	0.0%	0.0%	1.6E-29
2923	56914-82-0	3,4-Dichloro-1,2-thiazole-5-carbonyl chloride	186	88	1.1E-01	4.3E+05	4.6E-01	9.5	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+00	1.3E-01	4.6E+00	-9.51	-9.28	-10.80	-2.15	0.46	0.0%	0.0%	2.1E-35
2924	117-69-1	4-[(6-amino-1-hydroxy-3-sulpho-2-naphthyl)azo]-3-hydroxy-7-nitronaphthalene-1-sulphonic acid	534	350	3.4E-25	9.1E-06	5.0E+01	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+00	1.3E-01	4.6E+00	-8.04	-8.76	-10.60	-2.13	0.69	0.0%	0.0%	5.3E-24
2925	4137-56-8	609-920-2	358	186	2E-06	2.0E+02	1.3E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-7.78	-8.73	-10.63	-1.47	0.87	0.0%	0.0%	1.9E-39
2926	151213-15-9	3-Quinolinecarboxylic acid, 1-cyclopropyl-6,8-difluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-	389	321	5.3E-12	1.0E+02	1.2E+01	8.7	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-8.82	-8.82	-10.63	-3.09	0.64	0.0%	0.0%	2.4E-27
2927	1003859-14-1	Unknown	207	46	3.9E+00	9.6E+03	8.5E+00	5.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-8.00	-8.78	-10.65	-2.82	1.07	0.0%	0.0%	2.3E-29
2928	39255-32-8	ethyl 2-methylvalerate	144	-44	3.8E+02	1.4E+03	5.5E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.0E+01	1.4E-01	5.2E+00	-9.31	-10.18	-11.86	-2.27	0.63	0.0%	0.0%	5.0E-43
2929	25383-06-6	cis-propenylphosphonic acid	122	27	2.3E-02	1.4E+05	5.9E-01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-7.81	-8.73	-10.61	-0.32	1.29	0.0%	0.0%	3.3E-49
2930	698-29-3	4-amino-2-methylpyrimidine-5-carbonitrile	134	99	8.0E-02	4.6E+04	4.7E-01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-7.95	-8.72	-10.61	-1.79	0.97	0.0%	0.0%	1.1E-36
2931	23996-53-4	607-301-1	121	77	3E-02	4.7E+04	1.3E+00	0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-7.65	-8.69	-10.59	-2.09	1.28	0.0%	0.0%	2.2E-34
2932	2253-52-3	O,O-diisobutyl hydrogen dithiophosphate	242	-39	6.4E-01	1.6E+01	1.1E+04	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+00	1.3E-01	4.6E+00	-10.80	-10.56	-11.76	-4.21	1.71	0.0%	0.0%	2.0E-27
2933	58909-56-1	(6R-trans)-7-amino-8-oxo-3-[[(1,2,5,6-tetrahydro-2-methyl-5,6-dioxo-1,2,4-triazin-3-yl)thio]methyl]-5-thia-1-azabicy	371	339	2.0E-15	8.7E+04	1.1E-04	2.4	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-7.54	-8.69	-10.57	-3.39	2.86	0.0%	0.0%	5.1E-25
2934	101990-44-7	600-261-6	186	88	1.1E-01	4.3E+05	4.6E-01	9.5	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-7.73	-8.65	-10.58	-2.80	1.05	0.0%	0.0%	5.8E-29
2935	95-02-3	4-amino-2-methylpyrimidine-5-methylamine	138	101	1.0E-01	1.0E+06	6.0E-02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-7.74	-8.68	-10.59	-1.60	1.10	0.0%	0.0%	5.0E-38
2936	1154308-86-1	800-884-5	201	119	7.6E-05	8.5E+02	3.8E+01	-0.7	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.0E+01	1.4E-01	5.2E+00	-8.49	-9.48	-11.25	-1.42	0.54	0.0%	0.0%	4.2E-45
2937	96-98-0	3-nitro-p-toluic acid	181	118	4.5E-03	1.3E+03	1.7E+02	14.0	3.5E-06	3.5E-06	3.5E-07	conf	conf	1.1E+01	1.5E-01	5.4E+00	-9.28	-10.10	-11.81	-1.20	0.55	0.0%	0.0%	3.1E-52
2938	116-75-6	1,4-bis(mesitylamino)anthraquinone	475	280	2E-13	1.8E-06	7.4E+10	0.4	3.5E-06	1.1E-06	1.1E-06	conf	conf	6.2E+00	8.6E-02	3.2E+00	-8.32	-9.61	-11.02	-2.36	1.49	0.0%	0.0%	2.0E-35
2939	1739-84-0	1,2-dimethylimidazole	96	20	3.6E+01	3.7E+04	1.4E+01	8.2	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E+00	1.3E-01	4.6E+00	-9.20	-8.95	-10.65	-1.12	0.31	0.0%	0.0%	1.6E-42
2940	61636-08-6	2-ethoxy-6-hydroxypyrimidin-4(1H)-one	156	176	5.5E-08	1.6E+03	6.9E-02	4.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.1E+01	1.5E-01	5.4E+00	-8.41	-9.85	-11.75	-1.43	0.64	0.0%	0.0%	1.7E-49
2941	4637-24-5	1,1-dimethoxytrimethylamine	119	-58	3.7E+03	4.9E+05	3.1E-01	4.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.0E+01	1.4E-01	5.2E+00	-8.90	-9.38	-11.27	1.42	0.67	0.0%	0.0%	1.1E-41
2942	591-22-0	3,5-dimethylpyridine	107	-8	1.9E+02	2.3E+05	7.6E+01	6.2	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.0E+00	1.3E-01	4.6E+00	-9.01	-8.88	-10.67	-1.81	0.62	0.0%	0.0%	5.8E-37
2943	62899-75-6	cyclohexylethylcarbamoyl chloride	190	58	5.4E-01	3.2E+03	1.1E+02	-0.4	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.0E+01	1.4E-01	5.1E+00	-8.74	-9.54	-11.32	-2.31	0.86	0.0%	0.0%	3.7E-38
2944	35786-94-8	4,5-dimethyl-2-(propan-2-yl)phenol	164	53	6.3E-01	7.2E+02	1.1E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-10.07	-9.88	-11.42	-2.73	0.30	0.0%	0.0%	1.0E-35
2945	82543-09-7	3H-Cyclopropa[15,16]androsta-5,15-dien-17-one, 3-(2,2-dimethyl-1-oxopropoxy)-15,16-dihydro-7-hydroxy-, (3β,7β,4	401	197	7E-09	9.2E-01	1.1E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-8.75	-9.79	-11.33	-2.37	0.23	0.0%	0.0%	5.8E-38
2946	927-62-8	N,N-dimethylbutylamine	101	-71	6.2E+03	2.9E+04	3.2E+01	10.0	3.5E-06	6.2E-07	1.1E-06	conf	conf	9.2E+00	1.3E-01	4.7E+00	-10.82	-10.56	-11.95	-1.52	0.70	0.0%	0.0%	2.0E-50
2947	13360-63-9	butyl(ethyl)amine	101	-54	3.6E+03	7.5E+04	6.2E+01	10.9	3.5E-06	3.5E-06	3.5E-07	conf	conf	1.0E+01	1.4E-01	5.3E+00	-10.86	-10.72	-11.98	-1.79	0.85	0.0%	0.0%	2.5E-48
2948	99305-42-7	619-422-7	88	-88	1E+04	2.2E+04	3.5E+01	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-8.28	-9.43	-11.34	-1.04	0.36	0.0%	0.0%	2.6E-49
2949	82544-13-6	5,6 beta-Epoxy-7 beta-hydroxy-15 beta,16 beta-methylene-3 beta-pivaloyloxy-5 beta androstan-17-one	417	200	2.4E-09	3.4E+00	9.1E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-8.74	-9.78	-11.32	-2.13	0.42	0.0%	0.0%	1.1E-39
2950	82543-14-4	(25,4aR,4bS,6aS,7aS,8aS,8bS,8cR,10aR)-10a-Hydroxy-4a,6a-dimethyl-7-oxo-1,2,3,4,4a,4b,5,6,6a,7,7a,8,8a,8b,8c,10a-h	401	192	8.9E-09	5.4E+00	8.9E+03	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	9.1E+00	1.3E-01	4.5E+00	-7.35	-8.30	-9.96	-2.36	0.24	0.0%	0.0%	9.9E-28
2951	169280-10-8	ethyl 2-(4-cyclopropancarbonylphenyl)-2-methylpropanoate	260	107	4.4E-03	2.1E+00	8.3E+03	0	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.2E+00	1.3E-01	4.7E+00	-8.88	-9.46	-11.35	-2.41	0.59	0.0%	0.0%	1.3E-37
2952	641571-10-0	4-methyl-N-[4-methyl-1H-benzimidazol-1-yl]-5-(trifluoromethyl)phenyl]-3-[[4-[pyridin-3-yl]pyrimidin-2-yl]amino]ben	530	131	2.7E-16	1.5E-05	1.0E+05	5.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-9.72	-9.77	-11.32	-3.71	0.17	0.0%	0.0%	7.5E-28
2953	55184-72-0	sodium 1,4-diisotridecyl sulphonatosuccinate	585	87	9.9E-03	4.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.7E+00	1.1E-01	3.9E+00	-8.12	-8.44	-10.10	-2.01	0.72	0.0%	0.0%	3.4E-31
2954	17928-28-8	1,1,1,3,5,5,5-heptamethyl-3-[(trimethylsilyl)oxy]trisiloxane	311	-36	1.0E+02	2.4E-02	1.4E+08	14.0	3.5E-06	3.5E-09	3.5E-09	conf	conf	5.9E+00	8.3E-02	2.9E+00	-10.75	-10.48	-12.19	-4.62	0.41	0.0%	0.0%	1.3E-27
2955	81-81-2	warfarin	308	197	1.6E-09	4.0E+01	1.1E+02	4.9	3.5E-06	4.5E-07	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-8.17	-8.97	-10.79	-1.55	1.19	0.0%	0.0%	4.1E-40
2956	1453-58-3	3-methylpyrazole	82	18	2.8E+01	2.6E+04	4.1E+00	3.4	3.5E-06	3.5E-07	1.1E-07	conf	conf	8.9E+00	1.2E-01	4.5E+00	-7.64	-8.77	-10.64	-0.48	0.36	0.0%	0.0%	4.3E-48
2957	2084-69-7	1,2,3,4-tetrahydro-1,1,2,4,4,7-hexamethylnaphthalene	216	65	4.0E-01	7.0E-01	4.6E+06	0	3.5E-06	3.5E-07	1.1E-07	conf	conf	6.4E+00	8.9E-02	3.3E+00	-8.49	-9.06	-10.90	-3.78	0.19	0.0%	0.0%	1.3E-24
2958	84852-23-3	dipotassium hydrogen 7-aminonaphthalene-1,3,6-trisulphonate	460	87	9.9E-03	3.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.7E+00	1.1E-01	3.9E+00	-8.13	-8.44	-10.10	-1.84	0.64	0.0%	0.0%	1.7E-32
2959	219715-34-1	2-Methoxy-4-(trifluoromethyl)pyridine	177	8	1.7E+00	9.2E-01	1.1E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	8.2E+00	1.1E-01	4.1E+00	-10.66	-10.38	-11.99	-2.12	1.54	0.0%	0.0%	1.7E-45
2960	60857-05-8	tetrahydro-4-methylene-2-(2-methyl-1-propenyl)-2H-pyran	152	-21	8.4E+01	1.2E+03	3.7E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-10.86	-10.63	-11.79	-2.36	0.86	0.0%	0.0%	1.2E-41
2961	67584-55-8	2-[methyl[(nonafluorobutyl)sulphonyl]amino]ethyl acrylate	411	86	9.2E-02	9.4E+00	1.5E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.2E+00	1.3E-01	4.7E+00	-11.00	-10.82	-12.12	-2.36	0.24	0.0%	0.0%	1.7E-44
2962	68133-60-8	1-benzyl-3-carboxylatopyridinium sodium chloride	272	87	9E-03	1.9E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.6E+00	1.1E-01	3.8E+00	-8.14	-8.45	-10.10	-1.84	0.64	0.0%	0.0%	1.7E-32
2963	50-03-3	hydrocortisone 21-acetate	405	217	2.9E-11	1.2E+02	2.3E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.0E+01	1.4E-01	5.2E+00	-9.04	-10.28	-11.78	-1.68	0.67	0.0%	0.0%	1.5E-47
2964	88374-05-4	618-153-2	232	79	1.2E-01	3.5E+01	4.6E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-10.21	-9.99	-11.46	-2.80	0.48	0.0%	0.0%	2.2E-35
2965	51920-12-8	N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2-methoxy-5-methyl-4-[(methylamino)sulphonyl]phenyl]	583	350	2.0E-21	1.5E-02	9.3E+05	-1.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+00	1.3E-01	5.0E+00	-8.75	-9.47	-11.27	-1.83	1.05	0.0%	0.0%	1.1E-41
2966	2550-02-9	triethoxypropylsilane	206	0	3E+01	4.3E+02	6.0E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	8.4E+00	1.0E-01	4.3E+00	-10.50	-10.25	-11.64	-0.27	0.84	0.0%	0.0%	1.3E-59
2967	1320-51-0	(hydroxyethyl)urea	104	57	2.0E-01	1.1E+05	7.2E-03	-0.7	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.0E+01	1.4E-01	5.2E+00	-8.43	-9.87	-11.78	-0.91	1.71	0.0%	0.0%	1.1E-54
2968	2901-13-5	608-307-7	192	28	3.0E+00	1.1E+02	2.8E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-10.62	-10.41	-11.59	-2.37	0.65	0.0%	0.0%	6.8E-40
2969	1852-04-6	undecanedioic acid	216	135	4.2E-04	1.1E+03	4.8E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.6E+00	1.3E-01	4.8E+00	-7.57	-8.46	-10.01	-2.38	0.55	0.0%	0.0%	5.9E-28
2970	554-52-9	4-(2-aminoethyl)-2-methoxyphenol	167	86	3.6E-02	3.8E+03	4.8E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.0E+01	1.4E-01	5.2E+00	-9.44	-10.00	-11.82	-2.38	0.58	0.0%	0.0%	7.9E-42
2971	1160221-25-1	tert-butyl 3-[6-((([1-(2,2-difluoro-1,3-benzodioxol-5-yl)cyclopropyl]carbonyl)amino)-3-methylpyridin-2-yl]benzoate	509	267	8.0E-12	3.1E-03	2.4E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.0E+00	1.3E-01	4.4E+00	-9.61	-10.18	-10.44	-3.85	0.86	0.0%	0.0%	2.2E-21
2972	181997-71-7	605-954-7	215	78	7.1E-02	5.6E+01	3.0E+03	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.5E+00	-9.02	-8.75	-10.23	-2.33	0.25	0.0%	0.0%	7.0E-30
2973	166524-68-1	5-ethoxy-7-fluoro[1,2,4]triazolo[4,3-c]pyrimidine-3(2H)-thione	214	156	1.6E-04	4.1E+02	2.2E+01	-1.1	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.6E+00	1.3E-01	4.9E+00	-8.26	-9.30	-11.26	-3.13	0.64	0.0%	0.0%	1.8E-31
2974	10258-54-5	2-methoxyethyl cyanoacetate	129	6	2.7E+01	4.3E+04	4.3E-02	0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.0E+01	1.4E-01	5.2E+00	-8.60	-9.96	-11.82	-0.93	1.36	0.0%	0.0%	7.5E-55
2975	103953-71-5	1-[(2E)-3,7-dimethylocta-2,6-dien-1-yl]pyrrolidine-2,5-dione	235	161	1.6E-05	2.7E+02	2.9E+03	-0.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-8.68	-9.39	-11.28	-2.45	0.84	0.0%	0.0%	9.2E-37
2976	139007-06-0	604-106-3	219	24	4.3E-01	3.4E+01	1.5E+05	5.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E+00	1.3E-01	4.7E+00	-9.99	-9.79	-11.45	-1.38	0.33	0.0%	0.0%	3.3E-47
2977	14402-88-1	disodium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4-)-N,N',O,O',ON,ON']magnesate(2-)	359	87	9.9E-03	2.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.5E+00	1.0E-01	3.7E+00	-8.14	-8.46	-10.11	-0.54	0.73	0.0%	0.0%	6.9E-43
2978	2580-78-1	2-(3-(4-amino-9,10-dihydro-3-sulpho-9,10-dioxoanthracen-4-yl)aminobenzenesulphonyl)vinyl) disodium sulphate	627	87	9.9E-03	4.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.5E+00	1.0E-01	3.7E+00	-8.14	-8.46	-10.12	-0.83	0.71	0.0%	0.0%	1.7E-40
2979	713-95-1	dodecan-5-olide	198	19	1.3E-01	3.8E+01	3.5E+03	0	3.5E-06	3.5E-07	1.1E-07	conf	conf	8.2E+00	1.1E-01	4.2E+00	-8.64	-8.83	-10.69	-1.55	0.77	0.0%	0.0%	2.6E-39
2980	59776-88-4	methyl 2-oxopyrrolidin-1-acetate	157	70	3.1E-01	1.3E+05	8.5E-01	-1.8	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.0E+01	1.4E-01	5.2E+00	-8.56	-9.96	-11.78	-2.18	2.04	0.0%	0.0%	4.5E-43
2981	565-61-7	3-methylpentan-2-one	100	-67	2.7E+03	9.6E+03	1.4E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+00	1.3E-01	4.7E+00	-11.00	-10.75	-12.17	-1.34	1.05	0.0%	0.0%	2.6E-54
2982	6920-22-5	DL-hexane-1,2-diol	118	2	2.4E+00	2.3E+04	4.9E+00	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	1.0E+01	1.4E-01	5.1E+00	-10.27	-10.23	-11.83	-1.25	1.23	0.0%	0.0%	7.4E-52
2983	471-01-2	3,5,5-trimethylcyclohex-3-en-1-one	138	17	6.4E-01	6.1E+02	2.1E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E+00	1.3E-01	4.7E+00	-8.78	-9.60	-11.35	-0.90	0.20	0.0%	0.0%	9.7E-51
2984	10595-49-0	methyl trimethyl-3-[(1-oxododecyl)amino]propylammonium sulphate	411	87	9.9E-03	2.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.4E+00	1.0E-01	3.7E+00	-8.15	-8.46	-10.12	-1.67	2.16	0.0%	0.0%	7.6E-34
2985	42872-30-0	2-(m-benzoylphenyl)

3087	178671-69-7	605-830-2	404	234	5.3E-10	2.7E+03	2.9E-03	0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	9.2E+00	1.3E-01	4.7E+00	-8.42	-9.88	-11.81	-1.85	0.64	0.0%	0.0%	3.1E-46
3088	2050-46-6	1,2-diethoxybenzene	166	17	1.1E+01	9.8E+02	4.2E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	8.6E+00	1.2E-01	4.4E+00	-10.39	-10.19	-11.47	-1.64	0.31	0.0%	0.0%	3.9E-45
3089	93981-14-7	6-[(p-tosyl)amino]hexanoic acid, compound with 2,2',2''-nitrilotriethanol (1:1)	435	87	9.9E-03	3.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	6.8E+00	9.5E-02	3.4E+00	-8.18	-8.50	-10.16	-0.42	0.79	0.0%	0.0%	3.0E-44
3090	5413-60-5	3a,4,5,6,7,7a-hmahydro-4,7-methanoinden-6-yl acetate	192	35	2.8E+00	1.1E+03	7.1E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	8.9E+00	1.2E-01	4.4E+00	-10.72	-10.54	-11.96	-1.75	0.20	0.0%	0.0%	1.7E-44
3091	68223-93-8	diammonium 2,2'-dithiodiacetate	216	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	6.8E+00	9.4E-02	3.4E+00	-8.20	-8.50	-10.15	0.04	1.35	0.0%	0.0%	2.2E-48
3092	19430-93-4	3,3,4,4,5,5,6,6,6-nonafluorohexene	246	-106	1.8E+05	4.1E+00	2.5E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	6.6E+00	9.3E-02	3.3E+00	-11.93	-11.63	-14.92	-2.35	0.14	0.0%	0.0%	2.2E-72
3093	23202-81-5	methyl 5-deoxy 2,3-O-isopropylidene-β-D-ribofuranoside	188	32	1.7E+01	1.2E+04	3.0E+00	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	conf	7.8E+00	1.1E-01	4.0E+00	-9.43	-9.20	-10.81	-0.12	0.45	0.0%	0.0%	6.0E-53
3094	83929-47-9	methyl 4-[[(2,5-dichlorophenyl)amino]carbonyl]-2-nitrobenzoate	369	222	8.3E-09	1.1E-01	1.2E+03	12.7	3.5E-06	3.5E-06	3.5E-07	conf	conf	conf	8.7E+00	1.2E-01	4.5E+00	-9.21	-10.34	-11.91	-2.93	0.50	0.0%	0.0%	5.4E-38
3095	630113-05-2	N-(3-[[(dimethyl(3-[(2-methylacryloyl)amino]propyl)ammonio)acetyl]amino)propyl)-2-hydroxy-N,N,N-[◆,N◆,N◆,N◆ pe	537	87	9.9E-03	3.7E+03	3.0E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	6.7E+00	9.3E-02	3.3E+00	-8.19	-8.51	-10.17	-1.16	0.50	0.0%	0.0%	3.4E-38
3096	383412-05-3	1-methylhexyl chloroacetate	193	-2	9.9E+00	1.2E+02	3.2E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	8.3E+00	1.1E-01	4.2E+00	-11.33	-11.12	-12.33	-2.23	0.86	0.0%	0.0%	1.7E-47
3097	70833-40-8	O-(2-ethylhexyl) O,O-tert-pentyl peroxycarbonate	260	6	2.6E-01	1.3E+02	1.1E+05	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	8.3E+00	9.2E-02	3.3E+00	-11.28	-11.04	-12.32	-3.25	0.05	0.0%	0.0%	1.1E-38
3098	3775-90-4	2-tert-butylaminoethyl methacrylate	185	13	1.7E+01	1.9E+04	1.3E+02	9.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	8.8E+00	1.2E-01	4.5E+00	-10.61	-10.43	-11.94	-2.21	0.60	0.0%	0.0%	3.1E-44
3099	15206-55-0	methyl benzoylformate	164	35	2.7E+00	5.0E+03	3.1E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	8.8E+00	1.2E-01	4.5E+00	-10.49	-10.31	-11.91	-1.61	0.94	0.0%	0.0%	2.7E-49
3100	10563-29-8	N'-[3-aminopropyl]-N,N-dimethylpropane-1,3-diamine	159	40	5.8E+00	1.0E+06	3.4E-01	10.4	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	8.8E+00	1.2E-01	4.5E+00	-9.22	-9.85	-11.87	-1.41	0.61	0.0%	0.0%	7.4E-51
3101	22174-70-5	3,3'-[methylbis(oxymethylene)]bisheptane	272	33	1.1E-01	3.5E+00	3.4E+06	0	3.5E-06	3.5E-07	1.1E-07	conf	conf	conf	7.6E+00	2.8E-01	4.6E+00	-9.10	-10.93	-3.95	0.35	0.0%	0.0%	0.0%	1.1E-23
3102	542-08-5	isopropyl acetoacetate	144	-19	9.6E+01	1.7E+04	1.6E+00	10.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	8.6E+00	1.2E-01	4.4E+00	-10.48	-10.36	-11.89	-1.40	1.03	0.0%	0.0%	5.3E-51
3103	3148-73-0	N,N'-diacetylhydrazine	116	126	2.8E-03	4.8E+05	2.6E-02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	8.2E+00	1.1E-01	4.2E+00	-8.22	-9.29	-11.32	0.06	0.98	0.0%	0.0%	8.3E-60
3104	62037-80-3	Ammonium 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoate	347	87	9.9E-03	2.4E+03	3.0E+02	14.0	3.5E-06	3.5E-07	6.6E-09	conf	conf	conf	6.8E+00	9.4E-02	3.4E+00	-8.53	-10.18	-11.15	0.53	0.0%	0.0%	0.0%	2.3E-38
3105	83-73-8	diiodohydroxyquinoline	397	154	3.3E-06	5.4E+00	1.0E+04	7.7	3.5E-06	3.5E-07	1.1E-07	conf	conf	conf	7.3E+00	1.0E-01	3.7E+00	-8.57	-9.22	-10.88	-1.90	0.15	0.0%	0.0%	5.5E-38
3106	55514-22-2	3,3'-(1,4-Phenylene)bis(5,6-diphenyl-1,2,4-triazine)	541	350	9.4E-19	1.2E-06	2.6E+06	14.0	3.5E-06	3.5E-07	3.5E-08	conf	conf	conf	5.4E+00	7.6E-02	2.7E+00	-9.11	-9.92	-11.02	-6.76	1.61	0.0%	0.0%	3.9E-37
3107	7328-22-5	2-(2-butoxyethoxy)ethyl methacrylate	230	35	7.1E-01	1.3E+03	1.6E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	8.1E+00	1.1E-01	4.1E+00	-10.05	-9.82	-11.47	-1.25	0.27	0.0%	0.0%	1.2E-48
3108	24304-50-5	N,N'-(2,5-dimethyl-1,4-phenylene)bis[3-oxobutyramide]	304	231	2.1E-09	1.4E+03	9.8E-01	0.9	3.5E-06	3.5E-07	3.5E-07	conf	conf	conf	7.3E+00	1.0E-01	3.7E+00	-7.74	-8.87	-10.71	-1.65	1.12	0.0%	0.0%	1.3E-38
3109	1962-75-0	dibutyl terephthalate	278	6	3.4E-02	8.2E+00	4.1E+04	14.0	3.5E-06	8.8E-07	3.5E-07	conf	conf	conf	6.9E+00	9.6E-02	3.5E+00	-10.32	-10.13	-11.53	-3.70	0.52	0.0%	0.0%	2.6E-29
3110	58-55-9	theophylline	180	193	7.4E-08	9.3E+04	4.1E-01	8.7	3.5E-06	7.0E-09	3.5E-07	conf	conf	conf	5.0E+00	6.9E-02	2.4E+00	-7.55	-8.33	-9.35	-0.83	0.37	0.0%	0.0%	2.3E-34
3111	91-21-4	1,2,3,4-tetrahydroisoquinoline	133	42	5.2E+00	7.1E+02	5.3E+01	8.9	3.5E-06	3.5E-07	1.1E-06	conf	conf	conf	7.2E+00	1.0E-01	3.6E+00	-9.96	-9.73	-11.03	-2.20	0.75	0.0%	0.0%	3.0E-37
3112	59673-82-4	methyl 2-amino-4-[[(2,5-dichlorophenyl)amino]carbonyl]benzoate	339	216	2.1E-08	2.2E+00	1.8E+04	1.6	3.5E-06	1.1E-06	1.1E-07	conf	conf	conf	8.0E+00	1.1E-01	4.1E+00	-8.72	-9.28	-11.30	-2.38	0.11	0.0%	0.0%	1.5E-37
3113	31778-10-6	butyl 2-[[3-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-hydroxy-1-naphthyl]azo]benzoate	524	350	2.0E-19	1.7E-03	6.5E+07	-1.7	3.5E-06	3.5E-07	3.5E-08	conf	conf	conf	7.2E+00	1.0E-01	3.6E+00	-8.47	-8.82	-10.69	-1.83	1.05	0.0%	0.0%	5.4E-37
3114	23410-40-4	N-[3-(dimethoxymethylsilyl)-2-methylpropyl]ethylenediamine	220	56	1.1E+00	4.0E+04	1.0E+00	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	8.4E+00	1.2E-01	4.2E+00	-8.42	-10.06	-0.94	0.76	0.0%	0.0%	0.0%	1.4E-39
3115	10411-92-4	cis-4-tert-butylcyclohexyl acetate	198	11	9.1E+00	4.3E-01	2.6E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	6.2E+00	8.6E-02	3.1E+00	-11.94	-11.66	-14.40	-2.00	0.29	0.0%	0.0%	1.6E-70
3116	41611-76-1	1,4-bis[(2-ethyl-6-methylphenyl)amino]anthraquinone	475	280	9.8E-13	5.4E-06	5.8E+10	-0.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	4.9E+00	6.8E-02	2.5E+00	-8.46	-9.67	-11.18	-5.72	0.62	0.0%	0.0%	3.0E-15
3117	107-87-9	pentan-2-one	86	-68	5.3E+03	2.3E+04	5.6E+00	14.0	3.5E-06	9.4E-07	1.1E-06	conf	conf	conf	7.6E+00	1.1E-01	3.9E+00	-10.97	-10.78	-12.08	-0.19	0.60	0.0%	0.0%	5.1E-65
3118	6992-11-6	4-[(2,5-dichlorophenyl)azo]-N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxynaphthalene-2-carboxamide	492	332	1.8E-18	1.2E-03	6.2E+07	-1.7	3.5E-06	3.5E-07	3.5E-08	conf	conf	conf	7.1E+00	9.8E-02	3.6E+00	-8.48	-8.83	-10.70	-1.83	1.05	0.0%	0.0%	4.8E-37
3119	561-41-1	4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol	376	209	5.2E-10	4.9E-01	2.3E+04	6.3	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	7.3E+00	1.0E-01	3.7E+00	-8.88	-9.89	-11.42	-1.74	0.27	0.0%	0.0%	8.8E-44
3120	166524-64-7	605-444-4	158	82	9.0E-01	7.5E+04	8.3E-01	0.8	3.5E-06	3.5E-07	1.1E-07	conf	conf	conf	7.0E+00	9.7E-02	3.6E+00	-7.82	-8.82	-10.72	-3.92	3.13	0.0%	0.0%	1.3E-22
3121	622-29-7	benzylidene(methyl)amine	119	-39	1.0E+02	1.4E+03	5.0E+01	6.1	3.5E-06	3.5E-07	1.1E-06	conf	conf	conf	7.0E+00	9.7E-02	3.5E+00	-9.87	-9.61	-10.86	-2.28	0.73	0.0%	0.0%	7.1E-35
3122	103-45-7	phenethyl acetate	164	11	9.1E+00	1.3E+03	3.7E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	7.6E+00	1.1E-01	3.9E+00	-10.33	-10.12	-11.48	-1.71	0.28	0.0%	0.0%	1.4E-44
3123	106-58-1	1,4-dimethylpiperazine	114	5	1.3E+03	9.2E+05	4.2E-01	8.1	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	8.1E+00	1.1E-01	4.2E+00	-10.28	-10.15	-11.87	-0.72	0.39	0.0%	0.0%	2.3E-57
3124	35265-04-4	2-[(1-methylpropoxy)amino]ethanol	117	-11	2.3E+01	4.3E+05	1.8E+00	10.1	3.5E-06	3.5E-06	3.5E-06	conf	conf	conf	8.1E+00	1.1E-01	4.2E+00	-10.17	-10.25	-11.92	-1.55	0.77	0.0%	0.0%	7.2E-50
3125	120-46-7	1,3-diphenylpropane-1,3-dione	224	107	6.8E-03	1.3E+02	1.5E+02	8.3	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	7.6E+00	1.1E-01	3.9E+00	-9.75	-9.71	-11.45	-2.21	0.32	0.0%	0.0%	5.2E-40
3126	17526-94-2	N,N''-(4-methyl-m-phenylene)bis[N',N'-dimethylurea]	264	193	7.1E-07	2.6E+03	5.9E+00	-0.1	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	7.7E+00	1.1E-01	3.9E+00	-8.17	-9.35	-11.33	-2.14	2.17	0.0%	0.0%	1.0E-39
3127	23779-32-0	[3-(trietho xysilyl)propyl]urea	264	130	1.3E-03	3.7E+03	7.2E-01	-0.1	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	7.7E+00	1.1E-01	3.9E+00	-8.29	-9.55	-11.39	-0.83	0.58	0.0%	0.0%	1.1E-51
3128	221615-75-4	1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone	289	176	6.5E-06	2.0E+02	2.0E+01	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	conf	7.6E+00	1.1E-01	3.9E+00	-8.24	-9.30	-11.38	-1.33	0.73	0.0%	0.0%	5.2E-47
3129	138-24-9	N,N,N-trimethylaniliniun chloride	187	87	9.9E-03	1.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	5.9E+00	8.3E-02	3.0E+00	-8.26	-8.56	-10.21	-1.84	0.64	0.0%	0.0%	2.8E-33
3130	17527-29-6	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl acrylate	418	-8	2.9E+02	3.3E-01	5.9E+05	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	5.3E+00	7.4E-02	2.6E+00	-12.02	-11.76	-15.01	-3.35	1.19	0.0%	0.0%	1.4E-62
3131	68259-05-2	bis(2-chloroethyl) 3,3'-[(2,5-dimethyl-p-phenylene)bis(iminocarbonyl(2-hydroxy-1,3-naphthylene)azo)]di-p-toluate	926	350	1.1E-34	6.2E-12	6.5E+14	9.2	3.5E-06	3.5E-07	3.5E-08	conf	conf	conf	4.5E+00	6.3E-02	2.2E+00	-14.21	-14.21	-6.48	3.08	0.0%	0.0%	0.0%	3.5E-70
3132	5895-82-9	2,2,5,5-tetramethyl-1,4,2,5-dioxadisilinane	176	5	1.1E+03	2.3E+03	1.8E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	4.5E+00	6.4E-02	2.2E+00	-10.96	-10.45	-12.73	-2.18	0.64	0.0%	0.0%	1.2E-51
3133	97-61-0	2-methylvaleric acid	116	15	5.7E+01	2.9E+04	9.5E+01	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	7.3E+00	1.0E-01	3.7E+00	-9.14	-8.83	-10.31	-1.34	0.14	0.0%	0.0%	7.2E-38
3134	166524-74-9	605-446-5	400	222	8.4E-09	7.9E-02	3.2E+02	1.5	3.5E-06	3.5E-07	1.1E-07	conf	conf	conf	6.7E+00	9.3E-02	3.4E+00	-8.19	-8.88	-10.77	-3.03	0.44	0.0%	0.0%	1.0E-28
3135	50675-18-8	Tetrahydropyran-4-carboxaldehyde	114	-27	2.3E+01	2.8E+05	2.9E+00	14.0	3.5E-06	1.1E-06	3.5E-06	conf	conf	conf	7.5E+00	1.0E-01	3.8E+00	-9.53	-11.36	-1.23	0.42	0.0%	0.0%	0.0%	8.4E-48
3136	515-84-4	ethyl trichloroacetate	191	-11	2.3E+02	1.2E+03	1.7E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	7.5E+00	1.0E-01	3.8E+00	-11.46	-11.25	-12.71	-1.10	0.28	0.0%	0.0%	4.7E-62
3137	76811-98-8	616-390-6	500	339	9.4E-19	3.2E-02	3.9E+02	4.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	7.4E+00	1.0E-01	3.8E+00	-8.62	-9.47	-11.37	-3.84	1.13	0.0%	0.0%	3.1E-27
3138	41272-40-6	(4-[α-[4-dimethylamino)phenyl]benzylidene]cyclohexa-2,5-dien-1-ylidene)dimethylammonium acetate	389	87	9.9E-03	2.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	5.8E+00	8.1E-02	2.9E+00	-8.25	-8.57	-10.23	-2.81	0.66	0.0%	0.0%	1.5E-26
3139	137433-01-3	604-018-5	584	87	9.9E-03	4.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	5.8E+00	8.0E-02	2.9E+00	-8.25	-8.57	-10.23	-1.84	0.64	0.0%	0.0%	2.0E-33
3140	6284-40-8	meglumine	195	129	1.8E-06	1.0E+06	7.1E-04	14.0	3.5E-06	3.4E-07	3.5E-06	conf	conf	conf	6.6E+00	9.2E-02	3.4E+00	-8.00	-8.98	-10.76	0.17	0.65	0.0%	0.0%	2.5E-55
3141	624-54-4	pentyl propionate	144	-33	2.2E+02	9.4E+02	6.8E+02	0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	7.4E+00	1.0E-01	3.8E+00	-9.29	-10.32	-12.00	-1.32	0.46	0.0%	0.0%	7.3E-53
3142	32454-35-6	2-(4-bromophenyl)-2-methylpropanoic acid	243	103	1.5E-02	1.1E+02	1.5E+03	4.2	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	7.3E+00	1.0E-01	3.8E+00	-8.58	-9.58	-11.46	-1.77	0.13	0.0%	0.0%	7.2E-44
3143	85-73-4	phthalylsulfathiazole	403	287	3.2E-13	3.4E+01	3.8E+02	3.6	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	7.3E+00	1.0E-01	3.8E+00	-8.78	-9.66	-11.40	-1.35	0.57	0.0%	0.0%	5.1E-47
3144	826-55-1	2-phenylisobutyric acid	164	74	2.2E-01	4.2E+02	2.0E+02	4.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	7.3E+00	1.0E-01	3.8E+00	-8.69	-9.55	-11.46	-1.32	0.24	0.0%	0.0%	7.3E-48
3145	88-45-9	2,5-diaminobenzenesulphonic acid	188	161	6.6E-07	1.5E+04	2.8E-04	5.7	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	7.3E+00	1.0E-01	3.8E+00	-8.29	-9.39	-11.36	-1.12	0.76	0.0%	0.0%	1.1E-48
3146	7300-34-7	3,3'-[butane-1,4-diylbis(oxy)]bispropanamine	204	87	7.2E-02	6.2E+05	6.3E-01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	conf	7.3E+00	1.0E-01	3.7E+00	-7.62	-8.45	-10.11	-0.73	0.64	0.0%	0.0%	3.1E-41
3147	302-23-8	hydroxyprogesterone acetate	373	184	2.6E-06	2.3E+01	4.7E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	conf	6.2E+00	8.7E-02	3.2E+00	-8.50	-9.24	-10.92	-2.25	0.59	0.0%	0.0%	1.6E-35
3148	89-48-5	menthyl acetate	198	1	1.2E+01	1.6E+02	2.5E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	6.6E+00	9.2E-02	3.4E+00	-11.45	-11.25	-12.43	-2.18	0.64	0.0%	0.0%	8.0E-49
3149	98730-04-2	2,2-Dichloro-1-(3-methyl-2,3-dihydro-4H-1,4-benzoxazin-4-yl)ethanone	260	118	1.6E-03	2.1E+02	2.4E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	conf	6.4E+00	8.9E-02	3.3E+00	-8.97	-9.17	-10.90	-2.17	0.45	0.0%	0.0%	2.5E-36
3150	2425-85-6	1-(4-methyl-2-nitrophenylazo)-2-naphthol	307	200	3.5E-08	5.4E+00	2.8E+06	8.6	3.5E-06	3.5E-06	1.1E-07	conf	conf	conf	5.2E+00	7.2E-02	2.6E+00	-10.34	-10.84	-12.00	-3.05	0.91	0.0%	0.0%	1.0E-37
3151	22288-43-3	1,1,3,3-tetramethylbutyl 2-ethylperoxyhexanoate	272	53	2.7E-01	4.2E-01	1.4E+06	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	conf	4.6E+00	6.4E-02	2.2E+00	-11.42	-11.20	-12.68	-3.61	0.18	0.0%	0.0%	9.8E-39
3152	776-04-5	(2-trifluoromethylbenzenesulfonyl chloride	245	72	2.8E-01	7.6E+01	7.9E+03	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	conf	5.9E+00	8.3E-02	3.0E+00	-9.94	-9.70	-11.10	-1.61	0.42	0.0%	0.0%	4.1E-42
3153	3681-71-8	(2)-hex-3-enyl acetate	142	-33	1.5E+02	6.9E+02	4.1E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	7.0E+00	9.7E-02	3.6E+00	-11.50	-11.29	-12.63	-1.45	0.33	0.0%	0.0%	1.1E-57
3154	86604-78-6	4-methoxy-3,5-dimethylpyridine-2-methanol	167	74	1.6E-02	1.9E+04	1.1E+01	3.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	7.0E+00	9.7E-02	3.6E+00	-8.45	-9.47	-11.43	-1.52	0.86	0.0%	0.0%	8.6E-46
3155	77-83-8	ethyl 2,3-epoxy-3-phenylbutyrate	206	67	4.2E-01	6.6E+02	1.0E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	6.7E+00	9.4E-02	3.4E+00	-10.12	-9.90	-11.54	-1.65	0.52	0.0%	0.0%	1.1E-45
3156	2495-37-6	benzyl methacrylate	176	12	5.5E+00	2.5E+02	5.0E+02	0	3.5E-06	6.2E-07	3.5E-07	conf	conf	conf	6.4E+00	8.9E-02	3.3E+00	-8.73	-9.31	-11.17	-2.45	0.29	0.0%	0.0%	5.6E-36
3157	59587-44-9	2-ethylhexyl nonanoate	270	44	7.2E-02	1.4E-01	1.5E+07	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	4.6E+00	6.4E-02	2.4E+00	-8.98	-9.92	-11.73	-4.03	0.43	0.0%	0.0%	2.0E-28
3158	5661-03-0	octahydrocyclopenta[c]pyrrole	111	7	2.3E+02	1.5E+05	3.7E+01	10.9	3.5E-06	1.1E-06	1.1E-07	conf	conf	conf	6.9E+00	9.6E-02	3.5E+00	-9.88	-9.68	-11.41	-2.01	0.81	0.0%	0.0%	2.2E-41
3159	6969-71-7	1,2,4-triazolo[4,3-a]pyridin-3(2H)-one	135	122	7E-03	4.1E+04	2.8E+00	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	6.8E+00	9.5E-02	3.4E+00	-7.66	-8.50	-10.15	-4.07	3.06	0.0%	0.0%	1.9E-18
3160	156366-26-6	619-692-6	432	227	4.3E-09	4.0E+00	1.1E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	6.4E+00	8.9E-02	3.3E+00	-8.90	-9.95	-11.48	-2.96	0.51	0.0%	0.0%	2.2E-34
3161	14246-53-8	N-(1-oxooctyl)glycine	201	150	1.3E-04	1.8E+02	8.3E+01	3.5	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	6.8E+00	9.5E-02	3.5E+00	-8.89	-9.71	-11.48	-0.86	0.80	0.0%	0.0%	2.6E-52
3162	60113-43-1	2,6,6-trimethylbicyclo[3.1.1]heptane-3-carbaldehyde	166	20	2.1E+01	4.0E+02	1.9E+03	0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	6.4E+00	8.9E-02	3.3E+00	-9.05	-9.77	-11.51	-2.08	0.19	0.0%	0.0%	1.1E-41
3163	112-49-2	1,2-bis(2-methoxyethoxy)ethane	178	2	3.2E+01	2.8E+05	1.7E-01	0	3.5E-06	9.2E-07	1.1E-06	conf	conf	conf	6.7E+00	9.3E-02	3.4E+00	-8.32	-9.52	-11.37	1.20	0.17	0.0%	0.0%	1.5E-42
3164	355-04-4	1,1,1,2,2,3,3,4,5,5,5-undecafluoro-4-(trifluoromethyl)pentane	338	-89	3.0E+04	2.1E-01	1.0E+05	14.0	3.5E-06	3.5E-08	3.5E-08	conf	conf	conf	4.0E+00	5.6E-02	2.0E+00	-11.75	-11.44	-14.10	-2.90	0.25	0.0%	0.0%	6.0E-58
3165	76-12-0	tetrachloro-1,2-difluoroethane	204	-50	6.3E+03	1.1E+02	2.6E+03	14.0	3.5E-06	3.5E-08	1.1E-08	conf	conf	conf	3.9E+00	5.4E-02	1.9E+00	-11.63	-10.91	-13.58	-2.03	0.13	0.0%	0.0%	1.7E-61
3166	87-13-8	diethyl ethoxymethylenemalonate	216	42	4.6E+00	1.9E+03	8.9E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	6.7E+00	9.3E-02	3.5E+00	-10.68	-10.48	-12.02	-2.20	0.77	0.0%	0.0%	4.8E-45
3167	89-62-3	2-nitro-p-toluidine	152	85	6.0E-02	3.5E+02	3.7E+02	0	3.5E-06	2.9E-09	1.1E-07	conf	conf	conf	3.8E+00	5.3E-02	1.9E+00	-8.14	-8.48	-9.43	-1.96	0.70	0.0%	0.0%

3270	35077-00-0	1,1,1-triethoxy-N,N-diethylsilanamine	235	33	4.0E+00	2.5E+02	3.2E+00	1.5	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	2.3E+00	3.2E-02	1.2E+00	-8.85	-10.18	-12.03	-1.98	0.54	0.0%	0.0%	0.0%	5.1E-47
3271	29736-24-1	Disodium hydroxy(sulfonato)acetate	178	87	9.9E-03	1.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.8E+00	2.5E-02	8.8E-01	-8.79	-9.09	-10.74	-0.51	0.64	0.0%	0.0%	0.0%	1.3E-48
3272	22094-93-5	2,2'-[(2,2',5,5'-tetrachloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxobutyramide]	755	350	5.5E-22	4.6E-08	2.5E+09	0.5	3.5E-06	3.5E-09	3.5E-09	conf	conf	conf	1.4E+00	1.9E-02	6.6E-01	-10.33	-10.33	-10.33	-0.74	1.21	0.0%	0.0%	0.0%	4.9E-43
3273	6358-87-8	diethyl 2-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[4,5-dihydro-5-oxo-1-phenyl-1H-pyrazole-3-carboxylate	740	350	5.4E-21	4.0E-06	1.7E+09	0	3.5E-06	3.5E-07	3.5E-08	conf	conf	conf	1.4E+00	1.9E-02	7.2E-01	-9.07	-9.58	-11.41	-4.73	0.48	0.0%	0.0%	0.0%	2.7E-22
3274	93857-00-2	tripotassium propylsilanetriolate	236	87	9.9E-03	1.6E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.7E+00	2.4E-02	8.7E-01	-8.23	-9.06	-10.72	0.31	0.30	0.0%	0.0%	0.0%	3.0E-56
3275	98967-40-9	N-(2,6-difluorophenyl)-5-methyl[1,2,4]triazolo[1,5-a]pyrimidine-2-sulfonamide	325	190	2.0E-07	2.9E+02	3.2E+01	2.0	3.5E-06	3.7E-09	3.5E-07	conf	conf	conf	1.3E+00	1.9E-02	6.5E-01	-8.42	-8.97	-9.92	-1.58	2.08	0.0%	0.0%	0.0%	4.5E-33
3276	87135-01-1	3,3,10,10-tetramethoxy-2,11-dioxa-3,10-disiladodecane	327	74	6.9E-02	1.1E+02	1.9E+00	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	conf	2.0E+00	2.8E-02	1.0E+00	-9.89	-9.66	-11.39	-2.33	0.53	0.0%	0.0%	0.0%	1.3E-38
3277	119895-68-0	2,2-difluoro-benzo[1,3]dioxole-4-carbaldehyde	186	52	2.4E+00	8.3E+02	2.2E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	2.1E+00	2.9E-02	1.1E+00	-10.84	-10.62	-12.10	-2.15	0.32	0.0%	0.0%	0.0%	4.0E-46
3278	943516-53-8	619-015-4	229	175	1.1E-05	1.4E+03	1.5E+02	-0.8	3.5E-06	3.5E-07	3.5E-07	conf	conf	conf	2.0E+00	2.7E-02	1.0E+00	-8.76	-9.51	-11.30	-2.94	0.83	0.0%	0.0%	0.0%	3.2E-33
3279	507448-65-9	ethyl (2Z)-4,4,4-trifluoro-3-(methylamino)but-2-enoate	197	-18	1.7E+02	2.5E+04	1.3E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	2.3E+00	3.2E-02	1.2E+00	-11.24	-11.12	-12.52	-1.46	0.55	0.0%	0.0%	0.0%	1.5E-56
3280	73-22-3	L-tryptophan	204	279	8.0E-07	5.2E+06	6.0E-02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.8E+00	2.5E-02	8.8E-01	-8.14	-9.09	-10.56	-1.81	0.07	0.0%	0.0%	0.0%	5.6E-36
3281	204918-22-9	1-(allyloxy)-2-methyl-1-oxopropan-2-yl 2-chloro-5-isocyanatobenzoate	324	58	9.0E-03	1.9E+01	2.1E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	1.9E+00	2.7E-02	9.8E-01	-10.76	-10.58	-12.14	-2.10	0.56	0.0%	0.0%	0.0%	5.2E-47
3282	130198-05-9	1-[2-amino-1-(4-methoxyphenyl)ethyl]cyclohexanol hydrochloride	286	87	9.9E-03	2.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.7E+00	2.3E-02	8.4E-01	-8.80	-9.11	-10.76	-1.84	0.64	0.0%	0.0%	0.0%	1.6E-37
3283	1001164-15-7	3,5-bis[1-(4-propan-2-yl)phenyl]propan-2-yl]dihydro-1H-[1,3]oxazolo[3,4-c][1,3]oxazole	436	198	1.3E-07	6.2E-03	7.8E+08	6.1	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	1.1E+00	1.9E-02	6.6E-01	-10.47	-10.83	-11.34	-4.72	0.22	0.0%	0.0%	0.0%	1.6E-21
3284	68-22-4	norethisterone	298	161	3.1E-07	4.7E+00	9.6E+02	13.6	3.5E-06	3.0E-07	1.1E-07	conf	conf	conf	1.8E+00	2.5E-02	9.3E-01	-8.87	-9.63	-11.35	-2.23	0.65	0.0%	0.0%	0.0%	4.0E-39
3285	20325-40-0	3,3'-dimethoxybiphenyl-4,4'-ylenediammonium dichloride	317	87	9.9E-03	2.2E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.6E+00	2.3E-02	8.2E-01	-8.24	-9.08	-10.75	-1.84	0.64	0.0%	0.0%	0.0%	2.0E-37
3286	85536-87-4	7-acetamido-4-hydroxy-3-[[4-[[2-(sulphooxy)ethyl]sulphonyl]phenyl]azo]naphthalene-2-sulphonic acid, sodium salt	618	87	9.9E-03	4.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.6E+00	2.2E-02	8.0E-01	-8.80	-9.12	-10.79	-0.67	0.92	0.0%	0.0%	0.0%	1.3E-47
3287	5638-76-6	betahistine	136	28	1.8E-01	5.6E+02	9.8E+03	9.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	1.8E+00	2.5E-02	9.3E-01	-10.76	-10.47	-11.83	-1.88	0.88	0.0%	0.0%	0.0%	1.1E-44
3288	646-24-2	nonamethylenediamine	158	49	2.3E+00	1.3E+03	6.6E+01	10.8	3.5E-06	3.5E-07	3.5E-07	conf	conf	conf	1.8E+00	2.5E-02	9.3E-01	-10.17	-9.92	-11.47	-1.25	0.20	0.0%	0.0%	0.0%	1.4E-48
3289	902146-43-4	(2S)-2-Benzyl-N,N-dimethylaziridine-1-sulfonamide	240	129	1.3E-03	2.2E+03	3.8E+01	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	conf	1.8E+00	2.5E-02	9.4E-01	-8.66	-9.49	-11.35	-1.76	1.15	0.0%	0.0%	0.0%	5.2E-43
3290	1254469-57-1	4-(2-[2-(2-hydroxybenzylidene)hydrazino]-2-oxoethyl)-4-methylmorpholin-4-ium chloride	314	87	9.9E-03	2.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.6E+00	2.2E-02	7.9E-01	-8.82	-9.13	-10.79	-1.33	0.10	0.0%	0.0%	0.0%	6.0E-42
3291	173904-11-5	N,N'-[cyclohexane-1,3-diylbis(methylene)]bis[2-methylpropan-1-imine]	250	15	2.0E-01	8.4E+00	1.8E+05	7.2	3.5E-06	3.5E-07	3.5E-07	conf	conf	conf	1.5E+00	2.0E-02	7.3E-01	-11.04	-10.82	-11.83	-1.52	0.34	0.0%	0.0%	0.0%	1.8E-49
3292	19444-21-4	allyl 2-hydroxy-2-methylpropanoate	144	-2	2.0E+01	9.9E+04	4.3E+00	12.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	2.0E+00	2.8E-02	1.0E+00	-10.90	-10.75	-12.52	-1.86	0.46	0.0%	0.0%	0.0%	1.0E-52
3293	89-33-8	ethyl 5-oxo-1-phenyl-2-pyrazoline-3-carboxylate	232	143	2.1E-04	2.6E+05	1.3E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.9E+00	2.6E-02	9.3E-01	-8.06	-9.01	-10.67	-4.02	2.91	0.0%	0.0%	0.0%	1.1E-21
3294	117-21-5	3-chloropiridaic anhydride	183	51	4.4E-01	8.5E+05	1.5E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	1.8E+00	2.6E-02	9.4E-01	-9.43	-10.12	-12.03	0.42	0.29	0.0%	0.0%	0.0%	5.4E-71
3295	467430-13-3	Salt of (8α,9R)-cinchonan-9-ol and [(R)-[(1S)-2-methyl-1-(1-oxopropoxy)propoxy][4-phenylbutyl]phosphinoyl]acetat	679	87	9.9E-03	4.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.5E+00	2.0E-02	7.3E-01	-8.85	-9.17	-10.83	-1.84	0.64	0.0%	0.0%	0.0%	4.5E-38
3296	10016-20-3	cyclohexapentylose	973	350	9.9E-03	1.9E+16	1.7E-08	11.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	1.5E+00	2.0E-02	7.5E-01	-8.78	-9.94	-12.02	-0.61	0.42	0.0%	0.0%	0.0%	4.5E-60
3297	12236-64-5	N-[4-(aminophenyl)-4-[[5-[(aminocarbonyl)-2-chlorophenyl]azo]-3-hydroxynaphthalene-2-carboxamide	502	350	3.7E-21	1.1E-01	6.2E+05	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.6E+00	2.0E-02	8.0E-01	-8.43	-9.32	-10.87	-0.99	1.08	0.0%	0.0%	0.0%	1.5E-45
3298	31251-41-9	8-chloro-5,6-dihydro-11H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-one	244	132	5.6E-04	1.5E+00	9.8E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	1.8E+00	2.6E-02	9.3E-01	-10.67	-10.46	-12.11	-2.34	0.12	0.0%	0.0%	0.0%	1.5E-44
3299	1072896-13-1	N-(2-hydroxyethyl)-N'-(1-methyl-1-[3-(1-methylethenyl)phenyl]ethyl)urea	262	160	3.7E-07	1.1E+02	2.7E+02	-0.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	1.8E+00	2.6E-02	9.4E-01	-9.20	-10.04	-11.97	-2.51	0.79	0.0%	0.0%	0.0%	7.1E-42
3300	13349-82-1	(2-piperazin-1-yl)ethoxyethanol	174	90	5.2E-03	1.0E+06	1.4E-02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	1.8E+00	2.6E-02	9.4E-01	-8.86	-9.93	-11.98	-0.93	1.00	0.0%	0.0%	0.0%	2.0E-56
3301	124750-51-2	5-[4'-(Bromomethyl)biphenyl-2-yl]-1-trityl-1H-tetrazole	558	302	3.0E-14	1.8E-07	2.5E+08	0	3.5E-06	3.5E-08	3.5E-08	conf	conf	conf	1.1E+00	1.5E-02	5.6E-01	-9.76	-9.76	-11.51	-4.99	0.64	0.0%	0.0%	0.0%	6.1E-21
3302	2668-75-9	607-988-8	368	186	2.1E-06	2.4E+01	1.7E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	1.7E+00	2.4E-02	8.8E-01	-9.61	-10.51	-12.11	-2.27	0.57	0.0%	0.0%	0.0%	3.5E-45
3303	394735-17-2	Ethyl 3-cyclobutylalaninate	171	33	6.3E+00	7.8E+04	3.9E+01	7.7	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	1.8E+00	2.6E-02	9.5E-01	-10.99	-10.94	-12.58	-1.64	0.78	0.0%	0.0%	0.0%	2.6E-55
3304	42036-65-7	Dimethyl(2-oxocyclohexylmethyl)ammonium chloride	192	87	9.9E-03	1.3E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.4E+00	1.9E-02	6.8E-01	-8.33	-9.16	-10.82	-1.84	0.64	0.0%	0.0%	0.0%	4.9E-38
3305	117-61-3	benzidine-2,2'-disulphonic acid	344	277	4.3E-16	2.5E+03	6.6E-03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	1.8E+00	2.6E-02	9.5E-01	-9.12	-10.33	-12.49	-0.70	0.59	0.0%	0.0%	0.0%	5.6E-64
3306	51336-95-9	2-chloro-1-(3,4-difluorophenyl)ethanone	191	31	7.6E+00	4.5E+02	2.1E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	1.7E+00	2.4E-02	8.8E-01	-11.24	-11.02	-12.26	-3.75	0.51	0.0%	0.0%	0.0%	2.9E-34
3307	6410-41-9	N-(5-chloro-2,4-dimethoxyphenyl)-4-[[5-[(diethylamino)sulphonyl]-2-methoxyphenyl]azo]-3-hydroxynaphthalene-2-c	627	350	3.5E-20	4.6E-04	4.5E+07	9.3	3.5E-06	1.1E-06	1.1E-07	conf	conf	conf	1.1E+00	1.5E-02	5.3E-01	-10.52	-11.12	-11.75	-0.96	1.10	0.0%	0.0%	0.0%	8.1E-54
3308	89-57-6	5-aminosalicylic acid	153	129	8.1E-06	1.4E+04	9.5E+00	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	conf	1.7E+00	2.4E-02	8.7E-01	-8.14	-9.09	-10.73	-1.83	0.54	0.0%	0.0%	0.0%	1.3E-41
3309	26919-50-6	6-(methyl(phenylsulphonyl)amino)hexanoic acid, compound with 2,2',2''-nitrilotriethanol (1:1)	435	87	9.9E-03	3.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.3E+00	1.8E-02	6.4E-01	-8.91	-9.22	-10.88	-0.42	0.79	0.0%	0.0%	0.0%	9.3E-51
3310	76201-56-4	3-(dimethyl(3-[[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulfonyl]amino]propyl)ammonio)-2-hydroxypropane-1-s	650	290	4.0E-17	9.5E+00	7.6E-01	-0.2	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	1.7E+00	2.3E-02	8.5E-01	-8.91	-10.20	-12.03	-1.32	0.38	0.0%	0.0%	0.0%	3.7E-53
3311	939961-06-5	618-990-1	227	87	9.9E-03	2.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.3E+00	1.8E-02	6.4E-01	-8.51	-9.23	-10.88	-1.84	0.64	0.0%	0.0%	0.0%	1.7E-38
3312	58190-57-1	611-631-1	273	14	2.4E-01	4.3E+00	7.1E+08	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	conf	9.7E-01	1.4E-02	4.7E-01	-10.84	-11.10	-11.45	-0.43	0.27	0.0%	0.0%	0.0%	4.5E-56
3313	50-28-2	estradiol	272	152	2.7E-07	8.8E+00	8.7E+03	10.0	3.5E-06	9.5E-08	1.1E-06	conf	conf	conf	1.2E+00	1.6E-02	5.7E-01	-9.11	-9.68	-11.06	-4.64	1.61	0.0%	0.0%	0.0%	2.5E-20
3314	111-83-1	1-bromooctane	193	-18	6.9E+01	2.5E+00	4.1E+04	14.0	3.5E-06	5.0E-07	3.5E-07	conf	conf	conf	1.0E+00	1.4E-02	5.0E-01	-12.40	-12.11	-14.66	-2.95	0.33	0.0%	0.0%	0.0%	3.9E-63
3315	80675-49-6	2-(EE)-(2-methoxy-5-nitrophenyl)diazenyl]-N-(2-methoxyphenyl)-3-oxobutanamide	386	242	4.6E-10	8.0E+00	9.8E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.4E+00	1.9E-02	6.8E-01	-8.22	-9.18	-10.82	-2.73	0.70	0.0%	0.0%	0.0%	3.7E-31
3316	88-19-7	toluene-2-sulphonamide	171	91	8.1E-03	2.3E+03	8.3E+00	10.1	3.5E-06	3.5E-07	1.1E-07	conf	conf	conf	1.4E+00	2.0E-02	7.1E-01	-8.88	-9.54	-11.43	-1.68	1.26	0.0%	0.0%	0.0%	2.3E-44
3317	76-74-4	pentobarbital	226	229	4.1E-08	6.8E+02	1.0E+02	14.0	3.5E-06	3.4E-07	1.1E-06	conf	conf	conf	1.7E+00	2.4E-02	8.8E-01	-11.24	-11.02	-12.26	-3.75	0.51	0.0%	0.0%	0.0%	2.9E-34
3318	860035-10-5	1-([[2,5-dioxopyrrolidin-1-yl]oxy]carbonyl)oxyethyl 2-methylpropanoate	273	169	3.4E-06	1.9E+04	3.9E-02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	1.6E+00	2.2E-02	8.3E-01	-9.24	-10.44	-12.56	-0.92	1.52	0.0%	0.0%	0.0%	1.9E-62
3319	1261240-30-1	4-tert-butyl-2-(5-tert-butyl-2-oxo-2,3-dihydro-1-benzofuran-3-yl)phenyl 3,5-di-tert-butyl-4-hydroxybenzoate	571	288	1.7E-14	1.3E-06	1.3E+10	8.5	3.5E-06	1.1E-06	1.1E-07	conf	conf	conf	9.0E-01	1.3E-02	4.4E-01	-10.57	-10.60	-10.74	-6.61	0.88	0.0%	0.0%	0.0%	2.1E-37
3320	62-55-5	thioacetamide	75	-21	2.4E+02	1.5E+05	1.5E-01	13.4	3.5E-06	2.9E-09	1.1E-06	conf	conf	conf	9.0E-01	1.3E-02	4.4E-01	-9.70	-9.44	-10.44	-1.36	0.69	0.0%	0.0%	0.0%	9.0E-39
3321	93924-07-3	Alkanes, C10-14	170	-21	3.1E+01	3.5E-02	1.7E+06	14.0	3.5E-06	3.5E-07	1.1E-06	conf	conf	conf	9.0E-01	1.3E-02	4.4E-01	-12.55	-12.27	-15.04	-4.18	0.10	0.0%	0.0%	0.0%	1.6E-54
3322	96-12-8	1,2-dibromo-3-chloropropane	236	-7	5.9E+01	2.6E+02	4.8E+02	0	3.5E-06	1.5E-08	3.5E-08	conf	conf	conf	9.0E-01	1.3E-02	4.4E-01	-8.44	-9.13	-10.25	-1.49	0.80	0.0%	0.0%	0.0%	3.0E-36
3323	1048649-80-4	N-(2-chlorobenzyl)-1-phenylpropan-2-amine hydrochloride (1:1)	296	87	9.9E-03	2.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.1E+00	1.6E-02	5.7E-01	-8.96	-9.28	-10.93	-1.84	0.64	0.0%	0.0%	0.0%	6.9E-39
3324	17465-86-0	cyclocheptapentylose	1297	87	9.9E-03	9.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.1E+00	1.6E-02	5.7E-01	-8.94	-9.27	-10.94	-0.54	0.41	0.0%	0.0%	0.0%	3.0E-50
3325	82203-23-4	(1R)-1-[(4R,4aR,8aS)-2,6-bis(4-chlorophenyl)tetrahydro[1,3]dioxino[5,4-d][1,3]dioxin-4-yl]ethane-1,2-diol	427	229	1.4E-12	3.5E+00	4.7E+02	14.0	3.5E-06	1.1E-08	1.1E-06	conf	conf	conf	9.0E-01	1.3E-02	4.4E-01	-8.28	-9.08	-10.15	-2.06	0.64	0.0%	0.0%	0.0%	1.6E-31
3326	950773-38-3	(3R)-3-[(2-Benzyloxy)-5-bromophenyl]-N,N-diisopropyl-3-phenylpropan-1-amine	481	206	3.6E-08	1.9E-05	2.2E+08	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	conf	9.0E-01	1.3E-02	4.4E-01	-10.72	-11.23	-11.55	-4.88	0.33	0.0%	0.0%	0.0%	7.3E-22
3327	123348-27-6	2-bromo-7-iodo-9H-fluorene	371	134	2.8E-04	1.2E-02	1.2E+06	0	3.5E-06	1.1E-07	3.5E-08	conf	conf	conf	9.1E-01	1.3E-02	4.5E-01	-9.25	-9.40	-11.00	-3.44	0.27	0.0%	0.0%	0.0%	1.7E-27
3328	70-26-8	1-Chloro-3,5-dimethyladamantane	199	32	2.1E-01	4.8E+00	1.1E+05	14.0	3.5E-06	3.5E-07	1.1E-06	conf	conf	conf	9.0E-01	1.3E-02	4.4E-01	-12.30	-12.03	-14.07	-2.41	0.13	0.0%	0.0%	0.0%	1.3E-62
3329	94158-79-9	4,4'-[(6-chloro-1,3,5-triazine-2,4-diyl)diimino]bis[5-hydroxy-6-[[4-[[2-(sulphooxy)ethyl]sulphonyl]phenyl]azo]naph	1467	87	9.9E-03	1.0E+04	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.1E+00	1.5E-02	5.4E-01	-8.97	-9.29	-10.96	-1.84	0.64	0.0%	0.0%	0.0%	3.8E-39
3330	93771-36-9	20,20-Ethylenedioxy-17-hydroxy-1,4,6-pregnatrien-3-one	370	192	1.0E-08	3.2E+00	1.5E+04	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	1.1E+00	1.7E-02	6.4E-01	-9.63	-10.68	-12.19	-1.47	0.19	0.0%	0.0%	0.0%	3.0E-53
3331	1196069-20-1	3,5-bis[2,4-dimethylcyclohex-3-en-1-yl]dihydro-1H-[1,3]oxazolo[3,4-c][1,3]oxazole	332	147	7.7E-05	2.5E+01	6.0E+06	6.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.9E-01	1.4E-02	4.9E-01	-10.56	-11.11	-12.27	-3.06	0.49	0.0%	0.0%	0.0%	7.8E-40
3332	93-07-2	veratric acid	182	96	3.1E-03	3.5E+03	3.3E+01	4.3	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	1.4E+00	1.9E-02	7.1E-01	-9.51	-10.39	-12.17	-1.82	0.62	0.0%	0.0%	0.0%	8.0E-50
3333	52-90-4	L-cysteine	121	199	9.0E-05	8.0E+04	8.9E-04	2.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	1.4E+00	2.0E-02	7.3E-01	-9.23	-10.67	-12.62	-0.32	1.02	0.0%	0.0%	0.0%	2.0E-69
3334	2422-91-5	methylidynetri-p-phenylene trisocyanate	367	170	3.0E-06	9.4E+01	1.5E+07	0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.75	-10.68	-12.31	-3.50	0.24	0.0%	0.0%	0.0%	3.4E-64
3335	1037197-98-4	1-(2-chloroethoxy)-4-(1,2-diphenylvinyl)benzene	335	161	3.6E-06	6.6E-02	2.0E+06	14.0	3.5E-06	3.5E-07	1.1E-06	conf	conf	conf	9.9E-01	1.3E-02	4.5E-01	-10.53	-10.85	-11.90	-3.57	0.69	0.0%	0.0%	0.0%	1.6E-33
3336	17183-98-1	605-617-4	453	211	4.7E-08	5.8E-01	4.2E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	conf	1.1E+00	1.5E-02	5.3E-01	-9.37	-10.17	-11.71	-2.30	0.69	0.0%	0.0%	0.0%	1.6E-41
3337	654-70-6	4-amino-2-(trifluoromethyl)benzonitrile	186	64	7.1E-01	1.1E+03	1.4E+02	0.5	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	1.3E+00	1.9E-02	6.8E-01	-9.64	-10.42	-12.19	-2.24	0.46	0.0%	0.0%	0.0%	3.4E-46
3338	1219086-87-1	(2Z)-3-(3-chloro-2-fluorophenyl)-2-(4-chloro-2-fluorophenyl)acrylonitrile	310	129	3.0E-04	1.3E-01	3.4E+05	0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	8.1E-01	1.1E-02	4.0E-01	-9.03	-9.13	-10.20	-3.58	0.04	0.0%	0.0%	0.0%	1.5E-21
3339	123849-42-1	bis(2-propylheptyl) carbonate	343	9	8.5E-03	2.1E-03	8.5E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	8.1E-01	1.1E-02	3.9E-01	-11.24	-11.38	-12.50	-0.67	0.25	0.0%	0.0%	0.0%	1.2E-64
3340	92-72-8	5'-chloro-3-hydroxy-2',4'-dimethoxy-2-naphthanilide	358	236	1.0E-10	1.0E-01	5.2E+04	10.2	3.5E-06	1.1E-06	1.1E-07	conf	conf	conf	1.1E+00	1.6E-02	5.7E-01	-9.68	-10.73	-12.23	-3.16	0.25	0.0%	0.0%	0.0%	1.0E-38
3341	81653-77-2	(4S)-4-(phenylthio)-L-proline	223	301	3.8E-08	6.6E+02	3.5E-01	1.7	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	1.4E+00	1.9E-02	7.1E-01	-9.36	-10.80	-12.64	-1.97	0.75	0.0%	0.0%	0.0%	9.6E-53
3342	247569-56-8	2-Fluoro-5-(methylsulfonyl)benzoic acid	218	131	8.8E-04	1.2E+03	2.0E+00	2.7	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	1.3E+00	1.8E-02	6.8E-01	-9.03	-10.17	-12.16	-1.03	0.61	0.0%	0.0%	0.0%	3.7E-57
3343	77-09-8	phenolphthalein	318	218	8.4E-11	3.2E+01	1.1E+03	9.4	3.5E-06	1.1E-07	3.5E-07	conf	conf	conf	9.9E-01	1.4E-02	4.9E-01	-9.03	-9.61	-11.10	-1.95	0.57	0.0%	0.0%	0.0%	2.6E-39
3344	12567-73-6	619-635-5	440	87	9.9E-03	3.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.0E+00	1.4E-02	5.1E-01	-9.01	-9.33	-10.99	-1.84	0.64	0.0%	0.0%	0.0%	2.4E-39
3345	122-09-8	phentermine	149	29	3.2E+01	1.4E+01	1.6E+02	0	3.5E-06	3.5E-07	1.1E-06	conf	conf	conf	9.2E-01

3453	119-40-2	7-anilino-4-hydroxynaphthalene-2-sulphonic acid	315	228	1.7E-11	2.0E+01	6.8E+00	-0.4	3.5E-06	3.5E-07	1.1E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-8.60	-9.67	-11.56	-2.11	0.37	0.0%	0.0%	0.0%	8.2E-42
3454	2022-85-7	flucytosine	129	95	6.0E-04	4.9E+03	3.9E-02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-8.75	-9.68	-11.59	-1.23	1.48	0.0%	0.0%	0.0%	7.3E-50
3455	101-41-7	methyl phenylacetate	150	-1	2.1E+01	3.9E+04	1.2E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	1.0E+00	1.4E-02	5.0E-01	-9.80	-9.49	-11.06	-0.89	0.49	0.0%	0.0%	0.0%	3.4E-48
3456	61832-41-5	N-methyl-1-(methylthio)-2-nitrovinylamine	148	40	5.4E+00	2.8E+05	4.8E-01	7.6	3.5E-06	3.5E-07	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.50	-9.74	-11.61	-3.96	0.64	0.0%	0.0%	0.0%	1.4E-28
3457	53-84-9	nadide	663	90	2.7E-09	2.9E+03	6.3E-07	0.3	3.5E-06	3.5E-07	3.5E-07	conf	conf	conf	9.1E-01	1.3E-02	4.6E-01	-8.54	-9.66	-11.56	0.04	2.30	0.0%	0.0%	0.0%	6.7E-62
3458	947753-66-4	2-Ethylhexyl-2-cyano-3-(4-methoxyphenyl)-3-phenylprop-2-enoate	392	199	6.5E-08	2.5E-02	9.1E+06	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	6.9E-01	9.6E-03	3.4E-01	-10.95	-11.55	-12.31	-4.84	0.79	0.0%	0.0%	0.0%	7.2E-27
3459	18402-22-7	678-409-4	332	71	4.6E-02	1.4E+00	2.5E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	6.3E-01	8.8E-03	3.1E-01	-11.21	-11.50	-11.99	-3.35	0.73	0.0%	0.0%	0.0%	2.5E-35
3460	252285-60-2	2-[4-(4-ethoxyphenyl)-6-phenyl-1,3,5-triazin-2-yl]phenol	369	244	2.7E-11	1.1E+00	1.9E+04	3.3	3.5E-06	3.5E-07	3.5E-08	conf	conf	conf	9.1E-01	1.3E-02	4.6E-01	-9.15	-9.65	-11.55	-3.95	0.40	0.0%	0.0%	0.0%	8.3E-28
3461	1195231-94-7	2-[ethyl(4-nitrosophenyl)amino]ethyl [3-(triethoxysilyl)propyl]carbamate	442	194	6.3E-07	1.6E+00	1.3E+03	4.5	3.5E-06	3.5E-07	1.1E-07	conf	conf	conf	9.1E-01	1.3E-02	4.6E-01	-9.24	-9.80	-11.67	-2.73	0.82	0.0%	0.0%	0.0%	1.2E-37
3462	378-44-9	betamethasone	392	217	7.7E-12	6.5E+01	5.2E+01	13.0	3.5E-06	1.0E-07	1.1E-06	conf	conf	conf	7.6E-01	1.1E-02	3.8E-01	-9.07	-9.65	-11.12	-1.04	0.48	0.0%	0.0%	0.0%	2.4E-47
3463	1624-62-0	3-methyoxestra-1,3,5(10)-trien-17-one	284	141	2.6E-04	1.8E+00	9.8E+04	14.0	3.5E-06	1.1E-06	6.6E-10	conf	conf	conf	9.1E-01	1.3E-02	4.5E-01	-9.67	-9.40	-11.03	-2.48	0.10	0.0%	0.0%	0.0%	1.3E-34
3464	3439-73-4	[4-(2-chloroethoxy)phenyl]phenylmethanone	261	120	6.3E-04	5.3E+00	9.3E+03	0	3.5E-06	1.1E-06	1.1E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.78	-10.27	-12.31	-2.54	0.19	0.0%	0.0%	0.0%	1.6E-44
3465	38982-12-6	3-(9-anthryl)acrylaldehyde	232	132	1.2E-04	6.8E+00	1.5E+04	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	conf	8.2E-01	1.1E-02	4.1E-01	-9.33	-9.41	-11.06	-3.40	0.32	0.0%	0.0%	0.0%	3.4E-28
3466	846-48-0	boldenone	286	145	1.6E-06	7.0E+01	1.1E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.6E-01	1.3E-02	4.9E-01	-9.80	-10.74	-12.34	-1.91	0.46	0.0%	0.0%	0.0%	1.7E-50
3467	58861-48-6	2-(4-fluorophenyl)thiophene	178	62	2.6E-01	1.5E+01	6.0E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.87	-10.46	-12.34	-2.53	0.12	0.0%	0.0%	0.0%	7.0E-45
3468	52698-46-1	1,1,1-Trimethoxy-2-methylpropane	148	-44	1.5E+03	3.8E+03	1.1E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-12.10	-11.84	-13.44	-1.00	0.59	0.0%	0.0%	0.0%	5.4E-71
3469	38849-09-1	3-(9,10-ethano-9(10H)-anthryl)acrylaldehyde	260	135	2.6E-04	1.5E-01	6.6E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-11.11	-10.90	-12.46	-3.13	0.52	0.0%	0.0%	0.0%	7.2E-41
3470	50372-61-7	(4,5-dibromo-1H-pyrrol-2-yl)(phenyl)methanone	329	138	7.2E-04	5.2E+00	1.9E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-10.87	-10.79	-12.40	-2.49	1.52	0.0%	0.0%	0.0%	1.0E-45
3471	87428-99-7	Benzyl N-(2-benzylacrylyol)glycinate	309	194	3.5E-07	1.1E+00	4.6E+03	12.8	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.86	-10.77	-12.38	-2.70	0.67	0.0%	0.0%	0.0%	8.9E-44
3472	924726-92-1	(6a,9β,11β,16a)-6-fluoro-17-hydroxy-16-methyl-3,20-dioxo-9,11-epoxypregna-1,4-dien-21-yl benzoate	495	242	1.3E-12	1.7E-02	3.4E+03	13.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	9.1E-01	1.3E-02	4.6E-01	-9.69	-10.73	-12.32	-2.01	0.15	0.0%	0.0%	0.0%	2.2E-49
3473	923036-25-3	N-[(3R,4R)-1-benzyl-4-methylpiperidin-3-yl]-2-chloro-N-methyl-1H-pyrrolo[2,3-d]pyrimidin-4-amine	370	234	1.4E-09	5.1E-01	2.9E+03	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	9.1E-01	1.3E-02	4.5E-01	-8.48	-9.40	-11.03	-3.39	0.30	0.0%	0.0%	0.0%	5.2E-28
3474	27566-05-8	4-(2-benzylaminopropyl)phenol	241	125	3.8E-04	1.8E+03	2.8E+03	7.7	3.5E-06	1.1E-06	1.1E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.64	-10.62	-12.35	-2.81	0.27	0.0%	0.0%	0.0%	1.4E-42
3475	18109-80-3	butamirate	307	115	6.5E-03	3.0E+01	2.5E+03	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	9.1E-01	1.3E-02	4.5E-01	-9.81	-9.53	-11.12	-2.37	0.65	0.0%	0.0%	0.0%	4.4E-36
3476	2321-07-5	2-(6-hydroxy-3-oxo-(3H)-xanthen-9-yl)benzoic acid	332	227	5.4E-12	2.5E+02	2.2E+03	9.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.67	-10.71	-12.31	-2.31	0.37	0.0%	0.0%	0.0%	1.3E-46
3477	7148-78-9	(3,3-diethoxy-1-propenyl)benzene	206	23	3.1E-01	6.9E+02	1.5E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	8.3E-01	1.2E-02	4.3E-01	-11.04	-10.82	-12.42	-4.87	4.54	0.0%	0.0%	0.0%	2.1E-27
3478	113290-51-1	1-tert-butyl-3,5-diiodo-2-methoxybenzene	416	106	4.2E-03	1.5E-01	2.1E+06	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	conf	6.3E-01	8.9E-03	3.1E-01	-11.76	-11.65	-12.67	-3.03	0.12	0.0%	0.0%	0.0%	1.9E-43
3479	197721-70-3	5-Hydroxydrospirenone	385	210	3.9E-10	1.4E+03	1.0E+03	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.61	-10.66	-12.31	-1.80	0.29	0.0%	0.0%	0.0%	2.7E-51
3480	156755-23-6	6-BROMO-4-PHENYLCHROMAN-2-ONE	345	245	2.4E-05	2.5E+00	9.5E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	9.1E-01	1.3E-02	4.6E-01	-9.36	-9.40	-11.05	-2.85	0.51	0.0%	0.0%	0.0%	5.9E-32
3481	5292-53-5	diethyl (phenylmethylene)malonate	248	3	1.2E-01	6.0E+01	8.7E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	9.1E-01	1.3E-02	4.6E-01	-10.10	-9.81	-11.29	-2.53	0.26	0.0%	0.0%	0.0%	3.1E-36
3482	60803-26-1	2-tert-butyl-4,6-diiodophenol	402	123	4.0E-04	7.5E+00	5.8E+05	7.8	3.5E-06	3.5E-06	1.1E-06	conf	conf	conf	7.3E-01	1.0E-02	3.6E-01	-11.63	-11.79	-13.00	-2.96	0.31	0.0%	0.0%	0.0%	6.2E-47
3483	160583-22-2	2-phenylethyl 2-cyanoacrylate	201	73	2.7E-02	3.4E+02	1.3E+03	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.1E-01	1.3E-02	4.7E-01	-9.80	-10.44	-12.34	-2.47	0.27	0.0%	0.0%	0.0%	2.2E-45
3484	575-61-1	3-benzylidenephthalide	222	121	6.0E-04	6.2E+01	5.6E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-10.29	-10.66	-12.37	-2.70	0.40	0.0%	0.0%	0.0%	1.1E-43
3485	84852-49-3	[[[phosphonomethyl]imino]bis[ethylenenitrilobis(methylene)]]tetrakisphosphonic acid, potassium salt	612	87	9.9E-03	4.2E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	7.3E-01	1.0E-02	3.7E-01	-8.59	-9.43	-11.10	-0.59	1.21	0.0%	0.0%	0.0%	3.0E-51
3486	101-97-3	ethyl phenylacetate	164	11	1.2E-01	1.1E+03	3.7E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	9.1E-01	1.3E-02	4.6E-01	-10.59	-10.28	-11.63	-1.99	0.80	0.0%	0.0%	0.0%	2.3E-43
3487	86960-46-5	4-(decanoyloxy)benzoic acid	292	151	3.1E-05	1.2E+00	2.5E+02	4.2	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.3E-01	1.3E-02	4.8E-01	-9.89	-10.60	-12.36	-1.59	0.95	0.0%	0.0%	0.0%	2.7E-54
3488	908145-87-9	Diethyl N-[4-(4-oxobutyl)benzoyl]-L-glutamate	377	199	4.4E-08	1.7E+00	5.1E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	9.1E-01	1.3E-02	4.6E-01	-8.50	-9.37	-11.03	-2.25	0.81	0.0%	0.0%	0.0%	2.5E-36
3489	92878-95-0	618-883-1	246	115	3.2E-03	1.2E+02	4.9E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-10.60	-10.66	-12.37	-1.45	0.57	0.0%	0.0%	0.0%	3.8E-55
3490	1172131-64-7	2-(2-aminopropan-2-yl)-4-[(4-fluorobenzyl)carbamoyl]-1-methyl-6-oxo-1,6-dihydropyrimidin-5-yl pivalate	418	253	7.0E-11	3.7E+01	3.3E+02	12.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.52	-10.59	-12.30	-3.05	0.64	0.0%	0.0%	0.0%	3.4E-40
3491	143418-49-9	604-355-8	176	91	2.3E-03	2.1E+03	9.9E+02	7.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.72	-10.59	-12.35	-4.29	0.64	0.0%	0.0%	0.0%	5.5E-31
3492	76-89-1	methyl benzilate	242	110	1.7E-04	5.1E+02	1.6E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.65	-10.58	-12.36	-4.20	3.22	0.0%	0.0%	0.0%	1.0E-31
3493	261953-36-0	6-iodo indazole	246	110	2.3E-02	4.5E+02	2.3E+02	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.65	-10.40	-12.33	-4.12	2.82	0.0%	0.0%	0.0%	4.4E-32
3494	152-97-6	fluocortolone	376	205	5.2E-10	5.4E+01	1.1E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	9.1E-01	1.3E-02	4.6E-01	-8.34	-9.31	-10.96	-1.44	0.37	0.0%	0.0%	0.0%	1.9E-42
3495	877399-00-3	5-Bromo-3-[(1R)-1-(2,6-dichloro-3-fluorophenyl)ethoxy]pyridin-2-amine	380	172	1.7E-05	4.3E-01	1.3E+05	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.1E-01	1.3E-02	4.6E-01	-10.91	-11.01	-12.41	-2.66	1.08	0.0%	0.0%	0.0%	2.1E-44
3496	61010-04-6	2-chloro-3-(hydroxymethylene)cyclohex-1-ene-1-carbaldehyde	173	74	7.2E-03	8.2E+03	7.9E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.85	-10.67	-12.36	-2.17	1.74	0.0%	0.0%	0.0%	2.4E-48
3497	148528-05-6	2-Methylcotane-1,8-diamine	158	40	4.8E-00	2.4E+03	5.6E+01	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.50	-10.38	-12.32	-1.28	0.18	0.0%	0.0%	0.0%	2.6E-56
3498	18667-19-1	2-chloro-N-cyclohexyl-N-(cyclohexylcarbamoyl) acetamide	301	198	1E-07	4.4E+00	6.2E+04	-0.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.76	-10.45	-12.29	-2.95	0.02	0.0%	0.0%	0.0%	7.3E-41
3499	69399-57-1	614-960-9	237	214	2.8E-08	5.9E+03	1.6E+00	4.7	3.5E-06	3.5E-06	3.5E-07	conf	conf	conf	9.7E-01	1.3E-02	5.0E-01	-9.40	-10.71	-12.78	-0.81	1.05	0.0%	0.0%	0.0%	8.0E-66
3500	867022-57-9	N-(4-bromobenzyl)-N-pentanoyl-L-valine	370	193	7.4E-07	2.9E+00	3.9E+04	3.2	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.81	-10.49	-12.32	-3.00	0.51	0.0%	0.0%	0.0%	9.4E-41
3501	16251-77-7	3-phenylpropylaldehyde	148	1	1.1E-01	2.4E+03	2.8E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	9.2E-01	1.3E-02	4.1E-01	-10.77	-10.52	-11.90	-2.11	0.07	0.0%	0.0%	0.0%	2.9E-45
3502	99842-68-9	2-phenylethyl cyanoacetate	189	72	4.3E-02	1.5E+03	5.2E+01	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.49	-10.38	-12.32	-1.84	0.84	0.0%	0.0%	0.0%	5.8E-51
3503	35877-42-0	3-cyclohexyl-2-(cyclohexylimino)-1,3-oxazolidin-4-one	264	141	9.6E-05	2.7E+02	1.6E+04	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.78	-10.44	-12.30	-2.54	0.78	0.0%	0.0%	0.0%	1.7E-44
3504	4890-85-1	o-phenethylbenzoic acid	226	132	5.6E-04	2.2E+01	1.9E+04	3.6	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.93	-10.66	-12.37	-2.35	0.08	0.0%	0.0%	0.0%	9.5E-47
3505	5419-55-6	trilisopropyl borate	188	-43	1.1E+03	1.3E+05	6.8E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-11.30	-11.12	-12.45	-1.55	0.64	0.0%	0.0%	0.0%	5.4E-55
3506	39856-50-3	5-bromo-2-nitropyridine	203	77	5.7E-01	7.6E+02	3.2E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-10.81	-10.61	-12.34	-2.87	0.97	0.0%	0.0%	0.0%	5.2E-42
3507	61337-89-1	1-[3-(hydroxymethyl)pyridin-2-yl]-4-methyl-2-phenylpiperazine	283	176	1.6E-07	2.7E+04	4.3E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.30	-10.42	-12.28	-2.15	0.69	0.0%	0.0%	0.0%	9.4E-48
3508	329216-67-3	2-(4-Dibenzo[b,f][1,4]thiazepin-11-yl)piperazin-1-yl)ethanol	339	207	5.2E-10	5.4E+01	1.1E+02	5.8	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.1E-01	1.3E-02	4.6E-01	-9.45	-10.42	-12.28	-2.63	0.31	0.0%	0.0%	0.0%	1.6E-43
3509	84268-36-0	3-[3-(2H-Benzotriazol-2-yl)-5-tert-butyl-4-hydroxyphenyl]propionic acid	339	224	6.9E-10	2.4E+01	2.0E+03	-1.1	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.66	-10.38	-12.27	-2.68	0.30	0.0%	0.0%	0.0%	4.2E-43
3510	76028-96-1	(ZZ)-(5-amino-1,2,4-thiadiazol-3-yl)[[(1-tert-butoxy-2-methyl-1-oxopropan-2-yl)oxy]imino]acetic acid	330	194	5.7E-07	1.8E+02	1.7E+03	0.6	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.74	-10.58	-12.30	-1.37	0.41	0.0%	0.0%	0.0%	2.6E-55
3511	909782-32-7	4-amino-N-(2-methylquinolin-8-yl)benzenesulfonamide	313	215	1.6E-08	7.7E+01	1.6E+03	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	9.1E-01	1.3E-02	4.6E-01	-8.43	-9.37	-11.01	-2.09	0.39	0.0%	0.0%	0.0%	1.7E-37
3512	5128-28-9	4,6-Dinitro-2,1,3-benzoxadiazole 1-oxide	226	172	1.7E-05	1.3E+02	2.8E+01	0	3.5E-06	1.1E-06	1.1E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.05	-10.13	-12.23	-2.03	1.11	0.0%	0.0%	0.0%	2.0E-48
3513	24085-06-1	4-ACETOXY-3-(ACETOXYMETHYL)ACETOPHENONE	250	29	6.5E-02	2.0E+03	2.3E+01	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.39	-10.36	-12.33	-2.92	0.36	0.0%	0.0%	0.0%	1.8E-41
3514	16673-34-0	N-[2-(4-aminosulphonylphenyl)ethyl]-5-chloro-2-methoxybenzamide	369	239	6.2E-10	5.6E+01	3.2E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	9.1E-01	1.3E-02	4.6E-01	-8.36	-9.33	-10.97	-2.24	0.80	0.0%	0.0%	0.0%	5.0E-36
3515	2688-84-8	2-phenoxyaniline	185	91	1.1E-01	5.6E+01	1.9E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-10.99	-10.78	-12.37	-2.26	0.53	0.0%	0.0%	0.0%	1.3E-47
3516	120279-88-1	6-methyl-4-oxo-5,6-dihydro-4H-thieno[2,3-b]thiopyran-2-sulfonamide	263	175	1.0E-05	1.7E+02	1.9E+01	8.6	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.63	-10.59	-12.36	-1.65	1.19	0.0%	0.0%	0.0%	3.5E-53
3517	846023-54-9	1-(3-(2-methoxy 5-nitrophenoxy)propyl)-4-methylpiperazine	309	169	2.5E-05	2.3E+03	1.7E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.35	-10.39	-12.33	-1.81	0.76	0.0%	0.0%	0.0%	2.3E-51
3518	82419-35-0	8,9-Difluoro-3-methyl-6-oxo-2,3-dihydro-6H-1-oxa-3a-aza-phenalene-5-carboxylic acid	281	187	3.2E-05	1.2E+02	8.7E+01	5.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.54	-10.44	-12.34	-2.95	0.64	0.0%	0.0%	0.0%	2.4E-41
3519	57260-71-6	tert-butyl piperazine-1-carboxylate	186	65	1.1E+00	6.1E+03	1.3E+01	0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.59	-10.55	-12.35	-1.72	0.87	0.0%	0.0%	0.0%	2.1E-52
3520	52980-28-6	Ethyl 4-oxo-1,4-dihydroquinoline-3-carboxylate	217	129	1.4E-03	1.4E+02	2.4E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-10.00	-10.42	-12.33	-3.02	0.64	0.0%	0.0%	0.0%	1.1E-40
3521	72684-95-8	4-hydroxy-3,5-dimethoxybenzonitrile	179	99	8.1E-03	2.7E+03	1.8E+01	8.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.64	-10.40	-12.32	-2.47	0.76	0.0%	0.0%	0.0%	2.7E-45
3522	106939-34-8	ethyl (3S)-9,10-difluoro-3-methyl-7-oxo-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylate	309	146	3E-04	7.0E+00	9.5E+00	-1.2	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.26	-10.33	-12.33	-3.33	0.64	0.0%	0.0%	0.0%	5.5E-38
3523	2657-85-4	Benzamide, 4-amino-N-(3-aminophenyl)-	227	196	4.8E-07	2.0E+02	7.4E+00	4.1	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.47	-10.53	-12.33	-1.96	0.77	0.0%	0.0%	0.0%	5.7E-50
3524	43170-88-3	diethyl N-[4-[[2,4-diamino-6-pteridinyl]methyl]methylamino]benzoyl]-L-glutamate	511	317	2.6E-15	3.7E+00	7.2E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.11	-10.26	-12.25	-1.07	1.10	0.0%	0.0%	0.0%	9.8E-58
3525	1207628-34-4	Methyl (3aR,7aR)-4-oxooctahydro-1H-indole-1-carboxylate	197	76	1.4E-01	2.5E+04	3.5E+00	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.45	-10.53	-12.34	-1.44	0.97	0.0%	0.0%	0.0%	5.6E-55
3526	24683-26-9	ethyl 4-hydroxy-2-methyl-2H-1,2-benzothiazine-3-carboxylate 1,1-dioxide	283	182	5.3E-08	5.1E+02	3.0E+00	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	conf	9.1E-01	1.3E-02	4.6E-01	-8.37	-9.33	-10.98	-1.45	0.64	0.0%	0.0%	0.0%	1.6E-42
3527	66356-53-4	5-[[(2-aminoethyl)thio]methyl]-N,N-dimethyl-2-furfurylamine	214	86	4.5E-02	4.1E+04	5.9E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.42	-10.31	-12.31	-1.78	0.81	0.0%	0.0%	0.0%	2.1E-51
3528	144338-64-6	1,1'-(1,3-dioxolane-2,2-diyldimethanediyl)bis[1H-1,2,4-triazole]	236	147	1E-04	4.4E+03	1.5E-01	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-9.94	-10.23	-12.26	-0.62	2.13	0.0%	0.0%	0.0%	2.4E-62
3529	652-37-9	theophyllin-7-ylacetic acid	238	219	1.4E-08	2.9E+06	4.6E-02	3.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	conf	9.2E-01	1.3E-02	4.7E-01	-8.89	-10.20	-12.24	-1.39	1.38	0.0%	0.0%	0.0%	1.8E-54
3530

3636	145022-44-2	1-ethyl-1H-imidazol-3-ium trifluoromethanesulfonate	261	87	9.9E-03	1.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.6E-01	6.4E-03	2.3E-01	-9.37	-9.67	-11.33	-0.97	0.64	0.0%	0.0%	7.1E-50
3637	824-80-6	Sodium 4-fluorobenzene sulfinate	182	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.6E-01	6.4E-03	2.3E-01	-9.37	-9.68	-11.32	-1.84	0.64	0.0%	0.0%	3.7E-42
3638	3687-18-1	3-aminopropane-1-sulphonic acid	139	80	6.9E-03	1.2E+05	1.3E-03	0.7	3.5E-06	3.5E-06	3.5E-06	conf	conf	6.0E-01	8.4E-03	3.1E-01	-9.85	-11.32	-13.02	-0.73	1.08	0.0%	0.0%	2.8E-69
3639	6764-10-9	1-(4-chlorophenyl)sulfanyl-2-nitrobenzene	266	140	2.9E-04	2.8E+00	5.6E+04	14.0	3.5E-06	3.5E-08	3.5E-08	conf	conf	3.6E-01	5.1E-03	1.8E-01	-10.19	-10.02	-11.21	-2.66	0.17	0.0%	0.0%	2.3E-34
3640	26184-62-3	(2S)-pentan-2-ol	88	-64	9.7E+02	3.6E+04	1.8E+01	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	5.5E-01	7.7E-03	2.8E-01	-11.73	-11.54	-12.69	-0.88	0.38	0.0%	0.0%	3.4E-64
3641	909782-35-0	4-[[4,6-Bis[3-(diethylamino)propyl]amino]-1,3,5-triazin-2-yl]amino]-N-[2-(4,5,6,7-tetrachloro-1,3-dioxo-2,3-dihydro-	917	350	1.5E-24	9.2E-09	1.7E+10	9.4	3.5E-06	1.1E-07	1.1E-07	conf	conf	3.3E-01	4.6E-03	1.6E-01	-11.03	-11.09	-11.20	-7.49	1.94	0.0%	0.0%	3.8E-41
3642	69555-14-2	ethyl N-[(diphenylmethylidene)]glycinate	267	94	1.4E-03	1.3E+01	6.5E+03	4.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.5E-01	7.7E-03	2.8E-01	-10.07	-10.74	-12.59	-2.77	0.17	0.0%	0.0%	6.0E-45
3643	848484-93-5	2-[4-(Phenylmethoxy)phenyl]ethyldecanoate	383	179	9.3E-07	6.5E-04	1.9E+08	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.5E-01	4.8E-03	1.7E-01	-11.12	-11.65	-11.98	-4.31	0.50	0.0%	0.0%	3.1E-28
3644	118-41-2	3,4,5-trimethoxybenzoic acid	212	119	9.2E-04	2.6E+03	2.5E+01	4.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.5E-01	7.7E-03	2.8E-01	-9.62	-10.59	-12.54	-1.34	0.43	0.0%	0.0%	5.5E-58
3645	6615-00-5	613-901-4	288	164	2.9E-07	6.3E+01	5.9E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.5E-01	7.7E-03	2.8E-01	-9.45	-10.52	-12.53	-1.53	0.85	0.0%	0.0%	6.2E-56
3646	90-51-7	6-amino-4-hydroxynaphthalene-2-sulphonic acid	239	198	1E-09	1.2E+04	4.1E+02	0	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.5E-01	7.7E-03	2.8E-01	-9.26	-10.63	-12.50	-1.11	0.70	0.0%	0.0%	7.5E-60
3647	5637-42-3	611-382-9	160	114	6.4E-03	2.8E+03	5.4E+00	10.8	3.5E-06	3.5E-06	1.1E-06	conf	conf	5.7E-01	7.9E-03	2.9E-01	-10.35	-11.26	-13.07	-2.01	0.77	0.0%	0.0%	1.3E-56
3648	9016-45-9	Nonylphenol, ethoxylated	441	209	1.3E-10	1.9E-01	3.0E+04	14.0	3.5E-06	2.5E-07	1.1E-06	conf	conf	4.1E-01	5.7E-03	2.1E-01	-9.73	-10.55	-11.98	-2.13	0.68	0.0%	0.0%	2.8E-45
3649	98-32-8	3-amino-4-hydroxybenzenesulphonamide	188	155	4.4E-05	2.6E+04	9.3E-01	3.0	3.5E-06	3.5E-06	3.5E-07	conf	conf	5.5E-01	7.7E-03	2.8E-01	-9.63	-10.96	-13.05	-1.91	0.73	0.0%	0.0%	2.3E-57
3650	135-63-7	5'-chloro-2'-methoxy-2'-methyl-2-naphthanilide	312	219	1.9E-07	1.0E+00	1.3E+05	10.2	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.3E-01	6.1E-03	2.2E-01	-10.26	-11.31	-12.67	-3.62	0.27	0.0%	0.0%	1.6E-38
3651	26090-29-9	2-(Diethylamino)ethyl 4-[[2-(octyloxy)benzoyl]amino]benzoate	469	260	2.3E-11	1.0E-02	1.3E+07	8.8	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.5E-01	4.9E-03	1.7E-01	-11.18	-11.84	-12.53	-4.24	0.28	0.0%	0.0%	1.2E-32
3652	692-49-9	(2Z)-1,1,1,4,4,4-Hexafluorobut-2-ene	164	-127	3.3E+05	3.4E+01	8.3E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.6E-01	5.1E-03	1.8E-01	-12.95	-12.62	-15.62	-1.48	0.28	0.0%	0.0%	4.3E-91
3653	918504-27-5	N-[3-[(5-bromo-1H-pyrrolo[2,3-b]pyridin-3-yl)carbonyl]-2,4-difluorophenyl]propane-1-sulfonamide	458	261	2E-11	1.1E+00	1.6E+07	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.5E-01	4.8E-03	1.7E-01	-9.16	-10.14	-11.94	-2.94	0.42	0.0%	0.0%	4.0E-38
3654	53378-52-2	Sodium O,O-diisobutyl phosphorothioate	248	87	9.9E-03	1.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.9E-01	5.5E-03	2.0E-01	-9.43	-9.74	-11.39	-1.00	0.42	0.0%	0.0%	3.7E-50
3655	908020-52-0	ammonium difluoro[1,1,2,2-tetrafluoro-2-(pentafluoroethoxy)ethoxy]acetate	363	87	9.9E-03	2.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.7E-01	5.1E-03	1.9E-01	-9.42	-9.74	-11.39	-1.84	0.64	0.0%	0.0%	9.9E-43
3656	13117-18-9	603-467-1	749	350	1.8E-26	1.1E-01	1.9E+02	8.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	5.2E-01	7.3E-03	2.7E-01	-11.85	-11.59	-13.16	-0.90	0.70	0.0%	0.0%	6.8E-69
3657	7605-52-9	methyl cis-3-methylcyclohexanecarboxylate	156	-18	6.5E+01	3.0E+02	1.1E+03	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.6E-01	6.4E-03	2.3E-01	-12.36	-12.10	-13.46	-1.84	0.24	0.0%	0.0%	5.3E-62
3658	69904-10-5	615-027-9	207	208	7.2E-08	3.9E+04	3.0E-01	5.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.9E-01	6.8E-03	2.5E-01	-9.20	-10.47	-12.51	-1.57	0.95	0.0%	0.0%	2.3E-55
3659	1034138-69-4	2-[(E)-[4-[[4-(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)butyl][(ethyl)amino]-2-methylphenyl]diazenyl]-5-nitrobenzene-1	536	350	8.3E-18	1.4E-03	9.3E+06	2.1	3.5E-06	3.5E-07	1.1E-07	conf	conf	4.3E-01	6.1E-03	2.2E-01	-9.73	-10.19	-11.97	-3.43	1.11	0.0%	0.0%	1.5E-34
3660	99591-74-9	1,5,2,4-dioxadithiane 2,2,4,4-tetraoxide	180	110	2.6E-02	3.3E+05	1.2E+01	14.0	3.5E-06	1.1E-05	3.5E-06	conf	conf	5.2E-01	7.2E-03	2.7E-01	-10.4	-11.81	-13.64	-1.30	0.11	0.0%	0.0%	7.2E-70
3661	298692-41-8	620-216-4	181	67	1.4E-01	7.7E+05	1.2E-02	9.3	3.5E-06	3.5E-06	1.1E-06	conf	conf	5.1E-01	7.0E-03	2.6E-01	-9.89	-10.98	-13.11	-2.70	0.64	0.0%	0.0%	2.8E-50
3662	41202-77-1	1-(2,3-dichlorophenyl)piperazine	231	113	1.2E-02	1.2E+03	6.8E+02	14.0	3.5E-06	1.1E-07	3.5E-08	conf	conf	3.6E-01	5.1E-03	1.8E-01	-9.76	-9.88	-11.44	-2.58	0.62	0.0%	0.0%	4.9E-37
3663	122584-18-3	N-(2-Bromo-5-hydroxy-4-methoxybenzyl)-N-[2-(4-hydroxyphenyl)ethyl]formamide	380	212	5E-10	6.9E-05	5.4E+02	-0.4	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.7E-01	6.5E-03	2.4E-01	-8.65	-10.65	-12.56	-2.54	0.30	0.0%	0.0%	8.4E-47
3664	1232839-86-1	5-tert-butyl-3-methyl-1,2-phenylene dibenzoate	388	164	1.4E-06	3.3E-02	1.7E+07	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.2E-01	4.4E-03	1.6E-01	-11.32	-11.89	-12.56	-4.54	1.27	0.0%	0.0%	1.1E-30
3665	6843-66-9	dimethoxydiphenylsilane	244	75	3.9E-02	7.8E+00	1.0E+03	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.6E-01	6.4E-03	2.4E-01	-10.08	-10.73	-12.64	-1.84	0.47	0.0%	0.0%	5.1E-54
3666	853950-77-3	2-[(R)-[(3-Methyl-4-nitropyridin-2-yl)methyl]sulfinyl]-1H-benzimidazole	316	87	9.9E-03	2.2E+03	3.0E+02	0	3.5E-06	1.1E-06	1.1E-07	conf	conf	3.7E-01	5.1E-03	1.9E-01	-9.81	-10.61	-12.69	-1.76	0.85	0.0%	0.0%	2.5E-55
3667	130-13-2	sodium 4-aminonaphthalene-1-sulphonate	245	87	9.9E-03	1.3E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.6E-01	5.1E-03	1.8E-01	-9.90	-9.74	-11.40	0.45	0.64	0.0%	0.0%	1.6E-64
3668	103429-90-9	3-Methoxy-3-methylbutyl acetate	160	-20	2.0E+02	3.5E+03	2.9E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	4.6E-01	6.3E-03	2.3E-01	-11.42	-11.12	-12.55	-1.61	0.94	0.0%	0.0%	2.3E-55
3669	2001-94-7	dipotassium dihydrogen ethylenediaminetetraacetate	368	87	9.9E-03	2.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.6E-01	5.0E-03	1.8E-01	-9.46	-9.77	-11.43	-1.38	0.64	0.0%	0.0%	5.2E-47
3670	246035-38-1	methyl [(1Z)-1-(2-amino-1,3-thiazol-4-yl)-2-[(1,3-benzothiazol-2-yl)sulfanyl]-2-oxoethylidene]amino]oxyacetate	408	246	2.1E-10	7.2E-01	8.1E+02	0	3.5E-06	1.1E-07	1.1E-07	conf	conf	4.6E-01	6.4E-03	2.4E-01	-9.51	-10.50	-12.54	-3.26	0.29	0.0%	0.0%	1.2E-40
3671	119-70-0	5-amino-2-(p-aminoanilino)benzenesulphonic acid	279	218	9.5E-11	2.2E+03	1.6E-03	6.7	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.6E-01	6.4E-03	2.4E-01	-9.30	-10.53	-12.55	-1.53	0.86	0.0%	0.0%	4.2E-56
3672	119-79-9	5-aminonaphthalene-2-sulphonic acid	223	173	7.0E-08	2.3E+03	1.2E-01	0.3	3.5E-06	1.1E-06	1.1E-06	conf	conf	4.6E-01	6.4E-03	2.4E-01	-9.21	-10.52	-12.54	-1.84	0.88	0.0%	0.0%	4.5E-53
3673	849727-62-4	617-648-0	275	87	9.9E-03	1.9E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.5E-01	4.9E-03	1.8E-01	-9.47	-9.78	-11.44	-1.84	0.64	0.0%	0.0%	4.1E-43
3674	1355646-93-1	1-(3-tert-butyl-5-(6-hydroxy-2-naphthyl)-4-methoxyphenyl)pyrimidine-2,4(1H,3H)-dione	416	302	1.5E-16	1.3E-02	1.8E+05	9.4	3.5E-06	3.5E-07	1.1E-07	conf	conf	3.8E-01	4.6E-03	1.6E-01	-10.03	-10.97	-12.27	-3.82	0.17	0.0%	0.0%	8.1E-34
3675	143782-23-4	4-isothiocyanato-2-(trifluoromethyl)benzonitrile	228	85	7.8E-02	9.3E+00	2.5E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	3.7E-01	5.1E-03	1.9E-01	-11.38	-11.14	-12.40	-3.39	0.44	0.0%	0.0%	3.2E-38
3676	37486-69-4	1,1,1,2,4,4,5,7,7,8,10,10,11,13,13,14,16,16,17,17,18,18,18-tricosafluoro-5,8,11,14-tetrakis(tri-fluoromethyl)-3,6,9,12,1	950	101	1.8E-02	1.1E-10	1.6E+12	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	2.7E-01	3.8E-03	1.3E-01	-12.95	-12.95	-12.95	-7.44	0.64	0.0%	0.0%	4.5E-57
3677	221640-14-8	benzyl [(2S)-1-[(2-aminoethyl)amino]-3-(4-ethoxyphenyl)propan-2-yl]carbamate dihydrochloride	444	87	9.9E-03	3.1E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.5E-01	4.8E-03	1.7E-01	-8.91	-9.76	-11.42	-2.00	0.64	0.0%	0.0%	1.3E-41
3678	49715-04-0	chloromethyl chlorosulphate	165	40	6.9E+00	1.8E+04	9.3E+01	0	3.5E-06	3.5E-06	3.5E-06	conf	conf	4.6E-01	6.4E-03	2.4E-01	-10.62	-11.63	-13.18	-1.28	1.22	0.0%	0.0%	4.5E-65
3679	4224-62-8	6-Chlorohexanoic acid	151	56	1.3E+00	1.8E+03	2.0E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	4.6E-01	6.4E-03	2.4E-01	-11.88	-11.71	-13.21	-1.09	0.63	0.0%	0.0%	1.7E-67
3680	82104-74-3	1,3-dihydro-1-oxoisobenzofuran-5-carbonitrile	159	93	1.2E-02	2.8E+03	1.8E+00	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.6E-01	6.4E-03	2.3E-01	-9.13	-9.67	-11.32	-1.64	0.93	0.0%	0.0%	7.6E-44
3681	13115-71-4	(2S)-5-amino-2-[(aminoacetyl)amino]-5-oxopentanoic acid	203	308	1E-09	7.2E+04	6.6E-04	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	4.6E-01	6.4E-03	2.3E-01	-8.61	-9.60	-11.25	0.41	1.30	0.0%	0.0%	1.2E-62
3682	5324-06-1	1,3-bis[(2-hydroxyethyl)thio]propan-2-ol	212	117	4.8E-06	3.5E+04	8.1E-02	14.0	3.5E-06	3.5E-06	3.5E-06	conf	conf	4.6E-01	6.4E-03	2.4E-01	-10.02	-11.24	-13.12	0.28	0.84	0.0%	0.0%	5.0E-82
3683	98-37-3	3-amino-4-hydroxybenzenesulphonic acid	189	161	1.1E-06	1.3E+05	2.8E-03	14.0	3.5E-06	3.5E-06	3.5E-07	conf	conf	4.6E-01	6.4E-03	2.4E-01	-9.60	-10.79	-13.07	-0.32	0.63	0.0%	0.0%	1.7E-74
3684	282102-50-5	608-177-1	470	87	9.9E-03	1.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.4E-01	4.7E-03	1.7E-01	-9.49	-9.81	-11.46	-1.84	0.64	0.0%	0.0%	2.4E-43
3685	76-75-5	5-ethyl-5-(1-methylbutyl)-2-thiobarbituric acid	242	216	2.3E-08	3.4E+01	2.2E+02	7.5	3.5E-06	2.6E-07	1.1E-06	conf	conf	3.7E-01	5.1E-03	1.8E-01	-9.65	-10.32	-11.95	-2.42	0.85	0.0%	0.0%	1.7E-42
3686	62756-44-9	3-hydroxymethylpyridinium fluoride	129	87	9.9E-03	8.9E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.3E-01	4.6E-03	1.6E-01	-9.52	-9.82	-11.46	-1.84	0.64	0.0%	0.0%	2.4E-43
3687	1174931-74-1	695-716-9	449	216	2.1E-08	3.1E-01	5.2E+07	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	2.7E-01	3.8E-03	1.3E-01	-11.24	-11.89	-12.35	-2.53	0.06	0.0%	0.0%	4.9E-45
3688	73263-40-8	strontium bis[2-chloro-5-[(2-hydroxy-1-naphthyl)azo]toluene-4-sulphonate]	839	87	9.9E-03	3.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.3E-01	4.5E-03	1.6E-01	-9.49	-9.82	-11.48	-1.03	1.01	0.0%	0.0%	1.1E-50
3689	68227-78-1	N-(5-chloro-2-methylphenyl)-3-hydroxy-4-[[2-methoxy-5-[(phenylamino)carbonyl]phenyl]azo]naphthalene-2-carbo	565	350	1.1E-20	1.3E-04	5.1E+08	14.0	3.5E-06	1.1E-07	1.1E-08	conf	conf	3.2E-01	4.4E-03	1.5E-01	-10.95	-11.03	-11.28	-0.96	1.10	0.0%	0.0%	1.8E-49
3690	64-04-0	phenethylamine	121	11	5.5E+01	1.2E+03	2.2E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	3.6E-01	5.1E-03	1.8E-01	-11.39	-11.10	-12.42	-3.19	1.27	0.0%	0.0%	6.2E-40
3691	284462-37-9	608-211-5	243	189	1.2E-06	2.5E+04	6.3E+02	4.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	4.6E-01	5.5E-03	2.0E-01	-9.73	-10.72	-12.64	-2.00	0.91	0.0%	0.0%	6.5E-52
3692	1231148-36-4	14,14',15,15'-tetradehydro-7,7'-spiro8((dibenzo[b,g][1,9,4,6]dioxadiazacyclododecine]	517	291	1.7E-13	7.0E-04	8.5E+05	0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.7E-01	3.8E-03	1.4E-01	-9.93	-10.33	-12.15	-3.52	0.26	0.0%	0.0%	3.5E-35
3693	536759-91-8	Ethyl 1-(4-methoxyphenyl)-6-(4-nitrophenyl)-7-oxo-4,5,6,7-tetrahydro-1H-pyrazolo[3,4-c]pyridine-3-carboxylate	436	264	1.2E-11	2.7E+00	1.1E+04	-0.2	3.5E-06	1.1E-06	1.1E-07	conf	conf	3.5E-01	4.9E-03	1.8E-01	-10.05	-10.63	-12.66	-2.82	0.18	0.0%	0.0%	3.2E-45
3694	181525-38-2	605-935-3	231	181	2.4E-08	6.6E+02	6.2E-01	1.7	3.5E-06	3.5E-06	3.5E-07	conf	conf	4.0E-01	5.3E-03	2.0E-01	-10.18	-11.58	-13.19	-2.03	0.64	0.0%	0.0%	1.7E-57
3695	39672-75-8	(9beta,11beta,16alpha)-9,11-Epoxy-21-hydroxy-16,17-[(1-methylethylidene)bis(oxy)]-pregna-1,4-diene-3,20-dione	415	213	2.5E-10	4.4E+01	2.8E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.7E-01	5.1E-03	1.9E-01	-9.90	-10.97	-12.70	-0.92	0.25	0.0%	0.0%	7.4E-64
3696	583-39-1	benzimidazole-2-thiol	150	119	4.8E-06	1.1E+03	8.5E+01	11.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	3.7E-01	5.1E-03	1.9E-01	-9.86	-10.90	-12.71	-2.15	0.80	0.0%	0.0%	1.0E-51
3697	221640-21-7	1,2-Propanediamine, N1-(2-aminoethyl)-3-(4-ethoxyphenyl)-, hydrochloride (1:2), (2S)-	310	87	9.9E-03	2.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E-01	3.9E-03	1.4E-01	-9.57	-9.88	-11.54	-1.90	0.64	0.0%	0.0%	2.0E-43
3698	1122460-01-1	(1R,2S,5R)-5-methyl-2-(prop-2-yl)cyclohexyl (ethylamino)(oxo) acetate	255	134	6.4E-01	4.4E+01	7.2E+02	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	3.7E-01	5.1E-03	1.9E-01	-11.10	-11.81	-13.29	-2.00	0.74	0.0%	0.0%	7.9E-59
3699	947701-81-7	undec-10-en-1-yl 2-cyano-3,3-diphenylacrylate	402	206	2.0E-08	1.5E-03	1.9E+08	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	2.3E-01	3.2E-03	1.2E-01	-10.24	-11.19	-12.90	-4.24	0.90	0.0%	0.0%	1.7E-35
3700	61358-25-6	bis(4-tert-butylphenyl)iodonium hexafluorophosphate	538	87	9.9E-03	3.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E-01	3.9E-03	1.4E-01	-9.57	-9.88	-11.54	-3.03	1.18	0.0%	0.0%	2.4E-34
3701	39648-67-4	609-734-1	348	90	2.4E-08	4.4E-05	1.7E+05	1.5	3.5E-06	1.1E-07	1.1E-08	conf	conf	2.7E-01	3.8E-03	1.4E-01	-9.85	-11.47	-13.04	0.34	0.06	0.0%	0.0%	1.0E-83
3702	198979-98-5	tetra-1-naphthyl 3,3',5,5'-tetra-tert-butyl-6,6'-dimethylbiphenyl-2,2'-diyl bis(phosphite)	1071	87	9.9E-03	7.4E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E-01	3.8E-03	1.4E-01	-9.00	-9.86	-11.53	-1.84	0.64	0.0%	0.0%	6.3E-44
3703	5405-40-3	(3S)-3-hydroxy-4,4-dimethyldihydrofuran-2(3H)-one	130	31	5.5E-02	1.8E+05	1.1E-01	12.6	3.5E-06	3.5E-06	1.1E-06	conf	conf	3.7E-01	5.1E-03	1.9E-01	-10.09	-11.18	-13.24	-1.18	1.12	0.0%	0.0%	8.2E-67
3704	31775-89-0	3-[(3-sulfanylbutanoyl)oxy]-2,2-bis[[(3-sulfanylbutanoyl)oxy]methyl]propyl 3-sulfanylbutanoate	545	196	2.3E-09	8.5E-01	1.8E+04	9.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	3.1E-01	4.3E-03	1.6E-01	-10.27	-11.32	-12.80	-3.09	1.30	0.0%	0.0%	5.4E-44
3705	51076-95-0	2-chloro-1,1,1-trethoxyethane	197	11	1.7E+01	5.6E+02	7.2E+02	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	3.0E-01	4.2E-03	1.5E-01	-11.78	-11.53	-12.75	-2.05	0.71	0.0%	0.0%	4.6E-53
3706	66422-95-5	2-(2,4-diaminophenoxy)ethanol dihydrochloride	241	87	9.9E-03	1.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E-01	3.7E-03	1.3E-01	-9.60	-9.91	-11.56	-1.90	0.64	0.0%	0.0%	1.4E-43
3707	28950-61-0	tetrasodium 4,4' bis[[4-morpholino-6-(p-sulphonatoanilino)-1,3,5-triazin-2-yl]amino]stilbene-2,2'-disulphonate	1129	87	9.9E-03	7.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E-01	3.6E-03	1.3E-01	-9.59	-9.91	-11.58	-1.84	0.64	0.0%	0.0%	2.5E-44
3708	86357-14-4	617-838-3	381	305	1.9E-14	1.4E+04	1.6E-01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	3.5E-01	4.8E-03	1.7E-01	-8.74	-9.72	-11.38	-0.52	1.47	0.0%	0.0%	1.4E-54
3709	6448-95-9	3-hydroxy-4-[(2-methyl-5-nitrophenyl)azo]-N-phenylnaphthalene-2-carboxamide	426	290	1.2E-14	3.2E-02	1.7E+08	9.4	3.5E-06	3.5E-07	3.5E-08	conf	conf	2.0E-01	2.8E-03	9.9E-02	-11.17	-11.45	-11.82	-0.96	1.10	0.0%	0.0%	1.6E-54
3710	1164-92-7	601-431-2	332	145	8.6E-05	5.3E+00	1.2E+04	0	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.7E-01	3.8E-03	1.4E-01	-9.95	-10.32	-12.18	-2.51	0.52	0.0%	0.0%	9.9E-44
3711	84449-85-4	696-244-6	666	87	9.9E-03	4.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E-01	3.6E-03	1.3E-01	-9.60	-9.92	-11.58	-1.84	0.64	0.0%	0.0%	2.2E-44
3712	1132935-63-7	N-[6-[3-tert-butyl-5-(2,4,6-trimethylphenyl)-4-(2,6-dimethylpyrimidin-1(2H)-yl)-2-methoxyphenyl]-2-naphthyl]methanesulfonamide	494	350	1.3E-17	7.6E-03	1.9E+04	8.6	3.5E-06	3.5E-07	1.1E-07	conf	conf	2.7E-01	3.7E-03	1.3E-01	-9.86	-10.70	-12.28	-3.51	0.24	0.0%	0.0%	2.6E-36
3713	593-60-2	bromoethylene	107	-94	1.4E+05	6.1E+03	3.3E+01	14.0	3.5E-06	1.3E-07	6.6E-08	conf	conf	2.1E-01	2.9E-03	1.0E-01	-12.86	-12.17	-14.78	-0.48	0.73	0.0%	0.0%	4.7E-93
3714	117380-85-4	ethyl (1R,2S)-1-amino-2-vinylcyclopropanecarboxylate sulfate (2:1)	408	87	9.9E-03	2.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.5E-01	3.5E-03	1.3E-01	-9.61

3819	1073607-50-1	4-(2-{2-(2-Chloro-3-{2-[1,1-dimethyl-3-(4-sulfobutyl)-1H-benzo[e]indolium-2-yl]vinyl}cyclohex-2-en-1-ylidene)ethyli	845	87	9.9E-03	5.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E-01	1.8E-03	6.4E-02	-9.90	-10.22	-11.89	-1.84	0.64	0.0%	0.0%	4.7E-47
3820	437717-43-6	610-141-5	392	317	1.1E-18	1.2E+01	3.2E+00	0.6	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.4E-01	2.0E-03	7.3E-02	-9.51	-10.59	-12.42	-2.31	1.01	0.0%	0.0%	1.5E-47
3821	86404-04-8	(5R)-5-[(1S)-1,2-Dihydroxyethyl]-4-ethoxy-3-hydroxyfuran-2(5H)-one	204	144	1.5E-07	4.4E+05	4.9E-04	13.5	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.7E-01	2.3E-03	8.7E-02	-10.15	-11.36	-13.53	-1.25	0.90	0.0%	0.0%	3.4E-69
3822	74462-02-5	4,4'-Ethylhexane-1,1-diyldiphenol	298	163	6.5E-07	4.4E-01	1.1E+04	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	1.1E-01	1.6E-03	5.6E-02	-11.42	-12.02	-13.23	-3.54	0.52	0.0%	0.0%	3.1E-44
3823	19694-10-1	3-amino-4-chlorobenzamide	171	136	8.1E-04	6.6E+03	3.0E+00	1.5	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.5E-01	2.1E-03	7.9E-02	-10.19	-11.30	-13.11	-1.85	0.83	0.0%	0.0%	1.6E-58
3824	64-86-8	colchicine	399	242	4.2E-09	1.4E+01	7.2E+01	-1.0	3.5E-06	2.1E-07	3.5E-07	conf	conf	1.3E-01	1.8E-03	6.5E-02	-9.76	-10.51	-12.21	-2.93	1.16	0.0%	0.0%	2.1E-40
3825	197706-51-7	(2S)-6-fluoro-2-{[2R)-oxiran-2-yl]chromane	194	58	1.0E+00	7.7E+02	4.7E+02	14.0	3.5E-06	1.1E-06	1.1E-07	conf	conf	1.5E-01	2.1E-03	7.7E-02	-11.68	-11.48	-13.14	-2.27	1.25	0.0%	0.0%	1.1E-54
3826	3034-38-6	4-nitroimidazole	113	95	8.6E-05	4.6E+04	7.6E-01	0.2	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.5E-01	2.0E-03	7.5E-02	-9.76	-11.04	-13.04	-1.73	1.18	0.0%	0.0%	4.1E-59
3827	69739-16-8	(6R,7R)-7-[(Z2)-2-(2-amino-1,3-thiazol-4-yl)-2-(methoxyimino)acetyl]amino}-3-{[(5-carboxymethyl)-4-methyl-1,3-th	585	350	1.1E-20	3.1E+00	5.1E+01	14.0	3.5E-06	1.1E-07	1.1E-07	conf	conf	1.1E-01	1.6E-03	5.6E-02	-9.46	-10.33	-11.90	-1.86	0.91	0.0%	0.0%	6.2E-47
3828	173194-95-1	(6-hydroxy-2-naphthyl)boronic acid	188	158	7.1E-08	2.8E+03	1.6E+02	8.9	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.4E-01	2.0E-03	7.3E-02	-10.25	-11.34	-13.11	-1.90	0.64	0.0%	0.0%	5.6E-58
3829	59875-04-6	611-909-2	159	121	2.8E-03	7.0E+03	3.4E+00	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E-01	2.2E-03	7.9E-02	-9.36	-10.17	-11.82	-1.40	1.39	0.0%	0.0%	2.0E-50
3830	1103-38-4	barium bis[2-[(2-hydroxynaphthyl)azo]naphthalenesulphonate]	892	87	9.9E-03	6.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E-01	1.5E-03	5.5E-02	-9.97	-10.29	-11.95	-1.03	1.01	0.0%	0.0%	3.5E-55
3831	1176-81-4	21-Acetoxy-6alpha-fluoro-11beta-hydroxy-16alpha-methyl-4-pregnene-3,20-dione	421	207	6.9E-10	3.6E+00	2.8E+02	14.0	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.4E-01	1.9E-03	7.1E-02	-10.50	-11.52	-13.14	-1.84	0.72	0.0%	0.0%	5.5E-59
3832	3409-21-0	2-{2-(dimethylamino)ethyl}-2,3-dihydro-1H-inden-1-one	203	85	4.0E-02	7.0E+03	1.7E+02	9.3	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.4E-01	1.9E-03	7.1E-02	-10.90	-11.40	-13.18	-2.28	0.70	0.0%	0.0%	5.9E-55
3833	3222-49-9	5-methylnicotinic acid	137	77	2.1E-01	3.9E+03	1.9E+01	1.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.4E-01	1.9E-03	7.1E-02	-10.78	-11.18	-13.13	-0.91	0.69	0.0%	0.0%	1.5E-68
3834	191605-10-4	606-247-6	418	236	9.7E-10	1.8E+03	1.1E+04	1.1	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.4E-01	1.9E-03	7.1E-02	-10.55	-11.24	-13.10	-1.55	0.81	0.0%	0.0%	1.8E-61
3835	61320-65-8	Methyl 5-amino-4-cyano-3-methylthiophene-2-carboxylate	196	125	2.7E-03	1.3E+03	2.4E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.4E-01	1.9E-03	7.1E-02	-10.44	-11.25	-13.15	-1.42	0.52	0.0%	0.0%	2.3E-63
3836	16298-03-6	methyl 5-aminopyrazinecarboxylate	153	85	2.1E-01	8.7E+04	1.5E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.4E-01	1.9E-03	6.8E-02	-9.63	-10.23	-11.87	-1.64	0.96	0.0%	0.0%	1.2E-48
3837	82410-32-0	Ganciklovir	255	266	6.0E-15	5.3E+04	5.4E-02	2.2	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.4E-01	1.9E-03	7.0E-02	-9.87	-11.24	-13.11	-0.68	1.60	0.0%	0.0%	7.5E-71
3838	17270-01-8	Unknown	651	90	2.7E-06	6.8E-06	1.5E+09	14.0	3.5E-06	1.3E-07	6.6E-10	conf	conf	8.1E-02	1.1E-03	3.9E-02	-11.79	-11.59	-12.35	-4.74	0.92	0.0%	0.0%	7.9E-28
3839	87392-07-2	(2S)-tetrahydrofuran-2-carboxylic acid	116	33	1.8E-01	5.2E+04	1.5E+00	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.4E-01	1.9E-03	7.1E-02	-11.99	-11.83	-13.65	-0.30	0.59	0.0%	0.0%	2.1E-81
3840	143183-03-3	S-1,3-benzothiazol-2-yl (2Z)-(2-amino-1,3-thiazol-4-yl)[(trityloxy)imino]ethanethioate	579	336	1.8E-16	7.4E-06	2.5E+09	0	3.5E-06	3.5E-07	3.5E-08	conf	conf	1.1E-01	1.5E-03	5.6E-02	-10.15	-10.68	-12.50	-5.79	1.16	0.0%	0.0%	4.5E-22
3841	131-56-6	2,4-dihydroxybenzophenone	214	142	1.9E-05	2.5E+03	9.1E+02	7.8	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.1E-01	1.6E-03	5.8E-02	-10.21	-10.96	-12.63	-2.40	0.29	0.0%	0.0%	1.2E-48
3842	15934-01-7	triammonium hydrogen ethylenediaminetetraacetate	343	87	9.9E-03	2.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E-01	1.4E-03	5.1E-02	-10.01	-10.33	-11.98	-1.16	0.78	0.0%	0.0%	3.0E-54
3843	154477-55-1	methyl 2-[4-(4-{4-(hydroxyd(phenyl)methyl)piperidin-1-yl}butanoyl)phenyl]-2-methylpropanoate	514	263	2.8E-14	5.0E-02	2.0E+06	1.1	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.1E-02	1.3E-03	4.6E-02	-11.42	-12.34	-13.29	-3.83	1.32	0.0%	0.0%	5.9E-42
3844	924663-38-7	2-{[4-(3-methoxypropoxy)-3-methyl-1-oxidopyridin-2-yl]methyl}sulfinyl}-1H-benzimidazole	375	285	4.4E-16	6.4E+00	6.0E+00	3.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.3E-01	1.8E-03	6.6E-02	-9.95	-11.13	-13.11	-1.56	0.64	0.0%	0.0%	1.9E-61
3845	477-29-2	colchicoside	548	348	6.1E-23	1.1E+02	1.9E-01	-0.7	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.1E-01	1.6E-03	5.8E-02	-9.67	-10.71	-12.57	-2.05	2.34	0.0%	0.0%	2.1E-51
3846	1001320-38-2	O,S-dibutyl dithioimidodicarbonate	249	102	5.8E-03	2.3E+01	5.0E+03	8.5	3.5E-06	1.5E-06	1.1E-06	conf	conf	1.2E-01	1.7E-03	6.1E-02	-12.39	-12.82	-13.82	-3.59	1.53	0.0%	0.0%	1.2E-48
3847	73612-34-7	barium bis[6-chloro-4-[(2-hydroxy-1-naphthyl)azo]toluene-3-sulphonate]	889	87	9.9E-03	6.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.3E-02	1.3E-03	4.7E-02	-10.04	-10.36	-12.02	-1.03	1.01	0.0%	0.0%	7.1E-56
3848	111298-82-9	619-847-8	401	332	3.7E-14	2.7E+01	5.5E-01	2.5	3.5E-06	3.5E-07	3.5E-07	conf	conf	1.1E-01	1.5E-03	5.4E-02	-9.55	-10.70	-12.54	-1.48	0.65	0.0%	0.0%	1.7E-56
3849	24650-42-8	2,2-dimethoxy-1,2-diphenylethan-1-one	256	110	2.3E-03	7.3E+01	8.9E+02	0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E-01	1.6E-03	5.9E-02	-10.67	-11.33	-13.24	-1.66	0.11	0.0%	0.0%	8.3E-62
3850	210223-97-5	2,2-dimethoxy-N-(2-oxo-2-{[2-phenylethyl]amino}ethyl)ethanaminium chloride	303	87	9.9E-03	1.1E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E-01	1.5E-03	5.3E-02	-10.34	-12.00	-13.64	-1.84	0.64	0.0%	0.0%	4.3E-48
3851	120202-68-8	[(1R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methanesulfonic acid – methyl (2S)-(2-chlorophenyl)(6,7-dihydroth	554	87	9.9E-03	3.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E-02	1.3E-03	4.6E-02	-10.05	-10.37	-12.03	-1.84	0.64	0.0%	0.0%	2.4E-48
3852	54981-42-9	2-acetamido-5-chlorobenzenesulfonic acid - pyridine (1:1)	329	87	9.9E-03	2.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E-02	1.3E-03	4.6E-02	-10.06	-10.37	-12.03	-1.84	0.64	0.0%	0.0%	2.5E-48
3853	25628-08-4	N,N,N-triethylethanaminium 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonate	430	87	9.9E-03	3.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E-02	1.3E-03	4.6E-02	-10.06	-10.37	-12.03	-0.47	0.64	0.0%	0.0%	1.5E-61
3854	22450-96-0	N,N-dibutylbutan-1-aminium bis[2-(hydroxy-kO)benzoato(2-)-kO]borate(1-)	469	87	9.9E-03	3.2E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E-02	1.3E-03	4.6E-02	-9.49	-10.34	-12.00	-1.55	0.64	0.0%	0.0%	9.7E-51
3855	102601-34-3	sodium 3-(cyclohexylamino)-2-hydroxypropane-1-sulfonate	259	87	9.9E-03	1.8E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E-02	1.3E-03	4.6E-02	-10.06	-10.37	-12.03	-1.84	0.64	0.0%	0.0%	2.6E-48
3856	125700-67-6	603-087-9	321	87	9.9E-03	2.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E-02	1.3E-03	4.6E-02	-10.06	-10.37	-12.03	-1.84	0.64	0.0%	0.0%	2.5E-48
3857	674347-28-5	Lithium naphthalene-2-carboxylate	178	87	9.9E-03	1.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E-02	1.3E-03	4.6E-02	-10.07	-10.38	-12.02	-1.84	0.64	0.0%	0.0%	2.8E-48
3858	1266664-66-7	7R)-4-(5-Chloro-1,3-benzoxazol-2-yl)-7-methyl-1,4-diazepan-1-ium chloride	302	87	9.9E-03	2.1E+03	3.0E+02	0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E-02	1.3E-03	4.6E-02	-9.50	-10.34	-12.00	-2.32	0.64	0.0%	0.0%	7.7E-44
3859	872-36-6	vinylene carbonate	86	14	4.7E-01	4.3E+04	2.8E-01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	1.2E-01	1.7E-03	6.3E-02	-11.03	-11.70	-13.71	-2.35	0.21	0.0%	0.0%	1.7E-59
3860	4062-46-8	17β-hydroxy-1a-methyl-5-oandrostan-3-one acetate	347	150	4.7E-05	2.4E+00	3.1E+04	14.0	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.1E-02	1.3E-03	4.6E-02	-11.20	-11.22	-12.82	-2.64	0.47	0.0%	0.0%	1.1E-48
3861	60924-38-1	(3aS,4R,5S,6S,8R,9R,9aR,10R)-6-ethenyl-5-hydroxy-4,6,9,10-tetramethyl-1-oxodecahydro-3a,9-propanocyclopenta[8	457	230	1.1E-11	6.9E+00	3.2E+02	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	1.1E-01	1.5E-03	5.6E-02	-10.43	-11.51	-13.22	-1.86	0.70	0.0%	0.0%	1.4E-59
3862	1836-62-0	2-(2-Methoxyphenoxy)ethanamine	167	54	1.1E+00	1.3E+05	4.6E+00	9.1	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.1E-01	1.5E-03	5.7E-02	-11.00	-11.41	-13.26	-1.74	0.83	0.0%	0.0%	4.2E-61
3863	833-86-3	3-(1-pyrrolidinyl)propiphenone hydrochloride	240	87	9.9E-03	1.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.6E-02	1.2E-03	4.3E-02	-10.09	-10.40	-12.05	-1.84	0.64	0.0%	0.0%	1.5E-48
3864	14352-61-5	methyl cyclobutylacetate	156	-15	3.9E-01	2.6E+02	1.3E+03	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E-02	1.3E-03	4.6E-02	-12.31	-11.98	-13.63	-2.00	0.81	0.0%	0.0%	2.7E-62
3865	35130-97-3	(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl methanesulfonate	219	99	2.3E-02	9.9E+04	1.7E+00	8.8	3.5E-06	1.1E-06	1.1E-06	conf	conf	1.1E-01	1.5E-03	5.7E-02	-10.35	-11.34	-13.25	-1.13	1.01	0.0%	0.0%	1.7E-67
3866	2730-71-4	thiocolchicine	416	252	8.9E-11	3.7E+03	3.2E+02	-0.7	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.8E-02	1.4E-03	5.0E-02	-10.14	-10.82	-12.61	-2.92	0.53	0.0%	0.0%	6.9E-44
3867	153-00-4	metenolone	302	150	1.6E-06	3.5E+01	4.9E+03	14.0	3.5E-06	3.5E-07	3.5E-07	conf	conf	9.1E-02	1.3E-03	4.6E-02	-10.42	-11.15	-12.77	-1.94	0.26	0.0%	0.0%	2.8E-54
3868	2766-74-7	5-chlorothiophene-2-sulfonyl chloride	217	97	3.7E-02	4.7E+02	2.6E+03	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E-02	1.3E-03	4.5E-02	-10.69	-10.47	-12.07	-1.52	0.41	0.0%	0.0%	1.1E-51
3869	438193-30-7	Phosphonium, triphenyl[(trans-4-(1E)-1-propen-1-ylcyclohexyl]methyl-, iodide (1:1)	526	87	9.9E-03	3.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.2E-02	1.1E-03	4.1E-02	-10.10	-10.42	-12.08	-2.82	0.64	0.0%	0.0%	3.5E-40
3870	31981-44-9	17-hydroxy-19-norpregn-4-ene-3,20-dione 17-acetate	358	178	4.2E-06	6.2E+01	1.7E+03	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E-02	1.3E-03	4.6E-02	-9.56	-10.41	-12.05	-2.09	0.65	0.0%	0.0%	3.1E-46
3871	119302-20-4	(2β,3α,5α,16β,17β)-2-(morpholin-4-yl)-16-[pyrrolidin-1-yl]androstane-3,17-diol	447	228	4.4E-12	3.0E+01	5.4E+02	9.8	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E-02	1.3E-03	4.6E-02	-10.00	-10.92	-12.67	-2.28	0.62	0.0%	0.0%	3.9E-50
3872	2137-18-0	gestonorone	316	170	2.2E-07	9.3E+01	4.3E+02	13.9	3.5E-06	3.5E-07	1.1E-07	conf	conf	9.2E-02	1.3E-03	4.6E-02	-10.01	-10.92	-12.68	-1.65	0.33	0.0%	0.0%	3.0E-56
3873	380843-75-4	4-[(2,4-dichloro-5-methoxyphenyl)amino]-6-methoxy-7-{3-(4-methylpiperazin-1-yl)propoxy}quinoline-3-carbonitrile	530	278	1.3E-12	2.2E-01	2.1E+04	8.1	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.2E-02	1.3E-03	4.6E-02	-10.69	-11.75	-13.32	-3.62	0.40	0.0%	0.0%	5.9E-44
3874	13978-15-1	Octan-2-yl 2-cyanoacrylate	209	36	1.8E-01	4.0E+01	1.9E+04	0	3.5E-06	3.5E-07	1.1E-06	conf	conf	9.2E-02	1.3E-03	4.7E-02	-10.91	-11.48	-13.34	-2.77	0.27	0.0%	0.0%	8.2E-52
3875	53595-66-7	5-chlorothiophene-2-sulfonamide	198	117	9.7E-03	5.3E+03	6.8E+00	14.0	3.5E-06	3.5E-07	6.6E-08	conf	conf	9.1E-02	1.3E-03	4.6E-02	-9.75	-10.39	-12.04	-1.71	1.21	0.0%	0.0%	1.5E-49
3876	54605-02-6	611-173-2	539	239	2.3E-12	2.0E-01	1.0E+04	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.2E-02	1.3E-03	4.7E-02	-11.21	-12.47	-13.83	-2.55	0.23	0.0%	0.0%	1.1E-58
3877	18979-61-8	4-butylbenzene-1,3-diol	166	89	9E-03	9.4E+02	1.1E+03	9.6	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E-02	1.3E-03	4.7E-02	-11.32	-11.70	-13.36	-2.48	0.38	0.0%	0.0%	6.6E-55
3878	5534-13-4	9-fluoro-11β,17,21-trihydroxy-16β-methylpregna-1,4-diene-3,20-dione 17-propionate	449	229	3.7E-12	1.1E+01	8.9E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E-02	1.3E-03	4.6E-02	-9.40	-10.35	-11.99	-1.84	0.32	0.0%	0.0%	5.6E-48
3879	36130-02-6	609-203-4	461	224	3.3E-11	1.9E+00	5.1E+03	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.2E-02	1.3E-03	4.7E-02	-11.19	-12.45	-13.83	-2.25	0.11	0.0%	0.0%	8.5E-62
3880	51997-51-4	4-(Oxiran-2-ylmethoxy)-9H-carbazole	239	153	4.5E-05	8.0E+00	7.1E+02	0	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.2E-02	1.3E-03	4.7E-02	-10.51	-11.23	-13.29	-2.28	0.33	0.0%	0.0%	4.8E-56
3881	165115-73-1	2-(2-(2,4-difluorophenyl)prop-2-en-1-yl)propane-1,3-diol	228	86	4.6E-04	2.8E+02	5.2E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.2E-02	1.3E-03	4.7E-02	-10.89	-11.66	-13.37	-2.13	1.16	0.0%	0.0%	2.6E-58
3882	63432-37-1	2-(methylthio)-3-nitropyrazolo[1,5-a]pyridine	210	128	1.9E-03	3.5E+02	4.3E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E-02	1.3E-03	4.6E-02	-10.01	-10.38	-12.03	-2.42	0.50	0.0%	0.0%	3.6E-43
3883	87670-90-1	2-((1-((2-methoxyphenyl)amino)-1,3-dioxobutan-2-yl)diazenyl)benzoic acid	355	243	3.5E-10	2.7E+01	2.5E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.2E-02	1.3E-03	4.7E-02	-10.49	-11.57	-13.30	-4.00	2.80	0.0%	0.0%	1.4E-40
3884	936103-10-5	2-[(3-nitropyrazolo[1,5-a]pyridin-2-yl)oxy]ethanol	224	156	1.6E-03	3.8E+03	1.4E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E-02	1.3E-03	4.7E-02	-10.25	-11.34	-13.29	-1.85	0.39	0.0%	0.0%	2.2E-60
3885	398489-26-4	Tert-butyl 3-oxoazetidine-1-carboxylate	171	47	3.8E+00	1.7E+04	4.6E+01	0	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E-02	1.3E-03	4.7E-02	-10.72	-11.57	-13.35	-2.07	1.08	0.0%	0.0%	1.1E-58
3886	95748-46-2	benzyl (5-{[4-((5-[acetyl(hydroxy)amino]pentyl)amino)-4-oxobutanoyl](hydroxy)amino]pentyl)carbamate	495	332	1.1E-20	2.6E+02	5.5E+00	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E-02	1.3E-03	4.7E-02	-10.09	-11.24	-13.25	-1.53	1.05	0.0%	0.0%	3.4E-63
3887	116539-55-0	(1S)-3-(methylamino)-1-(2-thienyl)propan-1-ol	171	72	1.8E-02	6.4E+04	6.3E+00	10.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	9.2E-02	1.3E-03	4.7E-02	-10.31	-11.31	-13.31	-1.71	0.84	0.0%	0.0%	6.8E-62
3888	501925-98-0	hexane-1,6-diyl bis[(3-(trimethoxysilyl)propyl)carbamate]	529	189	2.1E-07	6.5E+00	3.1E+00	11.3	3.5E-06	1.1E-06	1.1E-06	conf	conf	9.2E-02	1.3E-03	4.7E-02	-10.44	-11.46	-13.36	-1.80	0.21	0.0%	0.0%	1.5E-61
3889	935859-71-5	2-(methylsulfonyl)-3-nitropyrazolo[1,5-a]pyridine	242	164	5.2E-05	2.1E+03	1.4E+00	0	3.5E-06	1.1E-06	1.1E-07	conf	conf	9.2E-02	1.3E-03	4.7E-02	-10.00	-11.25	-13.25	-2.01	0.18	0.0%	0.0%	2.5E-58
3890	956317-36-5	689-732-5	203	153	2.4E-04	3.6E+03	6.9E+01	14.0	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.2E-02	1.3E-03	4.7E-02	-11.18	-12.28	-13.88	-1.09	0.71	0.0%	0.0%	6.4E-75
3891	849793-87-9	Ethyl [(5-chlorothiophen-2-yl)sulfonyl]carbamate	270	143	2.8E-04	7.0E+02	8.3E+01	4.4	3.5E-06	3.5E-06	1.1E-06	conf	conf	9.2E-02	1.3E-03	4.7E-02	-11.18	-12.17	-13.89	-1.94	0.61	0.0%	0.0%	1.4E-65
3892	152845-00-6	Dilithium naphthalene-1,5-disulfonate	300	87	9.9E-03	2.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.8E-02	9.5E-04	3.4E-02	-10.19	-10.50	-12.15	-1.14	0.64	0.0%	0.0%	4.6E-56
3893	24916-90-3	9β,11β-epoxy-17,21-dihydroxy-16α-methylpregna-1,4-diene-3,20-dione	372	206	2.7E-10	6.7E+01	7.6E+01	13.2	3.5E-06	1.1E-06	1.1E-06	conf	conf	8.5E-02	1.2E-03	4.4E-02	-10.62	-11.67	-13.34	-1.05	0.26	0.0%	0.0%	2.7E-69
3894	944730-39-6	Tetrasodium (3,3',3'',3'''-{[29H,31H-phthalocyanine-1,8,15,22-tetrayl-14N29,N30,N31,N32]tetrasulfonyl}tetrapropan	1373	87	9.9E-03	9.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.4E-02	8.9E-04	3.2E-02	-10.20	-10.52	-12.19	-0.84	0.58	0.0%	0.0%	1.9E-59
3895	2441-41-0	N-Palmitoylglycine	313	202	1.7E-07	4.1E-01	7.1E+05	3.5	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.3E-02	1.0E-03	3.8E-02	-10.87	-11.65	-13.40	-3.94	0.31	0.0%	0.0%	6.9E-42
3896	765-63-9	2,2,3,3-Tetrafluorooxetane	130	-86	1.8E+05	1.6E+04	8.9E+01	14.0	3.5E-06	1.1E-06	3.5E-07	conf	conf	5.5E-02	7.6E-04	2.7E-02	-13.63	-13.22	-15.66	-2.38	0.64	0.0%	0.0%	1.2E-80
3897	23680-84-4	2-chloro-6,7-dimethoxyquinazolin-4-amine	240	153	2.0E-04	7.7E+02	3.2E+01	-0.2	3.5E-06	1.1E-06	3.5E-07	conf	conf	7.0E-02	9.7E-04	3.6E-02	-10.41	-11.44	-13.39	-2.22	0.75	0.0%	0.0%	1.3E-57
3898	20826-04-4	5-bromonicotinic acid	202	100	5.0E-02	1.

3994	591-51-5	phenyllithium	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	9.1E+01	-6.77	-7.07	-8.72	-1.84	0.64
3995	143-29-3	bis(2-(2-butoxyethoxy)ethoxy)methane	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+02	2.3E+00	8.2E+01	-6.81	-7.12	-8.77	-0.74	0.42
3996	10584-98-2	2-ethylhexyl 4,4-dibutyl-10-ethyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+02	2.1E+00	7.6E+01	-6.84	-7.15	-8.80	-3.10	1.24
3997	818-08-6	dibutyltin oxide	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+02	2.0E+00	7.2E+01	-6.87	-7.18	-8.83	-2.84	0.64
3998	631-61-8	ammonium acetate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+02	2.0E+00	7.1E+01	-6.87	-7.18	-8.83	-0.01	0.62
3999	683-18-1	dibutyltin dichloride	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.4E+01	-6.92	-7.23	-8.88	-3.53	1.06
4000	5205-93-6	N-(3-(dimethylamino)propyl)methacrylamide	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	6.2E+01	-6.93	-7.24	-8.89	-0.73	0.31
4001	288-32-4	imidazole	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	6.1E+01	-6.94	-7.25	-8.90	-0.63	0.22
4002	3091-25-6	trichlorooctylstannane	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	6.0E+01	-6.95	-7.26	-8.91	-3.67	0.64
4003	55310-46-8	sodium dibenzyldithiocarbamate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	6.0E+01	-6.95	-7.26	-8.91	-2.95	0.64
4004	7360-53-4	aluminium triformate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.6E+00	5.8E+01	-6.96	-7.27	-8.92	-2.89	0.70
4005	867-56-1	sodium (S)-lactate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+02	1.5E+00	5.4E+01	-6.99	-7.30	-8.95	0.07	0.83
4006	2440-22-4	2-(2H-benzotriazol-2-yl)-p-cresol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+02	1.5E+00	5.4E+01	-7.00	-7.30	-8.96	-1.66	1.40
4007	96-10-6	diethylaluminium chloride	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+02	1.5E+00	5.3E+01	-7.00	-7.31	-8.96	-1.84	0.64
4008	870-08-6	dioctyltin oxide	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+02	1.4E+00	5.2E+01	-7.01	-7.32	-8.97	-1.84	0.64
4009	557-20-0	diethylzinc	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+02	1.4E+00	5.1E+01	-7.02	-7.32	-8.97	-1.84	0.64
4010	13014-18-1	2,4-dichloro-1-(trichloromethyl)benzene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+02	1.4E+00	5.1E+01	-7.02	-7.33	-8.98	-0.88	0.23
4011	1191-15-7	diisobutylaluminium hydride	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.8E+01	1.4E+00	4.9E+01	-7.04	-7.34	-9.00	-1.84	0.64
4012	301-04-2	lead di(acetate)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.7E+01	1.4E+00	4.9E+01	-7.04	-7.35	-9.00	-2.10	0.70
4013	68649-12-7	1-Decene, tetramer, mixed with 1-decene trimer, hydrogenated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.37	-9.03	0.46	0.64
4014	77168-63-9	4-(Pyridin-4-yl)-1,3-thiazole-2(3H)-thione	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.37	-9.03	-1.84	0.64
4015	6921-34-2	benzylmagnesium chloride	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.37	-9.03	-1.84	0.64
4016	95-52-3	2-fluorotoluene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.37	-9.03	-1.71	0.64
4017	78182-00-0	(2-hydroxyethyl)(3-hydroxypropyl)dimethylammonium chloride	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.37	-9.03	-1.84	0.64
4018	1558-25-4	trichlorochloromethylsilane	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+01	1.3E+00	4.6E+01	-7.07	-7.37	-9.03	-1.84	0.64
4019	103-34-4	di(morpholin-4-yl) disulphide	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.6E+01	1.2E+00	4.3E+01	-7.09	-7.40	-9.05	-2.06	0.50
4020	2414-98-4	magnesium ethanolate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.5E+01	1.2E+00	4.3E+01	-7.10	-7.40	-9.05	0.41	0.72
4021	104-78-9	3-aminopropyldiethylamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.4E+01	1.2E+00	4.2E+01	-7.10	-7.41	-9.06	-0.90	0.98
4022	12108-13-3	tricarbonyl(methylcyclopentadienyl)manganese	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.5E+01	1.0E+00	3.8E+01	-7.15	-7.46	-9.11	-3.27	0.35
4023	35674-68-1	zinc bis[12-hydroxyoctadecanoate]	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.4E+01	1.0E+00	3.7E+01	-7.15	-7.46	-9.11	-3.07	0.58
4024	102-54-5	ferrocene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.0E+01	9.8E-01	3.5E+01	-7.18	-7.49	-9.14	-2.40	0.54
4025	68109-88-6	ethyl 9,9-dioctyl-4,7,11-trioxo-3,8,10-trioxa-9-stannatetradeca-5,12-dien-14-oate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.8E+01	9.5E-01	3.4E+01	-7.19	-7.50	-9.15	-1.84	0.64
4026	12626-81-2	Lead titanium zirconium oxide	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.8E+01	9.4E-01	3.4E+01	-7.20	-7.50	-9.15	-3.68	0.52
4027	77-58-7	dibutyltin dilaurate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.4E+01	9.0E-01	3.2E+01	-7.22	-7.52	-9.18	-3.02	0.64
4028	3087-36-3	titanium(4+) ethanolate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.3E+01	8.8E-01	3.2E+01	-7.23	-7.53	-9.18	0.73	0.57
4029	563-43-9	ethylaluminium dichloride	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.0E+01	8.3E-01	3.0E+01	-7.25	-7.56	-9.21	-1.84	0.64
4030	66069-34-9	[2R-(2a,3Z,5a)]-3-(2-hydroxyethylidene)-7-oxo-4-oxa-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, compound with	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.8E+01	8.0E-01	2.9E+01	-7.27	-7.57	-9.23	-0.23	0.95
4031	1071-93-8	adipohydrazide	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.0E+01	7.0E-01	2.5E+01	-7.33	-7.64	-9.29	-0.97	0.82
4032	133-14-2	bis(2,4-dichlorobenzoyl) peroxide	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.7E+01	6.5E-01	2.4E+01	-7.35	-7.66	-9.31	-1.84	0.64
4033	72-17-3	sodium lactate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.6E+01	6.5E-01	2.3E+01	-7.36	-7.67	-9.32	-0.25	0.50
4034	14882-18-9	bismuth oxide salicylate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.5E+01	6.3E-01	2.3E+01	-7.37	-7.68	-9.33	-1.84	0.64
4035	142-71-2	copper di(acetate)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.3E+01	6.1E-01	2.2E+01	-7.39	-7.70	-9.35	-3.32	0.60
4036	555-31-7	aluminium triisopropanolate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.2E+01	5.9E-01	2.1E+01	-7.40	-7.71	-9.36	-1.83	0.64
4037	22722-98-1	sodium dihydridobis(2-methoxyethanolato)aluminate(1-)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.2E+01	5.9E-01	2.1E+01	-7.40	-7.71	-9.36	-1.84	0.64
4038	66108-89-2	(R*,R*)-(±)-5-amino-N,N'-bis[2,3-dihydroxypropyl]-2,4,6-triiodoisophthaldiamide	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.2E+01	5.8E-01	2.1E+01	-7.41	-7.71	-9.36	-0.50	0.64
4039	52406-71-0	titanium(4+) 2-(dimethylamino)ethanolate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.9E+01	5.4E-01	1.9E+01	-7.44	-7.75	-9.40	-1.20	0.64
4040	15535-79-2	2,2-dioctyl-1,3,2-oxathiastannolan-5-one	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.5E+01	4.8E-01	1.7E+01	-7.49	-7.79	-9.44	-1.84	0.64
4041	25973-55-1	2-(2H-benzotriazol-2-yl)-4,6-ditert-pentylphenol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.5E+01	4.8E-01	1.7E+01	-7.49	-7.79	-9.45	-1.84	0.64
4042	68227-46-3	lactic acid, compound with 3-[2-(dimethylamino)ethyl] 1-(2-ethylhexyl) toluene-2,4-dicarbamate (1:1)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.4E+01	4.7E-01	1.7E+01	-7.50	-7.81	-9.46	-3.09	0.64
4043	142-72-3	magnesium di(acetate)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.3E+01	4.6E-01	1.7E+01	-7.51	-7.82	-9.47	0.20	0.27
4044	873-57-4	sodium piperidine-1-carbodithioate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.3E+01	4.6E-01	1.6E+01	-7.51	-7.82	-9.47	-1.84	0.64
4045	1070-10-6	titanium tetrakis(2-ethylhexanolate)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.2E+01	4.4E-01	1.6E+01	-7.53	-7.83	-9.48	-1.62	0.30
4046	14302-13-7	[1,3,8,16,18,24-hexabromo-2,4,9,10,11,15,17,22,23,25-decachloro-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.1E+01	4.3E-01	1.6E+01	-7.53	-7.84	-9.49	-0.60	0.64
4047	4985-85-7	N-(3-aminopropyl)iminodiethanol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.9E+01	4.0E-01	1.4E+01	-7.57	-7.87	-9.52	-2.21	0.64
4048	86675-46-9	617-903-6	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E+01	3.9E-01	1.4E+01	-7.58	-7.88	-9.54	-1.84	0.64
4049	100-50-5	cyclohex-3-ene-1-carbaldehyde	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E+01	3.8E-01	1.4E+01	-7.59	-7.90	-9.55	-1.31	0.64
4050	2269-22-9	aluminium tri-sec-butanolate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E+01	3.8E-01	1.4E+01	-7.59	-7.90	-9.55	-1.57	0.64
4051	100-99-2	triisobutylaluminium	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E+01	3.7E-01	1.3E+01	-7.60	-7.91	-9.56	-1.84	0.64
4052	15546-11-9	methyl (Z,Z)-8,8-dibutyl-3,6,10-trioxo-2,7,9-trioxa-8-stannatrideca-4,11-dien-13-oate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.6E-01	1.3E+01	-7.61	-7.92	-9.57	-2.61	0.56
4053	121-97-1	p-methoxypropiophenone	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.6E-01	1.3E+01	-7.62	-7.92	-9.57	-1.84	0.64
4054	75234-41-2	trisodium bis[2-[[2,4-dihydroxy-3-[[2-methyl-4-sulphophenyl]azo]phenyl]azo]benzoato(3-)]chromate(3-)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.5E+01	3.5E-01	1.2E+01	-7.63	-7.94	-9.59	-1.01	0.62
4055	103-82-2	phenylacetic acid	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+01	2.8E-01	1.0E+01	-7.72	-8.02	-9.67	-1.16	0.78
4056	99290-97-8	619-419-0	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+01	2.8E-01	1.0E+01	-7.72	-8.03	-9.68	-1.84	0.64
4057	85-98-3	1,3-diethyldiphenylurea	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+01	2.5E-01	9.1E+00	-7.77	-8.07	-9.72	-1.86	0.42
4058	1070-00-4	trioctylaluminium	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+01	2.4E-01	8.6E+00	-7.79	-8.10	-9.75	-1.84	0.64
4059	28305-25-1	calcium (S)-2-hydroxypropionate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+01	2.4E-01	8.5E+00	-7.80	-8.10	-9.75	-0.02	0.78
4060	93686-48-7	Phosphorous acid, tri-C12-14-alkyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+01	2.3E-01	8.1E+00	-7.82	-8.12	-9.77	-0.47	0.64
4061	83877-91-2	bis(ethyl acetoacetato-O1',O3)bis(2-methylpropan-1-olato)titanium	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+01	2.2E-01	8.0E+00	-7.82	-8.13	-9.78	0.09	0.36
4062	14320-04-8	[29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]zinc	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+01	2.0E-01	7.3E+00	-7.86	-8.17	-9.82	-1.84	0.64
4063	27858-32-8	bis(ethyl acetoacetato-O1',O3)bis(propan-2-olato)titanium	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+01	2.0E-01	7.2E+00	-7.87	-8.18	-9.83	-0.16	0.98
4064	74336-59-7	3-[(4-chloro-2-nitrophenyl)azo]-2-methylpyrazolo[5,1-b]quinazolin-9(1H)-one	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+01	1.9E-01	6.8E+00	-7.89	-8.20	-9.85	-1.84	0.64
4065	12542-85-7	trichlorotrimethyldialuminium	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+01	1.8E-01	6.4E+00	-7.92	-8.22	-9.88	-1.84	0.64
4066	753-73-1	dimethyltin dichloride	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+01	1.7E-01	6.0E+00	-7.95	-8.25	-9.90	-2.77	1.06
4067	12237-62-6	ferrate(4-), hexakis(cyano-C)-, methylated 4-[(4-aminophenyl)(4-imino-2,5-cyclohexadien-1-ylidene)methyl]benzene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+01	1.7E-01	6.0E+00	-7.95	-8.25	-9.90	-2.12	0.64
4068	12225-06-8	N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2-methoxy-5-[(phenylamino)carbonyl]phenyl]azo]naphth	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+01	1.7E-01	6.0E+00	-7.95	-8.26	-9.91	-1.83	1.05
4069	813-93-4	bismuth citrate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+01	1.7E-01	5.9E+00	-7.95	-8.26	-9.91	-1.84	0.64
4070	22673-19-4	dibutylbis(pentane-2,4-dionato-O,O')tin	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+01	1.6E-01	5.6E+00	-7.98	-8.28	-9.93	-3.05	0.64
4071	62202-86-2	butylethylmagnesium	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+01	1.6E-01	5.6E+00	-7.98	-8.29	-9.94	-1.84	0.64
4072	90480-58-3	Octanoic acid, zinc salt, basic	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+01	1.5E-01	5.5E+00	-7.98	-8.29	-9.94	-3.55	0.41
4073	814-94-8	tin(II) oxalate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+01	1.5E-01	5.2E+00	-8.01	-8.31	-9.96	-0.83	0.64
4074	68155-22-6	Amides, tall-oil fatty, N-(hydroxyethyl)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+01	1.4E-01	5.0E+00	-8.03	-8.33	-9.98	-1.84	0.64
4075	72207-62-6	Butanamide, 2,2'-[[3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl]bis(azo)]bis[3-oxo-, N,N'-bis(phenyl and 2,4-xylyl) derivs.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.9E+00	1.4E-01	5.0E+00	-8.03	-8.34	-9.99	-0.74	1.21
4076	69011-06-9	[phthalato(2-)]dioxotrioxad	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.9E+00	1.4E-01	4.9E+00	-8.03	-8.34	-9.99	-3.57	0.68
4077	1888-87-5	dichloroisobutylaluminium	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.6E+00	1.3E-01	4.8E+00	-8.04	-8.35	-10.00	-1.84	0.64
4078	23275-26-5	aluminium tri(hexanolate)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
4079	175217-23-9	605-753-4	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
4080	117829-74-0	601-495-1	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
4081	21178-63-2	chromium trioleate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-0.83	0.64
4082	14878-28-5	696-062-7	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
4083	1636-27-7	dipropylmalonic acid	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
4084	299-35-4	3-(4-amino-2-methylpyrimidin-5-ylmethyl)-5-(2-hydroxyethyl)-4-methylthiazole-2(3H)-thione	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
4085	874209-13-9	619-741-1	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
4086	68333-81-3	Alkanes, C4-12	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
4087	15245-44-0	lead 2,4,6-trinitro-m-phenylene dioxide	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09

4169	68647-86-9	Charcoal, coconut shell	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+04	1.5E+02	5.2E+03	-5.01	-5.31	-6.97	-1.84	0.64
4170	68515-48-0	1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+04	1.4E+02	5.2E+03	-5.01	-5.32	-6.97	-2.28	0.88
4171	67701-06-8	Fatty acids, C14-18 and C16-18-unsatd.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+04	1.4E+02	5.0E+03	-5.03	-5.33	-6.99	-0.33	0.38
4172	90640-84-9	Creosote oil, acenaphthene fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.9E+03	1.4E+02	4.9E+03	-5.03	-5.34	-6.99	-2.06	0.95
4173	68526-84-1	Alcohols, C8-10-iso-, C9-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.6E+03	1.3E+02	4.8E+03	-5.04	-5.35	-7.00	-2.04	0.64
4174	66071-94-1	Corn, steep liquor	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.6E+03	1.3E+02	4.8E+03	-5.04	-5.35	-7.00	-1.23	0.56
4175	68425-17-2	Syrups, corn, hydrogenated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.5E+03	1.3E+02	4.8E+03	-5.05	-5.35	-7.01	-1.84	0.64
4176	68037-01-4	Dec-1-ene, homopolymer, hydrogenated Dec-1-ene, oligomers, hydrogenated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.3E+03	1.3E+02	4.7E+03	-5.06	-5.37	-7.02	0.46	0.64
4177	68333-89-1	Benzene, (1-methylethyl)-, oxidized, polyphenyl residues	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.2E+03	1.3E+02	4.6E+03	-5.06	-5.37	-7.02	-1.07	0.64
4178	85535-85-9	Alkanes, C14-17, chloro	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.0E+03	1.3E+02	4.5E+03	-5.07	-5.38	-7.03	-2.84	1.40
4179	64742-91-2	Distillates (petroleum), steam-cracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.8E+03	1.2E+02	4.4E+03	-5.08	-5.39	-7.04	-2.70	0.22
4180	101316-84-1	Tar, brown-coal, low-temp.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.7E+03	1.2E+02	4.3E+03	-5.09	-5.40	-7.05	-1.59	0.64
4181	9049-71-2	Sucrose, propoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.5E+03	1.2E+02	4.3E+03	-5.10	-5.40	-7.05	0.48	0.97
4182	51000-52-3	vinyl neodecanoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.3E+03	1.2E+02	4.2E+03	-5.11	-5.41	-7.07	-2.68	0.91
4183	740817-83-8	Alcohols, C12-13-branched and linear	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.0E+03	1.1E+02	4.0E+03	-5.12	-5.43	-7.08	-3.00	0.63
4184	102242-52-4	Fatty acids, C6-24 and C6-24-unsatd., Me esters, distn. residues	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.7E+03	1.1E+02	3.9E+03	-5.14	-5.45	-7.10	-0.17	0.64
4185	52625-13-5	D-Glucitol, propoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.6E+03	1.1E+02	3.8E+03	-5.14	-5.45	-7.10	-1.84	0.64
4186	92128-68-2	Hydrocarbons, C5, ethylene-manuf.-by-product, hydrogenated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.6E+03	1.1E+02	3.8E+03	-5.15	-5.46	-7.11	-1.93	0.39
4187	25791-96-2	Glycerol, propoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.4E+03	1.0E+02	3.7E+03	-5.16	-5.46	-7.11	-1.84	0.64
4188	71808-39-4	Fatty acids, C16-18 and C18-unsatd., dimerized	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.2E+03	1.0E+02	3.6E+03	-5.17	-5.48	-7.13	0.07	1.05
4189	84649-84-3	Amines, C12-14-alkyldimethyl	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.1E+03	9.9E+01	3.5E+03	-5.18	-5.48	-7.14	-3.88	0.66
4190	8013-07-8	Soybean oil, epoxidized	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.7E+03	9.4E+01	3.4E+03	-5.20	-5.50	-7.16	-0.96	0.64
4191	61788-89-4	Fatty acids, C18-unsatd., dimers	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.1E+03	8.5E+01	3.1E+03	-5.24	-5.55	-7.20	-1.84	0.64
4192	91995-60-7	Ethers, C5-6-branched alkyl Me	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.9E+03	8.2E+01	2.9E+03	-5.26	-5.57	-7.22	-0.67	0.64
4193	68187-58-6	Pitch, petroleum, arom.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.6E+03	7.8E+01	2.8E+03	-5.28	-5.59	-7.24	-1.27	0.64
4194	68477-35-0	Distillates (petroleum), C3-6, piperylene-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+03	7.6E+01	2.7E+03	-5.29	-5.60	-7.25	-1.93	0.39
4195	42978-66-5	(1-methyl-1,2-ethanediyl)bis[oxy(methyl-2,1-ethanediyl)] diacrylate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.4E+03	7.6E+01	2.7E+03	-5.29	-5.60	-7.25	-1.47	0.61
4196	9003-29-6	Butene, homopolymer (products derived from either/or But-1-ene/But-2-ene)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.3E+03	7.4E+01	2.6E+03	-5.30	-5.61	-7.26	-4.28	0.64
4197	68915-38-8	Cyclohexane, oxidized, aq. ext.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.2E+03	7.2E+01	2.6E+03	-5.31	-5.62	-7.27	-0.53	0.33
4198	67701-05-7	Fatty acids, C8-18 and C18-unsatd.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.0E+03	7.0E+01	2.5E+03	-5.32	-5.63	-7.28	-1.51	0.64
4199	8006-64-2	Turpentine, oil	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.9E+03	6.8E+01	2.5E+03	-5.34	-5.64	-7.29	-1.80	0.27
4200	85586-07-8	Sulfuric acid, mono-C12-14-alkyl esters, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.9E+03	6.8E+01	2.4E+03	-5.34	-5.64	-7.30	-2.09	0.57
4201	84961-70-6	Benzene, mono-C10-13-alkyl derivs., distn. residues	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.9E+03	6.8E+01	2.4E+03	-5.34	-5.65	-7.30	-1.84	0.64
4202	27458-92-0	isotridecan-1-ol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.8E+03	6.6E+01	2.4E+03	-5.35	-5.66	-7.31	-3.31	0.32
4203	84650-02-2	Distillates (coal tar), benzole fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.6E+03	6.5E+01	2.3E+03	-5.36	-5.67	-7.32	-1.88	0.38
4204	85566-26-3	Fatty acids, C8-10, Me esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.5E+03	6.3E+01	2.2E+03	-5.37	-5.68	-7.33	-1.99	0.71
4205	8050-26-8	Resin acids and Rosin acids, esters with pentaerythritol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.5E+03	6.3E+01	2.2E+03	-5.37	-5.68	-7.33	0.20	0.63
4206	84650-03-3	Distillates (coal tar), light oils	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.5E+03	6.2E+01	2.2E+03	-5.38	-5.68	-7.34	-1.96	0.64
4207	161074-79-9	Alcohols, C12-13, branched and linear, ethoxylated, sulfates, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.4E+03	6.2E+01	2.2E+03	-5.38	-5.69	-7.34	-1.98	0.43
4208	68937-75-7	Fatty acids, C8-10	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.4E+03	6.1E+01	2.2E+03	-5.38	-5.69	-7.34	-2.01	0.66
4209	97280-83-6	Dodecene, branched	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.3E+03	6.0E+01	2.1E+03	-5.39	-5.70	-7.35	-3.76	1.03
4210	91051-01-3	Fatty acids, C16-18, zinc salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.3E+03	5.9E+01	2.1E+03	-5.40	-5.70	-7.36	-2.92	0.69
4211	1234694-02-0	1234694-02-0	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.3E+03	5.9E+01	2.1E+03	-5.40	-5.70	-7.36	-0.26	0.64
4212	26780-96-1	1,2-Dihydro-2,2,4-trimethylquinoline, oligomers	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.1E+03	5.7E+01	2.0E+03	-5.42	-5.72	-7.38	-1.03	0.98
4213	1079184-43-2	Ethanaminium, 2-hydroxy-N-(2-hydroxyethyl)-N,N-d imethyl-, esters with C16-18 and C18-unsatd. fatty acids, chlori	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.1E+03	5.7E+01	2.0E+03	-5.42	-5.72	-7.38	-2.18	0.26
4214	34590-94-8	(2-methoxymethethoxy)propanol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.0E+03	5.5E+01	2.0E+03	-5.43	-5.74	-7.39	0.71	0.48
4215	65997-03-7	Fatty acids, tall-oil, low-boiling	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.9E+03	5.5E+01	2.0E+03	-5.43	-5.74	-7.39	-1.05	0.77
4216	97489-15-1	Sulfonic acids, C14-17-sec-alkane, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.8E+03	5.3E+01	1.9E+03	-5.45	-5.75	-7.40	-1.70	0.54
4217	25686-28-6	4,4'-Methylenediphenyl diisocyanate, oligomers	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.7E+03	5.2E+01	1.9E+03	-5.46	-5.77	-7.42	0.37	0.26
4218	5392-40-5	citral	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.7E+03	5.2E+01	1.9E+03	-5.46	-5.77	-7.42	-1.35	0.81
4219	121158-58-5	Phenol, dodecyl-, branched	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.5E+03	4.9E+01	1.8E+03	-5.48	-5.79	-7.44	-2.50	1.32
4220	68002-71-1	Glycerides, C16-18	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.5E+03	4.9E+01	1.7E+03	-5.48	-5.79	-7.44	-0.27	0.72
4221	65996-83-0	Extracts, coal tar oil alk.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.4E+03	4.8E+01	1.7E+03	-5.49	-5.80	-7.45	-1.86	0.64
4222	68603-87-2	Carboxylic acids, di-, C4-6	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.4E+03	4.7E+01	1.7E+03	-5.50	-5.80	-7.45	-1.20	0.26
4223	68784-26-9	Phenol, dodecyl-, sulfurized, carbonates, calcium salts, overbased	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.3E+03	4.7E+01	1.7E+03	-5.50	-5.81	-7.46	0.07	0.42
4224	65997-04-8	Rosin, fumarated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.3E+03	4.6E+01	1.7E+03	-5.51	-5.81	-7.46	-1.80	0.28
4225	85566-16-1	Alcohols, C13-15-branched and linear	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.3E+03	4.6E+01	1.7E+03	-5.51	-5.82	-7.47	-2.01	0.64
4226	90640-81-6	Anthracene oil, anthracene paste	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.2E+03	4.5E+01	1.6E+03	-5.52	-5.83	-7.48	-1.30	0.64
4227	8050-31-5	Resin acids and Rosin acids, esters with glycerol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.2E+03	4.5E+01	1.6E+03	-5.52	-5.83	-7.48	0.20	0.63
4228	1207435-39-4	Fast Pyrolysis Bio-oil	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.2E+03	4.4E+01	1.6E+03	-5.53	-5.83	-7.49	-0.75	0.45
4229	160901-19-9	Alcohols, C12-13, branched and linear, ethoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.2E+03	4.4E+01	1.6E+03	-5.53	-5.83	-7.49	-3.21	0.57
4230	68955-98-6	Fatty acids, C16-18 and C18-unsatd., branched and linear	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.1E+03	4.3E+01	1.5E+03	-5.54	-5.85	-7.50	0.14	0.96
4231	97280-95-0	Nonene, branched	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.0E+03	4.2E+01	1.5E+03	-5.55	-5.86	-7.51	-2.68	1.28
4232	93924-10-8	Alkenes, C20-24 α-	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.9E+03	4.0E+01	1.4E+03	-5.57	-5.88	-7.53	-2.68	1.28
4233	9003-36-5	Formaldehyde, oligomeric reaction products with 1-chloro-2,3-epoxypropane and phenol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E+03	3.9E+01	1.4E+03	-5.58	-5.88	-7.53	-1.53	0.93
4234	75782-86-4	Alcohols, C12-13	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E+03	3.9E+01	1.4E+03	-5.58	-5.88	-7.54	-3.00	0.63
4235	85408-62-4	Fatty acids, C12-18 and C18-unsatd., 2-sulfoethyl esters, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E+03	3.9E+01	1.4E+03	-5.58	-5.89	-7.54	-2.75	0.32
4236	90640-67-8	Amines, polyethylenepoly-, triethylenetetramine fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E+03	3.9E+01	1.4E+03	-5.59	-5.89	-7.54	-1.30	0.76
4237	8028-48-6	Orange, sweet, ext.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E+03	3.7E+01	1.3E+03	-5.60	-5.91	-7.56	-1.78	0.75
4238	67701-01-3	Fatty acids, C12-18	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+03	3.7E+01	1.3E+03	-5.61	-5.91	-7.56	-1.51	0.64
4239	90990-08-2	Fatty acids, C8-18	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+03	3.7E+01	1.3E+03	-5.61	-5.91	-7.57	-1.51	0.64
4240	25637-99-4	hexabromocyclododecane	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+03	3.7E+01	1.3E+03	-5.61	-5.92	-7.57	-4.88	0.70
4241	39202-17-0	Methyl dodec-9-enoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+03	3.6E+01	1.3E+03	-5.61	-5.92	-7.57	-3.29	0.46
4242	25103-58-6	tert-dodecanethiol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+03	3.6E+01	1.3E+03	-5.61	-5.92	-7.57	-2.49	0.64
4243	90604-40-3	Alcohols, C12-15-branched and linear	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+03	3.6E+01	1.3E+03	-5.61	-5.92	-7.57	-2.63	0.95
4244	61790-51-0	Resin acids and Rosin acids, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.5E+03	3.5E+01	1.3E+03	-5.62	-5.93	-7.58	-1.87	1.14
4245	161907-77-3	ethanol, 2-butoxy-, manufacture of, by-products from	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.5E+03	3.5E+01	1.3E+03	-5.63	-5.93	-7.58	-0.20	0.64
4246	164383-22-6	C16-18 evennumbered, C18 unsaturated alkyl nitrile	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.5E+03	3.4E+01	1.2E+03	-5.64	-5.94	-7.60	-3.09	0.41
4247	84989-41-3	2-Oxetanone, 3-C12-16-alkyl-4-C13-17-alkylidene derivs.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+03	3.3E+01	1.2E+03	-5.65	-5.95	-7.60	-1.08	0.64
4248	85586-21-6	Fatty acids, C16-18, Me esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+03	3.3E+01	1.2E+03	-5.65	-5.96	-7.61	-0.58	0.64
4249	68784-12-3	2,5-Furandione, dihydro-, mono-C15-20-alkenyl derivs.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+03	3.3E+01	1.2E+03	-5.65	-5.96	-7.61	-1.38	0.31
4250	8001-78-3	Castor oil, hydrogenated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+03	3.3E+01	1.2E+03	-5.65	-5.96	-7.61	-1.17	0.64
4251	8013-17-0	Sugar, invert	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+03	3.3E+01	1.2E+03	-5.66	-5.96	-7.62	-1.84	0.64
4252	66455-17-2	Alcohols, C9-11	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+03	3.2E+01	1.1E+03	-5.67	-5.98	-7.63	-2.32	0.64
4253	91051-05-7	Fatty acids, essential, Et esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+03	3.2E+01	1.1E+03	-5.67	-5.98	-7.63	-1.07	1.02
4254	94581-15-4	Resin acids and Rosin acids, fumarated, esters with pentaerythritol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+03	3.2E+01	1.1E+03	-5.67	-5.98	-7.63	-1.84	0.64
4255	68037-95-6	Amines, C16-18 and C18-unsatd.-alkyl	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+03	3.1E+01	1.1E+03	-5.68	-5.99	-7.64	-3.75	0.77
4256	68526-86-3	Alcohols, C11-14-iso-, C13-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+03	3.1E+01	1.1E+03	-5.69	-5.99	-7.64	-3.20	0.48
4257	68526-89-6	Octene, hydroformylation products, high-boiling	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+03	3.0E+01	1.1E+03	-5.69	-6.00	-7.65	-0.58	0.54
4258	68938-03-4	Octene, hydroformylation products, low-boiling	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+03	3.0E+01	1.1E+03	-5.69	-6.00	-7.65	-1.50	0.27
4259	67701-28-4	Glycerides, C8-18 and C18-unsatd.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+03	3.0E+01	1.1E+03	-5.70	-6.01	-7.66	-0.27	0.72
4260	1345668-40-7	Raffinates (Fischer-Tropsch), C10-25-branched	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+03	2.9E+01	1.0E+03	-5.71	-6.02	-7.67	0.54	0.42
4261	91082-17-6	Sulfonic acids, C10-21-alkane, Ph esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+03	2.9E+01	1.0E+03	-5.71	-6.02	-7.67	-1.35	0.98
4262	90640-32-7	Amines, C16-18-alkyl	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+03	2.9E+01	1.0E+03	-5.71	-6.02	-7.67	-3.75	0.78
4263	63449-39-8	Paraffin waxes and Hydrocarbon waxes, chloro	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.9E+03	2.7E+01	9.7E+02	-5.74	-6.05	-7.70	-0.

4352	91995-17-4	anthracene oil, anthracene paste, distn. lights	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+02	1.3E+01	4.6E+02	-6.07	-6.37	-8.03	-1.30	0.64
4353	68551-11-1	1-Propene, hydroformylation products, high-boiling	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+02	1.3E+01	4.6E+02	-6.07	-6.37	-8.03	-1.15	0.64
4354	85995-91-1	Alkyl iodides, C8-14, γ-ω-perfluoro	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+02	1.3E+01	4.6E+02	-6.07	-6.37	-8.03	-1.84	0.64
4355	68526-57-8	Alkenes, C10-12, C11-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+02	1.3E+01	4.6E+02	-6.07	-6.37	-8.03	-3.04	0.82
4356	68526-82-9	Alkenes, C6-10, hydroformylation products, high-boiling	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+02	1.3E+01	4.6E+02	-6.07	-6.37	-8.03	-1.84	0.64
4357	141-91-3	2,6-dimethylmorpholine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+02	1.3E+01	4.6E+02	-6.07	-6.37	-8.03	-0.61	0.64
4358	38640-62-9	bis(isopropyl)naphthalene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.0E+02	1.3E+01	4.5E+02	-6.07	-6.38	-8.03	-2.11	0.70
4359	50586-59-9	Propylidynetrimethanol, ethoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.9E+02	1.2E+01	4.5E+02	-6.08	-6.38	-8.03	-0.17	1.00
4360	8000-41-7	Terpineol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.9E+02	1.2E+01	4.5E+02	-6.08	-6.38	-8.03	-1.25	0.23
4361	27138-31-4	oxydipropyl dibenzoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.9E+02	1.2E+01	4.5E+02	-6.08	-6.38	-8.04	-2.35	0.68
4362	68188-18-1	Paraffin oils, sulfochlorinated, saponified	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.9E+02	1.2E+01	4.4E+02	-6.08	-6.39	-8.04	-2.18	0.99
4363	119345-04-9	Benzene, 1,1'-oxybis-, tetrapropylene derivs., sulfonated, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.6E+02	1.2E+01	4.3E+02	-6.09	-6.40	-8.05	-1.55	1.01
4364	125904-11-2	Benzene, ethenyl-, ar-bromo derivs.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.5E+02	1.2E+01	4.3E+02	-6.10	-6.40	-8.05	-2.34	0.25
4365	24851-98-7	methyl 3-oxo-2-pentylcyclopentaneacetate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.5E+02	1.2E+01	4.3E+02	-6.10	-6.40	-8.06	-1.70	0.24
4366	1761-71-3	4,4'-methylenebis(cyclohexylamine)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.4E+02	1.2E+01	4.2E+02	-6.10	-6.41	-8.06	-1.12	0.82
4367	33703-08-1	diisononyl adipate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.4E+02	1.2E+01	4.2E+02	-6.10	-6.41	-8.06	-1.84	0.64
4368	91081-53-7	Rosin, reaction products with formaldehyde	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.4E+02	1.2E+01	4.2E+02	-6.10	-6.41	-8.06	-1.87	1.14
4369	28299-41-4	ditolyl ether	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.3E+02	1.2E+01	4.2E+02	-6.10	-6.41	-8.06	-3.63	0.80
4370	1213789-63-t	C16-18-(even numbered, saturated and unsaturated)-alkylamines	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.3E+02	1.2E+01	4.1E+02	-6.11	-6.42	-8.07	-3.75	0.78
4371	68140-01-2	Amides, coco, N-[3-(dimethylamino)propyl]	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.3E+02	1.2E+01	4.1E+02	-6.11	-6.42	-8.07	-3.40	0.64
4372	68649-95-6	Linseed oil, oxidized	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.2E+02	1.1E+01	4.1E+02	-6.11	-6.42	-8.07	-1.21	0.64
4373	68424-31-7	Fatty acids, C5-10, esters with pentaerythritol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.2E+02	1.1E+01	4.1E+02	-6.11	-6.42	-8.07	-0.45	0.91
4374	68610-51-5	Phenol, 4-methyl-, reaction products with dicyclopentadiene and isobutylene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.1E+02	1.1E+01	4.0E+02	-6.12	-6.43	-8.08	-1.84	0.64
4375	26952-14-7	hexadecene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.0E+02	1.1E+01	4.0E+02	-6.12	-6.43	-8.08	-2.68	1.28
4376	9051-51-8	2,2'-Oxydiethanol, propoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.9E+02	1.1E+01	4.0E+02	-6.13	-6.44	-8.09	-1.84	0.64
4377	85480-55-3	Benzenesulfonic acid, mono-C10-13-alkyl derivs., compds. with ethanolamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.9E+02	1.1E+01	3.9E+02	-6.13	-6.44	-8.09	-2.16	0.61
4378	97404-33-6	Fatty acids, C16-18, C16-18-alkyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.8E+02	1.1E+01	3.9E+02	-6.13	-6.44	-8.09	-1.00	0.64
4379	16096-31-4	1,6-bis(2,3-epoxypropoxy)hexane	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.8E+02	1.1E+01	3.9E+02	-6.13	-6.44	-8.09	-1.51	0.64
4380	68551-08-6	Alcohols, C9-11-branched	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.8E+02	1.1E+01	3.9E+02	-6.14	-6.44	-8.10	-2.87	0.41
4381	65997-06-0	Rosin, hydrogenated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.7E+02	1.1E+01	3.8E+02	-6.14	-6.45	-8.10	-1.48	0.81
4382	100085-61-8	Protein hydrolyzates, animal	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.7E+02	1.1E+01	3.8E+02	-6.14	-6.45	-8.10	-1.84	0.64
4383	68649-11-6	Dec-1-ene, dimers, hydrogenated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.7E+02	1.1E+01	3.8E+02	-6.14	-6.45	-8.10	0.46	0.64
4384	75880-28-3	4,4'-Methylenediphenyl diisocyanate, oligomeric reaction products with 2,4'-diisocyanatodiphenylmethane and [(m	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.6E+02	1.1E+01	3.8E+02	-6.15	-6.45	-8.11	0.42	1.23
4385	1190630-03-t	642-362-8	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.4E+02	1.0E+01	3.7E+02	-6.16	-6.46	-8.11	-1.84	0.64
4386	85507-79-5	diundecyl phthalate, branched and linear	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.1E+02	9.9E+00	3.6E+02	-6.17	-6.48	-8.13	-2.28	0.67
4387	57472-68-1	oxybis(methyl-2,1-ethanediyl) diacrylate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.1E+02	9.9E+00	3.6E+02	-6.18	-6.48	-8.13	-1.97	0.46
4388	26401-35-4	diisotridecyl adipate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.0E+02	9.8E+00	3.5E+02	-6.18	-6.49	-8.14	-0.29	0.64
4389	1328-53-6	polychloro copper phthalocyanine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.0E+02	9.7E+00	3.5E+02	-6.18	-6.49	-8.14	-0.60	0.64
4390	68936-98-1	Benzene, [1-methylethyl]-, distn. residues	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.9E+02	9.7E+00	3.5E+02	-6.19	-6.49	-8.14	-2.45	0.64
4391	90193-76-3	1,2-Benzenedicarboxylic acid, di-C16-18-alkyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.9E+02	9.6E+00	3.5E+02	-6.19	-6.50	-8.15	-1.84	0.64
4392	8050-25-7	Resin acids and Rosin acids, esters with triethylene glycol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.8E+02	9.5E+00	3.4E+02	-6.19	-6.50	-8.15	0.20	0.63
4393	68515-47-9	1,2-Benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.8E+02	9.5E+00	3.4E+02	-6.20	-6.50	-8.15	-2.83	0.52
4394	1218787-29-t	C12-18 evennumbered alkyl nitrile	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.8E+02	9.4E+00	3.4E+02	-6.20	-6.50	-8.15	-3.13	1.27
4395	11138-60-6	Decanoic acid, ester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol octanoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.7E+02	9.4E+00	3.4E+02	-6.20	-6.51	-8.16	-1.01	0.64
4396	102242-49-9	Alcohols, C6-24, distn. residues	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.7E+02	9.4E+00	3.4E+02	-6.20	-6.51	-8.16	0.83	1.15
4397	151006-60-9	Unknown	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.7E+02	9.3E+00	3.3E+02	-6.20	-6.51	-8.16	0.46	0.64
4398	68604-41-1	Fatty acids, C16-18 and C18-unsatd., Me esters, distn. residues	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.5E+02	9.0E+00	3.2E+02	-6.21	-6.52	-8.17	-0.17	0.64
4399	84605-29-8	Phosphorodithioic acid, mixed O,O-bis[1,3-dimethylbutyl and iso-Pr] esters, zinc salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.4E+02	8.9E+00	3.2E+02	-6.22	-6.53	-8.18	-1.71	0.37
4400	26898-17-9	dibenzylidene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.4E+02	8.8E+00	3.2E+02	-6.23	-6.53	-8.18	-3.91	1.00
4401	68784-31-6	Phosphorodithioic acid, mixed O,O-bis(sec-Bu and 1,3-dimethylbutyl) esters, zinc salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.3E+02	8.8E+00	3.1E+02	-6.23	-6.54	-8.19	-1.16	0.77
4402	85940-28-9	Phosphorodithioic acid, mixed O,O-bis[2-ethylhexyl and iso-Bu and iso-Pr] esters, zinc salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.1E+02	8.5E+00	3.1E+02	-6.24	-6.55	-8.20	-2.43	0.64
4403	68187-75-7	Oils, fish, oxidized	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.1E+02	8.5E+00	3.1E+02	-6.24	-6.55	-8.20	-1.84	0.64
4404	68609-97-2	Oxirane, mono[(C12-14-alkyloxy)methyl] derivs.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.1E+02	8.5E+00	3.0E+02	-6.24	-6.55	-8.20	-0.23	0.64
4405	3648-20-2	diundecyl phthalate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.1E+02	8.5E+00	3.0E+02	-6.24	-6.55	-8.20	-2.97	0.72
4406	29590-42-9	isooctyl acrylate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.1E+02	8.5E+00	3.0E+02	-6.24	-6.55	-8.20	-3.19	0.24
4407	1222-05-5	1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylindeno[5,6-c]pyran	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.0E+02	8.4E+00	3.0E+02	-6.25	-6.55	-8.20	-3.07	0.64
4408	70084-85-4	Fatty acids, hydrogenated tallow, distn. residues	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.0E+02	8.4E+00	3.0E+02	-6.25	-6.56	-8.21	-1.84	0.64
4409	161907-79-5	ethanol, 2-methoxy-, manufacture of, by-products from	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.9E+02	8.3E+00	3.0E+02	-6.25	-6.56	-8.21	-1.84	0.61
4410	68441-94-1	Heptanoic acid, mixed esters with pentaerythritol and valeric acid	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.9E+02	8.2E+00	2.9E+02	-6.26	-6.56	-8.22	-0.87	0.96
4411	160901-14-4	Fatty acids, tall-oil, oligomeric reaction products with maleic anhydride and rosin, calcium magnesium zinc salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.8E+02	8.1E+00	2.9E+02	-6.26	-6.57	-8.22	-0.50	0.64
4412	8007-24-7	Cashew, nutshell liq.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.7E+02	7.9E+00	2.8E+02	-6.27	-6.58	-8.23	-0.25	0.98
4413	4259-15-8	zinc bis[O,O-bis(2-ethylhexyl)] bis(dithiophosphate)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.6E+02	7.8E+00	2.8E+02	-6.28	-6.59	-8.24	-1.16	0.77
4414	92129-33-4	Quaternary ammonium compounds, di-C16-18-alkyldimethyl, chlorides	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.6E+02	7.8E+00	2.8E+02	-6.28	-6.59	-8.24	-3.13	0.87
4415	68920-66-1	Alcohols, C16-18 and C18-unsatd., ethoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+02	7.7E+00	2.8E+02	-6.29	-6.59	-8.24	-2.58	0.73
4416	97489-04-8	Oils, vegetable, sulfonated, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+02	7.7E+00	2.8E+02	-6.29	-6.59	-8.24	-0.65	0.53
4417	90641-05-7	Extract residues (coal), naphthalene and alk., distn. residues	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+02	7.6E+00	2.7E+02	-6.29	-6.60	-8.25	-1.99	0.88
4418	93821-38-6	Extract residues (coal), benzole fraction acid	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+02	7.6E+00	2.7E+02	-6.29	-6.60	-8.25	-2.47	0.64
4419	1490-04-6	DL-menthol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+02	7.6E+00	2.7E+02	-6.29	-6.60	-8.25	-1.64	0.64
4420	90622-59-6	Alkanes, C16-20-iso-	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+02	7.6E+00	2.7E+02	-6.29	-6.60	-8.25	-3.96	0.30
4421	68514-28-3	Humic acids, potassium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.4E+02	7.6E+00	2.7E+02	-6.29	-6.60	-8.25	-0.53	0.22
4422	27070-58-2	octadecene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.4E+02	7.6E+00	2.7E+02	-6.29	-6.60	-8.25	-2.68	1.28
4423	25321-41-9	xylenesulphonic acid	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.3E+02	7.4E+00	2.7E+02	-6.30	-6.61	-8.26	-0.38	0.64
4424	68515-43-5	1,2-Benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.3E+02	7.3E+00	2.6E+02	-6.31	-6.61	-8.26	-1.90	0.64
4425	85049-37-2	Fatty acids, C16-18 and C18-unsatd., 2-ethylhexyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.3E+02	7.3E+00	2.6E+02	-6.31	-6.61	-8.26	0.35	1.10
4426	73296-89-6	Sulfuric acid, mono-C12-16-alkyl esters, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.3E+02	7.3E+00	2.6E+02	-6.31	-6.61	-8.26	-2.11	0.41
4427	71302-83-5	615-276-3	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.2E+02	7.3E+00	2.6E+02	-6.31	-6.62	-8.27	-1.84	0.64
4428	31795-24-1	potassium methylsilanetriolate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.2E+02	7.3E+00	2.6E+02	-6.31	-6.62	-8.27	-1.84	0.77
4429	65997-13-9	Resin acids and Rosin acids, hydrogenated, esters with glycerol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.1E+02	7.1E+00	2.5E+02	-6.32	-6.63	-8.28	0.20	0.63
4430	91995-49-2	Distillates (coal tar), naphthalene oil crystn. mother liquor	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.0E+02	7.0E+00	2.5E+02	-6.33	-6.63	-8.28	-1.13	0.89
4431	98072-31-2	Alkenes, C7-9, hydroformylation products, distn. residues, heavy cracked fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.0E+02	6.9E+00	2.5E+02	-6.33	-6.64	-8.29	-1.84	0.64
4432	85711-26-8	Alcohols, C9-11-branched and linear	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.9E+02	6.8E+00	2.4E+02	-6.34	-6.65	-8.30	-2.32	0.64
4433	91031-48-0	Fatty acids, C16-18, 2-ethylhexyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.8E+02	6.7E+00	2.4E+02	-6.34	-6.65	-8.30	0.35	0.97
4434	57583-54-7	tetraphenyl m-phenylene bis(phosphate)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.8E+02	6.7E+00	2.4E+02	-6.35	-6.65	-8.30	-1.11	0.59
4435	68609-68-7	1-Hexanol, 2-ethyl-, manuf. of, by-products from, distn. residues	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.8E+02	6.6E+00	2.4E+02	-6.35	-6.66	-8.31	-1.15	0.25
4436	84989-04-8	Tar acids, methylphenol fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.8E+02	6.6E+00	2.4E+02	-6.35	-6.66	-8.31	-1.95	0.22
4437	1226892-43-t	Fatty acids, C18 unsat, reaction products with diethylenetriamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.7E+02	6.5E+00	2.3E+02	-6.36	-6.66	-8.31	-3.21	0.55
4438	6864-37-5	2,2'-dimethyl-4,4'-methylenebis(cyclohexylamine)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.6E+02	6.4E+00	2.3E+02	-6.36	-6.67	-8.32	-2.00	0.48
4439	85631-26-1	Fatty acids, C8-16	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.6E+02	6.4E+00	2.3E+02	-6.37	-6.68	-8.33	-1.54	1.35
4440	68910-05-4	Ethanol, 2-amino-, reaction products with ammonia, by-products from	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.5E+02	6.2E+00	2.2E+02	-6.38	-6.68	-8.33	-2.06	0.64
4441	308062-60-4	N-(C16-18)alkyl(C16-18)alkanamide	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.5E+02	6.2E+00	2.2E+02	-6.38	-6.68	-8.34	-2.82	0.64
4442	68953-84-4	1,4-Benzenediamine, N,N'-mixed Ph and tolyl derivs.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.4E+02	6.1E+00	2.2E+02	-6.39	-6.70	-8.35	-3.49	0.59
4443	1236007-63-t	Reaction mass of 6-O-alfa-D-glucopyranosyl-D-fructofuranose and 1-O-alfa-D-glucopyranosyl-D-fructofuranose and i	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.3E+02	6.0E+00	2.2E+02	-6.39	-6.70	-8.35	-1.84	0.64
4444	68411-27-8	Benzoic acid, C12-15-alkyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.2E+02	5.9E+00	2.1E+02	-6.40	-6.71	-8.36	-1.84	0.64
4445	1300-72-7	sodium xylenesulphonate	223

4535	1330-78-5	tris(methylphenyl) phosphate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+02	2.8E+00	1.0E+02	-6.72	-7.03	-8.68	-2.70	1.18
4536	68082-29-1	Fatty acids, C18-unsatd., dimers, oligomeric reaction products with tall-oil fatty acids and triethylenetetramine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+02	2.8E+00	1.0E+02	-6.73	-7.04	-8.69	-2.20	0.64
4537	26896-48-0	tricyclodecanedimethanol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+02	2.8E+00	9.9E+01	-6.73	-7.04	-8.69	-0.62	0.22
4538	68391-05-9	Quaternary ammonium compounds, di-C12-18-alkyldimethyl, chlorides	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+02	2.8E+00	9.9E+01	-6.73	-7.04	-8.69	-3.52	0.32
4539	68002-88-0	Fatty acids, C16-22	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.9E+02	2.7E+00	9.8E+01	-6.74	-7.04	-8.69	-1.84	0.64
4540	94279-90-0	Oils, animal, sulfated, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.9E+02	2.7E+00	9.7E+01	-6.74	-7.05	-8.70	-0.57	0.55
4541	61790-19-0	Oils, vegetable, sulfated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.9E+02	2.7E+00	9.7E+01	-6.74	-7.05	-8.70	-0.57	0.55
4542	68201-37-6	Octadecanoic acid, branched and linear	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.9E+02	2.6E+00	9.5E+01	-6.75	-7.06	-8.71	0.03	1.10
4543	68441-66-7	Decanoic acid, mixed esters with dipentaerythritol, octanoic acid and valeric acid	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.9E+02	2.6E+00	9.4E+01	-6.75	-7.06	-8.71	-1.84	0.64
4544	67746-08-1	Linseed oil, polymd.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.6E+00	9.2E+01	-6.76	-7.07	-8.72	-0.90	1.38
4545	68002-70-0	Glycerides, C16-22	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.6E+00	9.2E+01	-6.76	-7.07	-8.72	-0.17	0.55
4546	1226892-45-(	Fatty acids C18 unsat, reaction products with tetraethylenepentamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	9.2E+01	-6.76	-7.07	-8.72	-3.10	0.58
4547	27970-79-2	1-hydroxy-2-methylpentan-3-one	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	9.1E+01	-6.77	-7.07	-8.72	-1.84	0.64
4548	163292-61-3	605-322-0	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	9.1E+01	-6.77	-7.07	-8.72	-1.84	0.64
4549	1160806-44-1	Reaction mass of ethyl (2S,3S)-3,4-dibromo-2-methylbutanoate and ethyl (2R,3R)-3,4-dibromo-2-methylbutanoate a	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	9.1E+01	-6.77	-7.07	-8.72	-1.50	0.64
4550	68411-44-9	Benzene, butyl-, branched and linear	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	9.1E+01	-6.77	-7.07	-8.72	-2.68	0.64
4551	66319-07-1	1,4-anhydro-2,5-dideoxy-2-(methoxycarbonyl)-1-thiopent-3-ulose	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	9.1E+01	-6.77	-7.07	-8.72	-1.84	0.64
4552	68953-96-8	Benzenesulfonic acid, mono-C11-13-branched alkyl derivs., calcium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	9.0E+01	-6.77	-7.08	-8.73	-1.60	0.54
4553	95912-87-1	Fatty acids, C16-18, C12-18-alkyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	9.0E+01	-6.77	-7.08	-8.73	-0.17	1.22
4554	95912-88-2	Fatty acids, C16-18, isotridecyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	9.0E+01	-6.77	-7.08	-8.73	-1.00	0.64
4555	1229186-15-(	N-benzyl-N-C16-18 (even numbered)-alkyl-N-methyl-C16-18 (even numbered)-alkyl-1-aminium chloride	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	8.9E+01	-6.78	-7.08	-8.73	-2.87	0.31
4556	84649-98-9	Cinnamomum zeylanicum, ext.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	8.8E+01	-6.78	-7.09	-8.74	-2.78	0.64
4557	1245638-61-(	2-Propenoic acid, reaction products with pentaerythritol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.5E+00	8.8E+01	-6.78	-7.09	-8.74	-2.10	0.41
4558	1338-39-2	sorbitan laurate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.4E+00	8.8E+01	-6.78	-7.09	-8.74	-1.06	0.70
4559	84989-06-0	Tar acids, xylenol fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+02	2.4E+00	8.7E+01	-6.79	-7.09	-8.74	-1.71	0.35
4560	77745-66-5	triisotridecyl phosphite	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+02	2.4E+00	8.7E+01	-6.79	-7.09	-8.74	-1.84	0.64
4561	97925-95-6	Ethanol, 2,2'-iminobis-, N-(C13-15-branched and linear alkyl) derivs.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+02	2.4E+00	8.7E+01	-6.79	-7.10	-8.75	-3.79	0.91
4562	27253-26-5	diisotridecyl phthalate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+02	2.4E+00	8.6E+01	-6.79	-7.10	-8.75	-2.83	0.52
4563	29385-43-1	methyl-1H-benzotriazole	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+02	2.4E+00	8.6E+01	-6.79	-7.10	-8.75	-1.13	0.44
4564	25550-98-5	diisodecyl phenyl phosphite	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+02	2.3E+00	8.4E+01	-6.80	-7.11	-8.76	-2.40	0.64
4565	26544-38-7	dihydro-3-(tetrapropenyl)furan-2,5-dione	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+02	2.3E+00	8.3E+01	-6.80	-7.11	-8.76	-1.41	0.64
4566	126-86-1	2,4,7,9-tetramethyldec-5-yne-4,7-diol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+02	2.3E+00	8.3E+01	-6.81	-7.11	-8.77	-1.43	0.32
4567	68187-76-8	Castor oil, sulfated, sodium salt	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+02	2.3E+00	8.3E+01	-6.81	-7.12	-8.77	-0.99	0.44
4568	1218787-32-(	2,2'-(C16-18 (evennumbered, C18 unsaturated) alkyl imino) diethanol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+02	2.3E+00	8.2E+01	-6.81	-7.12	-8.77	-4.03	0.71
4569	68457-79-4	Phosphorodithioic acid, mixed O,O-bis(iso-Bu and pentyl) esters, zinc salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+02	2.3E+00	8.2E+01	-6.81	-7.12	-8.77	-1.71	0.37
4570	32210-23-4	4-tert-butylcyclohexyl acetate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+02	2.3E+00	8.1E+01	-6.82	-7.12	-8.77	-1.94	0.25
4571	68608-66-2	Acetic acid, chloro-, sodium salt, reaction products with 4,5-dihydro-2-undecyl-1H-imidazole-1-ethanol and sodium	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+02	2.2E+00	8.1E+01	-6.82	-7.13	-8.78	-1.67	0.82
4572	25550-51-0	hexahydromethylphthalic anhydride	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+02	2.2E+00	8.0E+01	-6.82	-7.13	-8.78	-0.67	0.29
4573	68610-97-9	614-668-1	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+02	2.2E+00	8.0E+01	-6.82	-7.13	-8.78	-1.84	0.64
4574	68583-51-7	Decanoic acid, mixed diesters with octanoic acid and propylene glycol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+02	2.2E+00	8.0E+01	-6.82	-7.13	-8.78	-1.89	0.64
4575	94279-37-5	1-Butene, chlorinated, epoxidized, distn. residues	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+02	2.2E+00	7.9E+01	-6.83	-7.13	-8.78	-1.84	0.64
4576	1338-41-6	sorbitan stearate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+02	2.2E+00	7.8E+01	-6.83	-7.14	-8.79	-1.84	0.64
4577	9032-08-0	Amylase, gluco-	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+02	2.2E+00	7.8E+01	-6.84	-7.14	-8.79	-0.38	0.28
4578	1160164-88-(	Alcohols, C18-22, distn. residues	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+02	2.2E+00	7.7E+01	-6.84	-7.14	-8.80	-0.50	0.64
4579	68439-75-8	Amines, di-C12-18-alkylmethyl	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+02	2.1E+00	7.7E+01	-6.84	-7.15	-8.80	-3.40	1.00
4580	68855-45-8	Phenol, dodecyl-, sulfurized, calcium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+02	2.1E+00	7.5E+01	-6.85	-7.16	-8.81	0.21	0.41
4581	140362-65-8	extract residues (coal tar), high-temperature, naphthalene oil alkaline, distn. overheads	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+02	2.1E+00	7.5E+01	-6.85	-7.16	-8.81	-1.64	0.64
4582	9000-90-2	Amylase, α-	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+02	2.1E+00	7.5E+01	-6.85	-7.16	-8.81	-0.73	1.05
4583	71786-60-2	Ethanol, 2,2'-iminobis-, N-C12-18-alkyl derivs.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+02	2.1E+00	7.5E+01	-6.85	-7.16	-8.81	-3.50	0.43
4584	67762-63-4	Fatty acids, tall-oil, Bu esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+02	2.1E+00	7.5E+01	-6.85	-7.16	-8.81	-0.89	0.64
4585	163206-31-3	Hexane, 1,6-diisocyanato-, homopolymer, 3,5-dimethyl-1H-pyrazole-blocked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+02	2.1E+00	7.4E+01	-6.86	-7.16	-8.81	-0.25	0.64
4586	68201-60-5	Resin acids and Rosin acids, maleated, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+02	2.1E+00	7.4E+01	-6.86	-7.16	-8.81	-1.81	0.28
4587	95371-11-2	Oils, animal, sulfonated, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+02	2.0E+00	7.3E+01	-6.86	-7.17	-8.82	-0.65	0.53
4588	68909-99-9	2-Propenenitrile, reaction products with ethylenediamine, hydrogenated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+02	2.0E+00	7.3E+01	-6.86	-7.17	-8.82	-0.95	0.36
4589	86089-17-0	tridecylamine, branched and linear	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+02	2.0E+00	7.3E+01	-6.86	-7.17	-8.82	-4.13	0.74
4590	159168-82-8	4,4'-Methylenediphenyl diisocyanate, oligomeric reaction products with 2,4'-diisocyanatodiphenylmethane, [(meth	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+02	2.0E+00	7.3E+01	-6.86	-7.17	-8.82	0.37	0.26
4591	947522-81-8	3-[C13-(branched)-alkyloxy]propionitrile	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+02	2.0E+00	7.2E+01	-6.87	-7.18	-8.83	-1.84	0.64
4592	68002-65-3	Nitriles, C16-18	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+02	1.9E+00	7.0E+01	-6.88	-7.19	-8.84	-1.84	0.64
4593	8016-11-3	Linseed oil, epoxidized	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+02	1.9E+00	7.0E+01	-6.88	-7.19	-8.84	-1.84	0.64
4594	65997-05-9	Rosin, oligomers	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+02	1.9E+00	7.0E+01	-6.88	-7.19	-8.84	-1.91	1.16
4595	85535-84-8	Alkanes, C10-13, chloro	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+02	1.9E+00	6.9E+01	-6.89	-7.19	-8.84	-2.12	0.64
4596	20566-35-2	2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl 3,4,5,6-tetrabromophthalate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+02	1.9E+00	6.9E+01	-6.89	-7.19	-8.85	-2.04	0.64
4597	68081-77-6	614-264-5	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+02	1.9E+00	6.8E+01	-6.89	-7.20	-8.85	-1.84	0.64
4598	130169-56-1	C12-14-(even numbered)-alkylamines	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+02	1.9E+00	6.8E+01	-6.89	-7.20	-8.85	-3.75	0.78
4599	68424-37-3	Fatty acids, C14-22	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+02	1.9E+00	6.8E+01	-6.89	-7.20	-8.85	-1.22	0.64
4600	91052-13-0	Glycerides, C8-18 and C18-unsatd. mono- and di-, acetates	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+02	1.9E+00	6.8E+01	-6.89	-7.20	-8.85	-1.12	0.68
4601	9005-00-9	Octadecan-1-ol, ethoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.9E+00	6.7E+01	-6.90	-7.20	-8.86	-2.80	0.51
4602	85186-86-3	Fatty acids, C8-18 and C18-unsatd., esters with neopentyl glycol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.6E+01	-6.91	-7.21	-8.86	-1.84	0.64
4603	84238-17-5	Fatty acids, palm-oil, hydrogenated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.6E+01	-6.91	-7.21	-8.86	-1.00	0.64
4604	68155-37-3	Amines, N-C12-18-alkyltrimethylenedi-	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.6E+01	-6.91	-7.21	-8.87	-3.12	0.64
4605	91722-33-7	Tar, wood	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.6E+01	-6.91	-7.21	-8.87	-1.84	0.64
4606	111-57-9	N-(2-hydroxyethyl)stearamide	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.6E+01	-6.91	-7.22	-8.87	-2.06	0.61
4607	13510B-88-2	Formaldehyde, polymer with benzenamine, hydrogenated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.6E+01	-6.91	-7.22	-8.87	-1.44	0.29
4608	68610-84-4	Benzenesulfonic acid, propenated, calcium salt, overbased	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.4E+01	-6.92	-7.23	-8.88	0.19	0.60
4609	25155-23-1	trixylyl phosphate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.4E+01	-6.92	-7.23	-8.88	-2.38	1.32
4610	92731-41-4	Ethanol, 2-amino-, reaction products with ammonia, 1-piperazineethanamine fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.4E+01	-6.92	-7.23	-8.88	-0.84	0.84
4611	90622-29-0	Alkenes, C13-14, hydroformylation products, distn. residues	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.4E+01	-6.92	-7.23	-8.88	-0.70	0.35
4612	90411-68-0	Hexanoic acid, 2-ethyl-, C16-18-alkyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.4E+01	-6.92	-7.23	-8.88	-1.84	0.64
4613	68477-42-9	Gases (petroleum), extractive, C3-5, butene-isobutylene-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	6.3E+01	-6.92	-7.23	-8.88	-1.81	0.23
4614	51728-26-8	Pentaerythritol, ethoxylated, esters with acrylic acid	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.7E+00	6.3E+01	-6.93	-7.23	-8.89	-1.53	0.85
4615	103170-26-9	3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate, oligomers, reaction products with 2-butanone oxime	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.7E+00	6.3E+01	-6.93	-7.24	-8.89	-0.30	0.64
4616	36078-10-1	dodecyl oleate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	6.2E+01	-6.93	-7.24	-8.89	-0.33	0.25
4617	110839-12-8	Toluene diisocyanate, oligomeric reaction products with water	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	6.2E+01	-6.93	-7.24	-8.89	-1.84	0.64
4618	135800-37-2	Fatty acids, C8-16, 2-ethylhexyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	6.1E+01	-6.94	-7.25	-8.90	-0.64	0.64
4619	68187-89-3	Acid chlorides, coco	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	6.0E+01	-6.95	-7.25	-8.90	-1.95	1.02
4620	161907-80-8	ethanol, 2-methoxy-, manufacture of, by-products from, esters with boric acid	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	6.0E+01	-6.95	-7.25	-8.90	-0.04	0.46
4621	84539-54-8	Acetic acid, oxo-, sodium salt, reaction products with ethylenediamine and hydroxybenzenesulfonic acid monosodi	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	6.0E+01	-6.95	-7.25	-8.91	-0.61	0.70
4622	68604-44-4	Fatty acids, C16-18 and C18-unsatd., tetraesters with pentaerythritol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	6.0E+01	-6.95	-7.26	-8.91	-0.28	0.76
4623	92908-35-5	Urea, reaction products with formaldehyde and glyoxal	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	6.0E+01	-6.95	-7.26	-8.91	-0.26	0.70
4624	2215-35-2	zinc O,O,O',O'-tetraks(1,3-dimethylbutyl) bis(phosphorodithioate)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	5.9E+01	-6.95	-7.26	-8.91	-1.71	0.37
4625	39423-51-3	Propylidynetrimethanol, propoxylated, reaction products with ammonia	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	5.9E+01	-6.95	-7.26	-8.91	-1.84	0.64
4626	1345668-41-(	Unknown	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.7E+00	5.9E+01	-6.95	-7.26	-8.91	-2.01	0.49
4627	1218787-30-(	2,2'-(C16-18 (evennumbered) alkyl imino) diethanol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf

4718	68783-88-0	Soybean oil, deodorizer distillate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.5E+01	1.1E+00	3.8E+01	-7.15	-7.46	-9.11	-1.00	0.64
4719	27138-01-8	α,α',α'-tetramethylxylene-α,α-diol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.5E+01	1.0E+00	3.8E+01	-7.15	-7.46	-9.11	-0.41	0.64
4720	68603-75-8	Amines, N-tallow alkyltrimethylenedi-, propoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.4E+01	1.0E+00	3.7E+01	-7.16	-7.46	-9.11	-3.99	0.45
4721	91050-88-3	Fatty acids, C6-18, triesters with trimethylolpropane	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.4E+01	1.0E+00	3.7E+01	-7.16	-7.46	-9.11	-1.84	0.64
4722	64147-40-6	Castor oil, dehydrated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.4E+01	1.0E+00	3.7E+01	-7.16	-7.46	-9.11	-0.17	0.58
4723	1273322-45-4	C16-18(even numbered)-alkylamine acetate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.4E+01	1.0E+00	3.7E+01	-7.16	-7.46	-9.12	-3.47	0.49
4724	73037-34-0	disodium oxybis[methylbenzenesulphonate]	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.3E+01	1.0E+00	3.7E+01	-7.16	-7.47	-9.12	-0.95	0.64
4725	80939-62-4	Amines, C11-14-branched alkyl, monohexyl and dihexyl phosphates	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.3E+01	1.0E+00	3.7E+01	-7.16	-7.47	-9.12	-2.53	0.49
4726	158318-67-3	Fatty acids, C16-18 and C18-unsatd., Me esters, epoxidized	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.3E+01	1.0E+00	3.6E+01	-7.16	-7.47	-9.12	-0.25	0.74
4727	118800-30-9	Oxirane, methyl-, polymer with oxirane, ether with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol (3:1), 2-propenoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.3E+01	1.0E+00	3.6E+01	-7.17	-7.47	-9.12	-1.87	0.56
4728	90989-41-6	Aromatic hydrocarbons, C6-10, C8-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.3E+01	1.0E+00	3.6E+01	-7.17	-7.47	-9.12	-2.70	0.22
4729	85049-33-8	Fatty acids, C8-18 and C18-unsatd., esters with pentaerythritol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.2E+01	1.0E+00	3.6E+01	-7.17	-7.47	-9.13	-1.84	0.64
4730	160901-09-7	Alcohols, C9-11, branched and linear, ethoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.1E+01	9.9E-01	3.6E+01	-7.17	-7.48	-9.13	-1.84	0.64
4731	67989-52-0	4,4'-Isopropylidenediphenol, oligomeric reaction products with 1-chloro-2,3-epoxypropane, reaction products with	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.0E+01	9.8E-01	3.5E+01	-7.18	-7.49	-9.14	-1.84	0.64
4732	1384855-91-7	2-Propenoic acid, reaction products with dipentaerythritol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.0E+01	9.7E-01	3.5E+01	-7.18	-7.49	-9.14	-1.75	0.22
4733	91722-14-4	Soybean oil, epoxidized, acrylate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.9E+01	9.7E-01	3.5E+01	-7.19	-7.49	-9.14	-1.59	0.64
4734	26316-40-5	Ethylenediamine, ethoxylated and propoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.9E+01	9.6E-01	3.4E+01	-7.19	-7.50	-9.15	-0.26	1.16
4735	25339-53-1	decene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.9E+01	9.5E-01	3.4E+01	-7.19	-7.50	-9.15	-2.68	1.28
4736	31831-53-5	2-Oxepanone, polymer with 1,4-butanediol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.8E+01	9.4E-01	3.4E+01	-7.20	-7.50	-9.16	-0.82	0.30
4737	68391-08-2	Alcohols, C8-14, γ-ω-perfluoro	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.7E+01	9.4E-01	3.4E+01	-7.20	-7.50	-9.16	-3.10	0.28
4738	25448-25-3	trisodecyl phosphite	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.7E+01	9.4E-01	3.4E+01	-7.20	-7.51	-9.16	-1.84	0.64
4739	61789-45-5	Fatty acids, dehydrated castor-oil	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.7E+01	9.3E-01	3.3E+01	-7.20	-7.51	-9.16	-0.22	1.19
4740	63310-16-7	9-Octadecenoic acid (Z)-, monoester with 1,2,3-propanetriol ester with boric acid (H3BO3)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.6E+01	9.3E-01	3.3E+01	-7.20	-7.51	-9.16	-0.60	0.64
4741	41637-38-1	Poly[oxy-1,2-ethanediyl], α,α'-[[1-(methylethylidene)di-4,1-phenylene]bis[ω-[[2-methyl-1-oxo-2-propen-1-yl]oxy]-	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.6E+01	9.2E-01	3.3E+01	-7.21	-7.51	-9.17	-1.61	0.64
4742	68425-34-3	Petrolatum (petroleum), oxidized, calcium salt	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.6E+01	9.2E-01	3.3E+01	-7.21	-7.52	-9.17	0.17	1.10
4743	68956-56-9	Hydrocarbons, terpene processing by-products	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.6E+01	9.2E-01	3.3E+01	-7.21	-7.52	-9.17	-2.44	0.64
4744	68122-64-5	Soybean oil, polymd.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.6E+01	9.2E-01	3.3E+01	-7.21	-7.52	-9.17	-0.55	1.28
4745	94667-33-1	Poly[oxy-1,2-ethanediyl], α-[2-(didecylmethylammonio)ethyl]-ω-hydroxy-, propanoate (1:1)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.6E+01	9.2E-01	3.3E+01	-7.21	-7.52	-9.17	-3.68	0.40
4746	67762-53-2	Fatty acids, C5-9, tetraesters with pentaerythritol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.6E+01	9.1E-01	3.3E+01	-7.21	-7.52	-9.17	-1.34	1.14
4747	71662-46-9	1,2-Benzenedicarboxylic acid, di-C8-10-alkyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.4E+01	8.9E-01	3.2E+01	-7.22	-7.53	-9.18	-2.99	0.77
4748	75782-87-5	Alcohols, C14-15	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.4E+01	8.9E-01	3.2E+01	-7.22	-7.53	-9.18	-2.08	0.64
4749	65996-87-4	Extract residues (coal), tar oil alk.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.4E+01	8.9E-01	3.2E+01	-7.22	-7.53	-9.18	-1.64	0.64
4750	3010-96-6	2,2,4,4-tetramethylcyclobutane-1,3-diol, mixed isomers	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.4E+01	8.9E-01	3.2E+01	-7.22	-7.53	-9.18	-0.46	0.64
4751	96152-43-1	Phenol, dodecyl-, branched, sulfurized	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.4E+01	8.9E-01	3.2E+01	-7.22	-7.53	-9.18	0.16	0.40
4752	122-32-7	1,2,3-propanetryl trioleate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.3E+01	8.8E-01	3.2E+01	-7.23	-7.53	-9.18	-1.84	0.64
4753	92129-53-8	Resin acids and Rosin acids, reaction products with formaldehyde, potassium salt	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.3E+01	8.8E-01	3.2E+01	-7.23	-7.53	-9.19	-1.87	1.14
4754	61791-12-6	Castor oil, ethoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.3E+01	8.8E-01	3.1E+01	-7.23	-7.54	-9.19	-1.84	0.64
4755	85586-34-1	Soybean oil, epoxidized, ether with ethylene glycol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.3E+01	8.7E-01	3.1E+01	-7.23	-7.54	-9.19	0.92	1.15
4756	106276-80-6	Reaction products of benzene-1,4-diamine and methyl 2,3,4,5-tetrachloro-6-cyanobenzoate and sodium methanola	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.2E+01	8.7E-01	3.1E+01	-7.23	-7.54	-9.19	-0.50	0.64
4757	85029-52-3	Acacia mearnsi, ext., reaction products with ammonium chloride and formaldehyde	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.2E+01	8.6E-01	3.1E+01	-7.24	-7.54	-9.19	-1.64	0.33
4758	85186-92-1	Fatty acids, C14-18 and C16-18-unsatd., mixed esters with neopentyl glycol and trimethylolpropane	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.1E+01	8.5E-01	3.1E+01	-7.24	-7.55	-9.20	0.17	0.76
4759	90506-45-9	Phosphoric acid, C16-18-alkyl esters, potassium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.1E+01	8.5E-01	3.1E+01	-7.24	-7.55	-9.20	-0.50	0.64
4760	94108-97-1	2-[[2,2-bis[[(1-oxoalyl)(ox)methyl]butox]methyl]-2-ethyl-1,3-propanediyl diacrylate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.1E+01	8.5E-01	3.0E+01	-7.24	-7.55	-9.20	-2.90	0.64
4761	1226892-49-4	Fatty acids, C18-unsaturated, reaction products with amines, polyethylenepoly- (triethylenetetramine, pentaethyle	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.1E+01	8.4E-01	3.0E+01	-7.24	-7.55	-9.20	-3.06	0.54
4762	67762-52-1	Fatty acids, C5-9, hexaesters with dipentaerythritol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.0E+01	8.4E-01	3.0E+01	-7.25	-7.55	-9.20	-0.17	0.58
4763	85711-46-2	Fatty acids, C14-18 and C16-18-unsatd., maleated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.0E+01	8.4E-01	3.0E+01	-7.25	-7.56	-9.21	-1.04	0.83
4764	68131-40-8	Alcohols, C11-15-secondary, Ethoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.9E+01	8.2E-01	3.0E+01	-7.25	-7.56	-9.21	-2.41	0.70
4765	68131-72-6	Polyphosphoric acids, esters with triethanolamine, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.8E+01	8.1E-01	2.9E+01	-7.26	-7.57	-9.22	0.15	0.79
4766	68187-84-8	Castor oil, oxidized	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.8E+01	8.1E-01	2.9E+01	-7.26	-7.57	-9.22	-0.87	0.72
4767	144086-02-2	2-Propenoic acid, polymer with 2,2-bis(hydroxymethyl)-1,3-propanediol, methyloxirane and oxirane	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.7E+01	8.0E-01	2.9E+01	-7.27	-7.58	-9.23	-1.49	0.79
4768	68002-42-6	4,4'-Isopropylidenediphenol, oligomeric reaction products with 1-chloro-2,3-epoxypropane, reaction products with	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.7E+01	8.0E-01	2.9E+01	-7.27	-7.58	-9.23	-1.84	0.64
4769	83897-91-0	titanium tetra(octanolate), branched and linear	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.7E+01	7.9E-01	2.8E+01	-7.27	-7.58	-9.23	-1.69	0.26
4770	25618-55-7	1,2,3-Propanetriol, homopolymer	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.7E+01	7.9E-01	2.8E+01	-7.27	-7.58	-9.23	-1.84	0.64
4771	68515-51-5	1,2-Benzenedicarboxylic acid, di-C6-10-alkyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.7E+01	7.9E-01	2.8E+01	-7.27	-7.58	-9.23	-2.99	0.77
4772	97592-79-5	2-Propanol, 1,1'-[[3-[(3-aminopropyl)amino]propyl]imino]bis-, N-tallow alkyl derivs.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.7E+01	7.9E-01	2.8E+01	-7.27	-7.58	-9.23	-4.05	0.53
4773	39322-78-6	Phosphoric acid, dodecyl ester, potassium salt	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.7E+01	7.9E-01	2.8E+01	-7.27	-7.58	-9.23	0.19	0.64
4774	91031-45-7	Fatty acids, C16-18, 1,2-ethanediylbis(oxy-2,1-ethanediyl) esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.6E+01	7.8E-01	2.8E+01	-7.28	-7.58	-9.23	-1.73	0.90
4775	90640-43-0	Amines, N-C12-14-alkyltrimethylenedi-	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.6E+01	7.8E-01	2.8E+01	-7.28	-7.58	-9.23	-4.27	0.45
4776	100209-45-8	Protein hydrolyzates, vegetable	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.6E+01	7.8E-01	2.8E+01	-7.28	-7.58	-9.24	-1.84	0.64
4777	85631-54-5	2-Propenoic acid, γ-ω-perfluoro-C8-14-alkyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.6E+01	7.8E-01	2.8E+01	-7.28	-7.59	-9.24	-3.04	0.35
4778	68153-95-7	Amines, di-C12-18-alkyl	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+01	7.7E-01	2.8E+01	-7.29	-7.59	-9.24	-3.29	0.64
4779	7212-44-4	3,7,11-trimethyldodeca-1,6,10-trien-3-ol,mixed isomers	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+01	7.6E-01	2.7E+01	-7.29	-7.59	-9.25	-2.85	0.21
4780	70225-05-7	615-086-0	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+01	7.6E-01	2.7E+01	-7.29	-7.60	-9.25	-1.84	0.64
4781	53988-10-6	1,3-dihydro-4(or 5)-methyl-2H-benzimidazole-2-thione	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+01	7.6E-01	2.7E+01	-7.29	-7.60	-9.25	-1.64	0.66
4782	22393-85-7	tetradecyl oleate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+01	7.6E-01	2.7E+01	-7.29	-7.60	-9.25	-0.83	0.79
4783	84539-53-7	Acetic acid, oxo-, sodium salt, reaction products with cresol and ethylenediamine, iron sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+01	7.6E-01	2.7E+01	-7.29	-7.60	-9.25	-0.67	1.08
4784	68424-19-1	Fatty acids, C16-18 and C18-unsatd., compds. with triethanolamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.4E+01	7.5E-01	2.7E+01	-7.30	-7.60	-9.25	-1.84	0.64
4785	77538-19-3	Docosanoic acid, ester with 1,2,3-propanetriol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.4E+01	7.5E-01	2.7E+01	-7.30	-7.60	-9.26	0.07	0.97
4786	68442-22-8	Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu) esters, zinc salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.3E+01	7.5E-01	2.7E+01	-7.30	-7.61	-9.26	-1.71	0.37
4787	26762-93-6	diisopropylbenzene hydroperoxide	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.3E+01	7.4E-01	2.7E+01	-7.30	-7.61	-9.26	-2.19	0.35
4788	97489-11-7	Resin acids and Rosin acids, fumarated, esters with glycerol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.3E+01	7.4E-01	2.7E+01	-7.30	-7.61	-9.26	-1.84	0.64
4789	94441-92-6	sodium N-(2-carboxyethyl)-N-(2-ethylhexyl)-β-alaninate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.3E+01	7.4E-01	2.6E+01	-7.30	-7.61	-9.26	-0.41	0.64
4790	68603-38-3	Amides, C16-18 and C18-unsatd., N,N-bis(hydroxyethyl)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.3E+01	7.4E-01	2.6E+01	-7.30	-7.61	-9.26	-2.35	0.48
4791	28390-91-2	4,4'-Methylenedianiline, oligomeric reaction products with 1-chloro-2,3-epoxypropane	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.2E+01	7.2E-01	2.6E+01	-7.31	-7.62	-9.27	-2.11	0.79
4792	91050-82-7	Fatty acids, C16-18, tetraesters with pentaerythritol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.2E+01	7.2E-01	2.6E+01	-7.31	-7.62	-9.27	-0.28	0.76
4793	1365085-43-7	Fatty acids, C8-10 (even numbered), 3-methylbutyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.2E+01	7.2E-01	2.6E+01	-7.31	-7.62	-9.27	-0.36	0.99
4794	68475-37-6	Resin acids and Rosin acids, polymd., esters with glycerol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.1E+01	7.1E-01	2.6E+01	-7.32	-7.63	-9.28	0.20	0.63
4795	26748-41-4	tert-butyl peroxyneodecanoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.1E+01	7.1E-01	2.5E+01	-7.32	-7.63	-9.28	-3.39	0.43
4796	96690-55-0	Tar acids, distin. residues	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.1E+01	7.1E-01	2.5E+01	-7.32	-7.63	-9.28	-1.84	0.64
4797	68390-97-6	Amines, C16-18-alkyldimethyl	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.0E+01	7.0E-01	2.5E+01	-7.32	-7.63	-9.28	-3.88	0.66
4798	85186-95-4	Fatty acids, C12-16, esters with neopentyl glycol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.0E+01	7.0E-01	2.5E+01	-7.32	-7.63	-9.28	0.17	0.76
4799	91078-64-7	Naphthalenesulfonic acids, branched and linear Bu derivs., sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.0E+01	7.0E-01	2.5E+01	-7.33	-7.63	-9.28	-0.92	0.64
4800	102242-48-8	Alcohols, C6-24 and C6-24-unsatd., distn. residues	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.0E+01	6.9E-01	2.5E+01	-7.33	-7.64	-9.29	0.83	1.15
4801	17671-27-1	docosyl docosanoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.9E+01	6.8E-01	2.5E+01	-7.34	-7.64	-9.29	-1.84	0.64
4802	91744-38-6	Glycerides, C16-18 mono-, di- and tri-, hydrogenated, citrates, potassium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.9E+01	6.8E-01	2.4E+01	-7.34	-7.65	-9.30	-1.84	0.64
4803	186321-96-0	Fatty acids, tall-oil, reaction products with bisphenol A, epichlorohydrin, glycols/ tolyl ether and triethylenetetramin	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.8E+01	6.7E-01	2.4E+01	-7.34	-7.65	-9.30	-3.19	0.55
4804	1258274-08-4	Aromatic hydrocarbons, C10-13, reaction products with branched nonene, sulfonated, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.8E+01	6.7E-01	2.4E+01	-7.34	-7.65	-9.30	-0.85	0.49
4805	68424-50-0	Fatty acids, tall-oil, C12-15-alkyl esters, sulfated, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.8E+01	6.7E-01	2.4E+01	-7.35	-7.65	-9.31	-0.97	0.55
4806	68440-34-6	Fatty acids, tallow, zinc salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.8E+01	6.6E-01	2.4E+01	-7.35	-7.66	-9.31	-2.89	0.69
4807	100402-60-6	d-Glucose, ether with glycerol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.7E+01	6.6E-01	2.4E+01	-7.35	-7.66	-9.31	0.32	0.64
4808	52624-57-4	610-877-7	223	87	9.9E-03	1.5E+03	3.0E+02

4901	26301-10-0	Oxirane, 2-methyl-, polymer with oxirane, ether with β-D-fructofuranosyl α-D-glucopyranoside	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.9E+01	4.0E-01	1.4E+01	-7.57	-7.88	-9.53	0.04	0.81
4902	29253-36-9	isopropylnaphthalene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.9E+01	4.0E-01	1.4E+01	-7.57	-7.88	-9.53	-3.38	0.41
4903	84082-70-2	Peppermint, ext.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.9E+01	4.0E-01	1.4E+01	-7.57	-7.88	-9.53	-2.54	0.64
4904	92128-40-0	Glycerides, C10-20 and C10-20-unsatd., oxidized	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E+01	3.9E-01	1.4E+01	-7.57	-7.88	-9.53	-0.44	0.64
4905	68921-51-7	2-Butenedioic acid (E)-, di-C12-18-alkyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E+01	3.9E-01	1.4E+01	-7.58	-7.88	-9.54	-0.34	0.64
4906	84418-71-3	Phosphoric acid, mono- and bis(branched and linear pentyl) esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E+01	3.9E-01	1.4E+01	-7.58	-7.89	-9.54	-0.95	0.33
4907	68183-39-1	Benzene-1,2,4-tricarboxylic acid 1,2-anhydride, oligomeric reaction products with ethane-1,2-diol and glycerol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E+01	3.9E-01	1.4E+01	-7.58	-7.89	-9.54	-1.84	0.64
4908	68440-25-5	Fatty acids, tall-oil, reaction products with ethanolamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E+01	3.9E-01	1.4E+01	-7.58	-7.89	-9.54	-2.25	0.64
4909	68517-10-2	614-560-4	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E+01	3.8E-01	1.4E+01	-7.59	-7.90	-9.55	-1.84	0.64
4910	160901-12-2	Fatty acids, C18-unsatd., dimers, hydrogenated, dimethyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E+01	3.8E-01	1.4E+01	-7.59	-7.90	-9.55	-1.84	0.64
4911	81457-65-0	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, [[3-[(1-methylethoxy)propyl]amino]sulfonyl derivs.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E+01	3.8E-01	1.4E+01	-7.59	-7.90	-9.55	-1.84	0.64
4912	101896-27-9	Distillates (coal tar), naphthalene oils, methylnaphthalene fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E+01	3.8E-01	1.4E+01	-7.59	-7.90	-9.55	-1.99	0.88
4913	163149-28-8	Unknown	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E+01	3.8E-01	1.4E+01	-7.59	-7.90	-9.55	0.64	0.29
4914	1229648-98-7	Condensation prod of N-C12-C18-alkylpropane-1,3-diamine, N-(3-aminopropyl)-N-C12-C18-alkylpropane-1,3-diamin	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E+01	3.8E-01	1.4E+01	-7.59	-7.90	-9.55	-3.80	0.60
4915	25360-10-5	1,1-dimethylheptanethiol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E+01	3.8E-01	1.4E+01	-7.59	-7.90	-9.55	-3.57	0.64
4916	85114-00-7	2-ethylhexanoic acid, monoester with propane-1,2-diol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E+01	3.8E-01	1.3E+01	-7.60	-7.90	-9.55	-1.57	0.25
4917	68411-04-1	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, [[3-[(dimethylamino)propyl]amino]sulfonyl derivs.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.7E-01	1.3E+01	-7.60	-7.90	-9.56	-1.84	0.64
4918	91002-07-2	Fatty acids, C16-18, barium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.7E-01	1.3E+01	-7.60	-7.90	-9.56	-0.58	0.57
4919	25640-78-2	(1-methylethyl)-1,1'-biphenyl	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.7E+01	3.7E-01	1.3E+01	-7.60	-7.91	-9.56	-3.61	0.20
4920	68213-23-0	Alcohols, C12-18, ethoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.7E-01	1.3E+01	-7.60	-7.91	-9.56	-3.19	0.37
4921	1419212-76-2	Reaction products of tall oil fatty acids with diethylenetriamine and maleic anhydride	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.7E-01	1.3E+01	-7.61	-7.91	-9.56	-1.84	0.64
4922	61791-39-7	1H-Imidazole-1-ethanol, 4,5-dihydro-, 2-nortall-oil alkyl derivs.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.7E-01	1.3E+01	-7.61	-7.92	-9.57	-3.38	0.60
4923	63705-03-3	1,2,3-Propanetriol, homopolymer, diisooctadecanoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.7E-01	1.3E+01	-7.61	-7.92	-9.57	-0.59	0.33
4924	85536-06-7	Glycerides, C8-18	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.7E-01	1.3E+01	-7.61	-7.92	-9.57	-1.31	0.58
4925	68002-61-9	Quaternary ammonium compounds, (C16-18 and C18-unsatd. alkyl)trimethyl, chlorides	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.6E-01	1.3E+01	-7.61	-7.92	-9.57	-4.03	0.47
4926	8007-43-0	Sorbitan, (Z)-9-octadecenoate (2:3)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.6E-01	1.3E+01	-7.62	-7.92	-9.57	0.79	0.59
4927	147900-93-4	Fatty acids, C18-unsatd., trimers, compds. with oleylamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.6E-01	1.3E+01	-7.62	-7.92	-9.57	-1.19	0.89
4928	68187-30-4	l-Glutamic acid, N-coco acyl derivs., disodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.6E-01	1.3E+01	-7.62	-7.92	-9.57	-1.16	0.30
4929	91744-39-7	Glycerides, C16-18 mono-, di- and tri-, hydrogenated, citrates, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.6E-01	1.3E+01	-7.62	-7.92	-9.57	-0.50	0.64
4930	36425-16-8	4,4'-Isopropylidenediphenol, oligomeric reaction products with 1-chloro-2,3-epoxypropane, reaction products with	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.6E-01	1.3E+01	-7.62	-7.92	-9.57	-1.84	0.64
4931	67784-87-6	Glycerides, palm-oil mono- and di-, hydrogenated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.6E-01	1.3E+01	-7.62	-7.93	-9.58	0.07	1.13
4932	85865-69-6	Fatty acids, C16-18, iso-Bu esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+01	3.6E-01	1.3E+01	-7.62	-7.93	-9.58	0.16	1.15
4933	85940-40-5	Fatty acids, tall-oil, reaction products with pentaethylenehexamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.5E+01	3.6E-01	1.3E+01	-7.62	-7.93	-9.58	-2.56	0.20
4934	85186-80-7	Fatty acids, C14-18 and C18-unsatd., branched and linear, Me esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.5E+01	3.5E-01	1.3E+01	-7.63	-7.93	-9.59	-1.84	0.64
4935	61617-00-3	1,3-dihydro-4(or 5)-methyl-2H-benzimidazole-2-thione, zinc salt	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.5E+01	3.5E-01	1.3E+01	-7.63	-7.93	-9.59	-2.40	0.37
4936	68909-18-2	Pyridinium, 1-(phenylmethyl)-, ethyl methyl derivs., chlorides	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.5E+01	3.4E-01	1.2E+01	-7.64	-7.94	-9.59	-2.59	1.10
4937	85711-45-1	Fatty acids, C16-18 and C18-unsatd., esters with pentaerythritol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+01	3.4E-01	1.2E+01	-7.64	-7.95	-9.60	-1.10	0.72
4938	1219458-14-4	N-(3-aminopropyl)-N'-C16-18 (evennumbered), C18 unsaturated alkyl -propane-1,3-diamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+01	3.4E-01	1.2E+01	-7.64	-7.95	-9.60	-3.73	0.61
4939	2579-20-6	1,3-Cyclohexanedimethanamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+01	3.4E-01	1.2E+01	-7.64	-7.95	-9.60	-1.18	0.23
4940	68153-02-6	Nitriles, C16-22	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+01	3.4E-01	1.2E+01	-7.64	-7.95	-9.60	-1.84	0.64
4941	218451-68-4	Reaction products of coconut oil with polyethyleneglycol and 2-ethyl-2-(hydroxymethyl)propane-1,3-diol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+01	3.4E-01	1.2E+01	-7.64	-7.95	-9.60	-1.36	0.39
4942	68308-74-7	Amides, tall-oil fatty, N,N-di-Me	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+01	3.3E-01	1.2E+01	-7.65	-7.95	-9.61	-2.57	0.52
4943	68081-91-4	Alcohols, C12-18, ethoxylated, sulfates, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+01	3.3E-01	1.2E+01	-7.65	-7.96	-9.61	-2.04	0.50
4944	61791-42-2	Ethanesulfonic acid, 2-(methylamino)-, N-coco acyl derivs., sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+01	3.3E-01	1.2E+01	-7.65	-7.96	-9.61	-1.89	0.50
4945	1226892-50-3	Amides, fatty acids C18 unsat, reaction products with polyethylene amines	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+01	3.3E-01	1.2E+01	-7.65	-7.96	-9.61	-3.10	0.58
4946	157707-73-8	Fatty acids, C18-unsatd., dimers, oligomeric reaction products with fatty acids, C16-18 and C18-unsatd., branched a	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+01	3.3E-01	1.2E+01	-7.65	-7.96	-9.61	-2.22	0.64
4947	61791-19-3	Fatty acids, tall-oil, reaction products with ethanolamine, ethoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+01	3.3E-01	1.2E+01	-7.65	-7.96	-9.61	-2.50	0.38
4948	93925-25-8	Phosphonic acid, mixed C12-20-alkyl and C14-18-unsatd. alkyl derivs.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+01	3.3E-01	1.2E+01	-7.65	-7.96	-9.61	-0.50	0.64
4949	39236-46-9	N,N'-methylenebis[N'-[3-(hydroxymethyl)-2,5-dioxoimidazolidin-4-yl]urea]	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.2E-01	1.2E+01	-7.66	-7.97	-9.62	-1.29	0.67
4950	15647-08-2	2-ethylhexyl diphenyl phosphite	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.2E-01	1.2E+01	-7.66	-7.97	-9.62	-1.84	0.64
4951	68988-45-4	Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu and pentyl) esters, zinc salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.2E-01	1.2E+01	-7.66	-7.97	-9.62	-2.27	0.50
4952	27614-71-7	[tetrachloro-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]copper	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.2E-01	1.2E+01	-7.66	-7.97	-9.62	-0.60	0.64
4953	68512-13-0	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, brominated chlorinated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.2E-01	1.1E+01	-7.67	-7.97	-9.62	-0.60	0.64
4954	1426148-68-4	Alcohols, C6-C8-(even numbered, linear)-ethoxylated (	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.2E-01	1.1E+01	-7.67	-7.98	-9.63	-0.81	0.27
4955	60209-82-7	isodecyl pivalate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.2E-01	1.1E+01	-7.67	-7.98	-9.63	-1.22	0.64
4956	38172-91-7	2-Propyn-1-ol, compd. with 2-methyloxirane (1:?)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.2E-01	1.1E+01	-7.67	-7.98	-9.63	-0.34	0.64
4957	1219826-66-4	N-(3-aminopropyl)-N-N-(C16-18 evennumbered, 18 unsaturated)-alkylpropane-1,3-diamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.2E-01	1.1E+01	-7.67	-7.98	-9.63	-3.57	0.68
4958	897381-19-0	Reaction products of ethane-1,2-diol and 1,2-epoxybutane	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.2E-01	1.1E+01	-7.67	-7.98	-9.63	-1.84	0.64
4959	94166-87-7	Aluminum, benzoate C16-18-fatty acids complexes	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.2E-01	1.1E+01	-7.67	-7.98	-9.63	-0.50	0.64
4960	71808-53-2	Quaternary ammonium compounds, C12-18-alkylbis(hydroxyethyl)methyl, chlorides	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.2E-01	1.1E+01	-7.67	-7.98	-9.63	-2.93	0.93
4961	70750-57-1	Terpenes and terpenoids, turpentine-oil, α-pinene fraction, oligomers	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.1E-01	1.1E+01	-7.67	-7.98	-9.63	-3.27	0.31
4962	61792-09-4	pentasodium pentahydrogen [[[(phosphonatomethyl)imino]bis(ethane-2,1-diylnitrilobis(methylene)]]tetrakisphosp	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.1E-01	1.1E+01	-7.67	-7.98	-9.63	-0.59	1.21
4963	68784-17-8	Isooctadecanoic acid, reaction products with tetraethylenepentamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.3E+01	3.1E-01	1.1E+01	-7.67	-7.98	-9.63	-0.55	1.30
4964	9001-62-1	Lipase, triacylglycerol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+01	3.1E-01	1.1E+01	-7.67	-7.98	-9.63	-0.83	0.54
4965	68424-85-1	Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl, chlorides	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+01	3.1E-01	1.1E+01	-7.68	-7.99	-9.64	-3.16	0.61
4966	84988-79-4	Fatty acids, C16-18 and C18-unsatd., iso-Bu esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+01	3.0E-01	1.1E+01	-7.69	-7.99	-9.65	-1.84	1.18
4967	162303-51-7	Tetra-n-butyl titanate, polymer with water	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+01	3.0E-01	1.1E+01	-7.69	-8.00	-9.65	0.00	0.33
4968	1275611-65-1	695-101-5	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+01	3.0E-01	1.1E+01	-7.69	-8.00	-9.65	-1.84	0.64
4969	95009-22-6	Cocoa, powd., alkalized	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	3.0E-01	1.1E+01	-7.69	-8.00	-9.65	-1.53	0.64
4970	101227-09-2	Fatty acids, C16-18, 2-hexyldecyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	3.0E-01	1.1E+01	-7.70	-8.01	-9.66	0.50	1.00
4971	91031-27-5	Fatty acids, C6-18, 2,2-dimethyl-1,3-propanediyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	3.0E-01	1.1E+01	-7.70	-8.01	-9.66	0.17	1.00
4972	133779-11-0	Amines, N-C16-18-alkyl (evennumbered) propane-1,3-diamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	2.9E-01	1.1E+01	-7.70	-8.01	-9.66	-3.95	0.51
4973	1000817-22-6	Fatty acids, C8-18 and C18-unsatd., reaction products with diethanolamine and propylene oxide	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	2.9E-01	1.1E+01	-7.70	-8.01	-9.66	-2.37	0.40
4974	68171-33-5	isopropyl isodecanoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	2.9E-01	1.1E+01	-7.70	-8.01	-9.66	-0.76	0.64
4975	19321-40-5	pentaerythritol tetraoleate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	2.9E-01	1.0E+01	-7.71	-8.01	-9.66	-0.75	0.75
4976	75627-31-5	Poly(oxy-1,2-ethanediyl), α-[3-[(carboxymethyl)methylamino]-2-hydroxypropyl]-ω-[4-nonylphenoxy]-, sodium salt (	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	2.9E-01	1.0E+01	-7.71	-8.02	-9.67	-2.54	0.28
4977	67701-33-1	Glycerides, C14-18 mono- and di-	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	2.9E-01	1.0E+01	-7.71	-8.02	-9.67	0.07	1.13
4978	68784-48-5	Titanium, diethylene glycol propylene glycol triethanolamine complexes	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	2.9E-01	1.0E+01	-7.71	-8.02	-9.67	-0.25	1.24
4979	18016-43-8	oleic acid, compound with N-(2-aminoethyl)ethane-1,2-diamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	2.9E-01	1.0E+01	-7.71	-8.02	-9.67	-2.02	0.49
4980	2451-62-9	1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	2.9E-01	1.0E+01	-7.71	-8.02	-9.67	-1.53	0.64
4981	6284-43-1	2,3-dihydroxypropyl 12-hydroxyoctadecanoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	2.9E-01	1.0E+01	-7.71	-8.02	-9.67	0.07	0.97
4982	100545-48-0	Octadecanoic acid, 12-hydroxy-, reaction products with ethylenediamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+01	2.9E-01	1.0E+01	-7.71	-8.02	-9.67	-1.84	0.64
4983	649747-80-8	Fatty acids, C8-10 (even numbered), 2-ethylhexyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+01	2.9E-01	1.0E+01	-7.72	-8.02	-9.67	-0.36	0.99
4984	82324-60-5	Reaction mass of ammonium 4-amino-3-nitrobenzenesulfonate and sodium 4-amino-3-nitrobenzenesulfonate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+01	2.8E-01	1.0E+01	-7.72	-8.02	-9.67	-1.84	0.64
4985	1334537-35-7	696-028-1	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+01	2.8E-01	1.0E+01	-7.72	-8.02	-9.67	-1.84	0.64
4986	68551-92-8	Fatty acids, C18-unsatd., dimers, ethoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+01	2.8E-01	1.0E+01	-7.72	-8.02	-9.68	-0.50	0.64
4987	109331-54-6	4,4'-Methylenediphenyl diisocyanate, oligomeric reaction products with 2,4'-diisocyanatodiphenylmethane	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+01	2.8E-01	1.0E+01	-7.72	-8.03	-9.68	-2.02	0.64
4988	37288-54-3	Mannanase, endo-1,4-β-	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+01	2.8E-01	1.0E+01	-7.72	-8.03	-9.68	-0.83	0.34
4989	85586-35-2	Soybean oil, epoxidized, reaction products with methanol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E

5084	1424148-94-4	6-(3-pentapropenyl-2,5-dioxopyrrolidin-1-yl)hexanoic acid	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+01	1.5E-01	5.5E+00	-7.99	-8.30	-9.95	-1.67	0.82
5085	92077-08-2	dihydro-3-(tripropenyl)furan-2,5-dione	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+01	1.5E-01	5.5E+00	-7.99	-8.30	-9.95	-1.84	0.64
5086	1178870-70-4	695-121-4	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+01	1.5E-01	5.5E+00	-7.99	-8.30	-9.95	-1.84	0.64
5087	78169-20-7	Sulfonium compounds, C11-14-alkylbis(hydroxyethyl), 2-hydroxyethyl sulfates (salts)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+01	1.5E-01	5.5E+00	-7.99	-8.30	-9.95	-3.31	1.29
5088	54261-67-5	zinc bis[bis(dodecylphenyl)] bis(dithiophosphate)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+01	1.5E-01	5.5E+00	-7.99	-8.30	-9.95	-1.89	0.74
5089	97553-05-4	fatty acids, C16-18 and C18-unsatd., isooctyl esters, epoxidized	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+01	1.5E-01	5.4E+00	-7.99	-8.30	-9.95	-0.01	0.85
5090	161075-00-9	Hexafluoropropene, oxidized, oligomers, reduced, fluorinated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+01	1.5E-01	5.4E+00	-7.99	-8.30	-9.95	-2.40	0.64
5091	173011-06-8	1-Butanamine, N-butyl-, reaction products with polyethylene-polypropylene glycol ether with trimethylolpropane (	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+01	1.5E-01	5.3E+00	-8.00	-8.31	-9.96	-1.62	0.75
5092	55066-48-3	3-methyl-5-phenylpentanol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+01	1.5E-01	5.3E+00	-8.00	-8.31	-9.96	-1.82	0.64
5093	1330-61-6	isodecyl acrylate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+01	1.4E-01	5.1E+00	-8.02	-8.32	-9.98	-2.78	0.64
5094	141773-73-1	2-(1-{[3',3'-dimethyl-1'-cyclohexyl]ethoxy}-2-methyl propyl propanoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+01	1.4E-01	5.1E+00	-8.02	-8.33	-9.98	-2.59	0.28
5095	42594-17-2	(octahydro-4,7-methano-1H-indenediyl)bis(methylene) diacrylate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+01	1.4E-01	5.0E+00	-8.02	-8.33	-9.98	-2.70	0.64
5096	84082-30-4	Rape oil, sulfated, sodium salt	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+01	1.4E-01	5.0E+00	-8.02	-8.33	-9.98	-1.26	0.51
5097	90640-45-2	Amines, N-C16-22-alkyltrimethylenedi-	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+01	1.4E-01	5.0E+00	-8.02	-8.33	-9.98	-3.00	0.64
5098	9002-92-0	Dodecan-1-ol, ethoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+01	1.4E-01	5.0E+00	-8.03	-8.33	-9.98	-2.48	0.30
5099	28654-73-1	[N,N,N',N',N'',N''-hexaethyl-29H,31H-phthalocyaninetrimethylaminato(2-)-N29,N30,N31,N32]copper	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.9E+00	1.4E-01	5.0E+00	-8.03	-8.34	-9.99	-1.84	0.64
5100	5831-80-1	N,N-dibutyloleamide	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.8E+00	1.4E-01	4.9E+00	-8.03	-8.34	-9.99	-1.84	0.64
5101	68439-46-3	Alcohols, C9-11, ethoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.9E+00	1.4E-01	4.9E+00	-8.04	-8.34	-9.99	-2.46	0.38
5102	1313206-64-2	Amines,N-(C16-18 and C18 unsaturated alkyl) trimethylenedi-,diacetates.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.7E+00	1.3E-01	4.8E+00	-8.04	-8.35	-10.00	-3.24	0.54
5103	1024699-81-3	3-(methacryloylamino)-N,N,N-trimethylpropan-1-aminium 4-((C10-13-sec-alkyl)benzenesulfonate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.6E+00	1.3E-01	4.8E+00	-8.05	-8.35	-10.00	-2.06	0.64
5104	646505-08-4	Poly[oxy(methyl-1,2-ethanediyl)], α-hydro-ω-[[3-[[3-(dimethylamino)propyl]amino]-1-oxo-2-butenyl]oxy]-, ether wi	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.6E+00	1.3E-01	4.8E+00	-8.05	-8.35	-10.00	-0.65	0.29
5105	135458-18-3	695-088-6	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.6E+00	1.3E-01	4.8E+00	-8.05	-8.35	-10.00	-1.84	0.64
5106	70024-64-5	Aluminum, hydrobis[2-methylprop1-, reaction products with isoprene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.5E+00	1.3E-01	4.7E+00	-8.05	-8.36	-10.01	-1.84	0.64
5107	67938-21-0	di(isooctadecanoic) acid, diester with oxydi(propanediol)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.5E+00	1.3E-01	4.7E+00	-8.05	-8.36	-10.01	-0.67	0.67
5108	1219826-47-7	N-C16-18-(even number)-,C18-unsaturated)-alkyl-1-C16-18-(even numbered, C18-unsaturated)-amine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.4E+00	1.3E-01	4.7E+00	-8.05	-8.36	-10.01	-4.75	0.64
5109	30374-01-7	isooctyl 3-mercaptopropionate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.4E+00	1.3E-01	4.7E+00	-8.06	-8.36	-10.01	-3.86	0.64
5110	51240-95-0	1,1,3,3-tetramethylbutyl peroxyneodecanoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.3E+00	1.3E-01	4.7E+00	-8.06	-8.36	-10.02	-0.70	0.64
5111	25151-96-6	2,2-bis(hydroxymethyl)-1,3-propanediyl oleate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.2E+00	1.3E-01	4.6E+00	-8.06	-8.37	-10.02	0.17	0.89
5112	105839-18-7	Fatty acids, C16 and C18-unsatd., polymers with bisphenol A, Bu glycidyl ether, epichlorohydrin and triethylenetetra	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.02	-3.27	0.47
5113	1424149-03-6	sodium/triethanolamine 4-((2-hydroxyethyl)amino)-3-pentapropenyl-4-oxobutanoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.32	0.57
5114	68411-20-1	Butanal, reaction products with aniline	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.47	0.56
5115	68611-64-3	Urea, reaction products with formaldehyde	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.15	0.64
5116	1225478-65-4	2,6-dimethylindan-1-amine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
5117	201872-72-2	Reaction mass of dimethyl 2,2,4-trimethylhexanedioate and dimethyl 2,4,4-trimethylhexanedioate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-0.72	0.64
5118	85632-63-9	Amines, N-(3-aminopropyl) tallow alkyltrimethylenedi-	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-3.89	0.64
5119	90622-71-2	Alkyl iodides, C6-18, perfluoro	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
5120	1079258-99-5	619-721-2	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
5121	68784-40-7	Propanenitrile, 3-amino-, N-coco alkyl derivs.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-3.48	0.64
5122	689-67-8	6,10-dimethylundeca-5,9-dien-2-one	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-2.17	0.64
5123	61792-11-8	3,7-dimethylnona-2,6-dienenitrile	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-2.54	0.64
5124	90990-11-7	Fatty acids, C18-22	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
5125	41524-32-7	[1R*,6S*]-6-(ethoxycarbonyl)-N,N-dimethyl-6-phenylcyclohex-2-en-1-aminium monooxalate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.50	0.64
5126	225375-65-5	Silsesquioxanes, 3-phosphonopropyl, Et Me esters, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	0.58	0.64
5127	84989-11-7	distillates (coal tar), upper, fluorene-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
5128	85909-49-5	isohexadecene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
5129	136294-06-1	Reaction mass of ammonium 2-amino-4-[(4-amino-6-chloro-1,3,5-triazin-2-yl)amino]benzenesulfonate and sodium :	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
5130	1424148-97-1	sodium/triethanolamine- 6-(2,5-dioxo-3-pentapropenylpyrrolidin-1-yl)hexanoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.67	0.82
5131	65996-86-3	Extract oils (coal), tar base	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
5132	68477-64-5	Gases (petroleum), acetylene manuf. off	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
5133	84836-98-6	Coconut oil, hydrogenated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
5134	27157-94-4	O,O-bis[methylphenyl] hydrogen dithiophosphate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
5135	27215-95-8	nonene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.6E+00	-8.07	-8.37	-10.03	-1.84	0.64
5136	3738-00-9	dodecahydro-3a,6,6,9a-tetramethylnaphtho[2,1-b]furan	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.5E+00	-8.07	-8.38	-10.03	-2.46	0.29
5137	91031-91-3	Fatty acids, coco, isotridecyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.5E+00	-8.07	-8.38	-10.03	-2.86	0.64
5138	236391-76-7	Acetic acid, 2-(1-oxopropoxy)-, 1-(3,3-dimethylcyclohexyl)ethyl ester	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+00	1.3E-01	4.5E+00	-8.07	-8.38	-10.03	-2.24	0.35
5139	65870-94-2	Hexanoic acid, 3,5,5-trimethyl-, 1,1'-[2-ethyl-2-[[(3,5,5-trimethyl-1-oxohexyl)oxy]methyl]-1,3-propanediyl] ester	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.0E+00	1.3E-01	4.5E+00	-8.07	-8.38	-10.03	-0.22	0.44
5140	91052-49-2	Glycerides, C12-18 mono- and di-	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.9E+00	1.2E-01	4.5E+00	-8.08	-8.38	-10.03	-1.46	0.33
5141	68071-07-8	Phenol, 4,4'-(1-methylethylidene)bis-, polymer with 2-(chloromethyl)oxirane, dodecanoate 2-propenoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.9E+00	1.2E-01	4.5E+00	-8.08	-8.38	-10.03	-2.22	0.57
5142	1309955-79-2	2-[(2-hydroxypropyl)](C16-18 sat. C18 unsat. alkylamino)propan-1-ol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.9E+00	1.2E-01	4.4E+00	-8.08	-8.39	-10.04	-3.45	0.48
5143	68410-23-1	Fatty acids, C18-unsatd., dimers, reaction products with polyethylenepolyamines	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.8E+00	1.2E-01	4.4E+00	-8.08	-8.39	-10.04	-2.25	0.64
5144	85116-88-7	Fatty acids, C14-18 and C16-18-unsatd., isotridecyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.8E+00	1.2E-01	4.4E+00	-8.08	-8.39	-10.04	-0.83	0.79
5145	93924-11-9	Alkenes, C24-28 α-	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.6E+00	1.2E-01	4.3E+00	-8.09	-8.40	-10.05	-2.68	1.28
5146	12650-88-3	Lysozyme (chicken egg white)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.6E+00	1.2E-01	4.3E+00	-8.09	-8.40	-10.05	-1.84	0.64
5147	106233-09-4	Alcohols, C16-18, ethoxylated, phosphates	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.5E+00	1.2E-01	4.2E+00	-8.10	-8.41	-10.06	-2.63	0.62
5148	68921-53-9	2-Butenediol acid (E)-, di-C18-22-alkyl esters	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.5E+00	1.2E-01	4.2E+00	-8.10	-8.41	-10.06	-1.84	0.64
5149	91770-03-5	Fatty acids, tall-oil, reaction products with boric acid (H3BO3) and diethanolamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.5E+00	1.2E-01	4.2E+00	-8.10	-8.41	-10.06	-0.57	1.10
5150	91050-89-4	Fatty acids, C8-10, triesters with trimethylolpropane	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.4E+00	1.2E-01	4.2E+00	-8.10	-8.41	-10.06	0.28	0.87
5151	68814-95-9	Amines, tri-C8-10-alkyl	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.3E+00	1.2E-01	4.1E+00	-8.11	-8.42	-10.07	-2.80	1.03
5152	84988-61-4	Phosphoric acid, isononyl ester	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.2E+00	1.1E-01	4.1E+00	-8.11	-8.42	-10.07	-0.83	0.48
5153	1233873-37-6	Benzaldehyde, 2-hydroxy, dodecyl-, oxime, branched	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.1E+00	1.1E-01	4.1E+00	-8.12	-8.42	-10.07	-2.02	1.28
5154	90411-76-0	Hydrochloric acid, reaction products with aniline and nitrobenzene, sulfonated, sodium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.0E+00	1.1E-01	4.0E+00	-8.12	-8.43	-10.08	-0.77	0.45
5155	71010-76-9	Decanoic acid, mixed esters with heptanoic acid, octanoic acid, pentaerythritol and valeric acid	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.0E+00	1.1E-01	4.0E+00	-8.12	-8.43	-10.08	-1.84	0.64
5156	32167-31-0	Poly[oxy-1,2-ethanediyl], α,α'-2-butyne-1,4-diylbis[ω-hydroxy-	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.7E+00	1.1E-01	3.9E+00	-8.14	-8.44	-10.10	-1.27	0.64
5157	68002-54-0	Tall oil, compd. with ethanolamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.7E+00	1.1E-01	3.8E+00	-8.14	-8.45	-10.10	-1.44	0.95
5158	159034-91-0	Propyldinetrimethanol, ethoxylated, esters with acrylic acid, reaction products with diethylamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.7E+00	1.1E-01	3.8E+00	-8.14	-8.45	-10.10	-1.51	0.64
5159	68515-81-1	Nonanol, branched and linear	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.6E+00	1.1E-01	3.8E+00	-8.15	-8.45	-10.10	-2.06	0.38
5160	68092-28-4	Tall oil, compd. with diethanolamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.6E+00	1.1E-01	3.8E+00	-8.15	-8.45	-10.10	-1.31	1.32
5161	66072-08-0	Naphthenic acids, potassium salts	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.6E+00	1.1E-01	3.8E+00	-8.15	-8.45	-10.10	-2.25	0.72
5162	68131-39-5	Alcohols, C12-15, ethoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.6E+00	1.1E-01	3.8E+00	-8.15	-8.45	-10.10	-2.95	0.70
5163	75247-18-6	[N,N,N',N',N'',N''-hexaethyl-29H,31H-phthalocyaninetrimethylaminato(2-)-N29,N30,N31,N32]copper tris(dodecylber	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.5E+00	1.1E-01	3.8E+00	-8.15	-8.46	-10.11	-1.44	0.64
5164	1225197-81-4	Amides, Fatty acids C18 unsaturated, reaction products with tetraethylenepentamine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.4E+00	1.0E-01	3.7E+00	-8.16	-8.47	-10.12	-3.07	0.57
5165	68411-76-7	Cyclohexane, oxidized, non-volatile residue	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.3E+00	1.0E-01	3.6E+00	-8.16	-8.47	-10.12	-0.53	0.37
5166	1499182-59-4	806-914-3	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.2E+00	1.0E-01	3.6E+00	-8.17	-8.48	-10.13	-1.84	0.64
5167	68201-32-1	Asphalt, sulfonated, sodium salt	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.9E+00	9.6E-02	3.5E+00	-8.19	-8.49	-10.15	0.48	1.15
5168	9005-67-8	Sorbitan monostearate, ethoxylated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.8E+00	9.5E-02	3.4E+00	-8.19	-8.50	-10.15	-0.88	0.32
5169	1072957-71-1	N-[9-(difluoromethylidene)-1,2,3,4-tetrahydro-1,4-methanonaphthalen-5-yl]-3-(difluoromethyl)-1-methyl-1H-pyraz	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.8E+00	9.5E-02	3.4E+00	-8.19	-8.50	-10.15	-4.12	0.73
5170	71500-39-5	methyl 3,5,5-trimethylhexanoate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.8E+00	9.5E-02	3.4E+00	-8.19	-8.50	-10.15	-1.84	0.64
5171	84082-68-8	Myristica fragrans, ext.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.2E+00	8.6E-02	3.1E+00	-8.23	-8.54	-10.19	-2.16	0.64
5172	83846-43-9	Benzoic acid, 2-hydroxy-, mono-C>13-alkyl derivs., calcium salts (2:1)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.0E+00	8.4E-02	3.0E+00	-8.25	-8.55	-10.20	-1.84	0.64
5173	68443-84-5	trisononanoic acid, trieter with 2,2'-[oxybis(methylene)]bis[2-(hydroxymethyl)propane-1,3-diol] t

5267	101541-04-2	N-palmitoylisoleucine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.6E-02	5.1E-04	1.8E-02	-10.46	-10.77	-12.42	-1.84	0.64
5268	1254940-85-4	3-(4-isobutylcyclohexyl)propanal	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.5E-02	4.8E-04	1.7E-02	-10.49	-10.79	-12.45	-2.41	0.64
5269	90480-71-0	Pentadecanol, branched and linear	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E-02	1.7E-04	5.9E-03	-10.95	-11.26	-12.91	-1.84	0.64
5270	10305-38-1	3-(hexyloxy)propane-1,2-diol	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E-04	1.3E-05	4.6E-04	-12.07	-12.37	-14.03	-1.84	0.64
REACH - petroleum products																								
n			*326*	*326*	*326*	*326*	*326*	*326*	*326*	*326*	*326*	*326*	*326*	*326*	*326*	*326*	*326*	*326*	*326*	*326*	*326*			
sum												***1.9E+09***		***3.3E+06***	***8.4E+04***	***1.6E+06***								
av												*5.9E+06*	*3.3E+06*	*1.9E+04*	*2.6E+02*	*5.0E+03*						*-1.54*	*0.64*	
std												*2.4E+07*	*1.5E+07*	*8.0E+04*	*1.1E+03*	*2.1E+04*						*1.09*	*0.27*	
2.5-p			*223*	*87*	*9.9E-03*	*1.5E+03*	*3.0E+02*		*3.5E-06*	*1.3E-07*	*6.6E-09*	*1.3E+02*	*8.2E+01*	*4.2E-01*	*5.6E-03*	*1.1E-01*	*-9.42*	*-9.79*	*-11.42*	*-4.28*	*0.46*			
50-p			*223*	*87*	*9.9E-03*	*1.5E+03*	*3.0E+02*	*14.0*	*3.5E-06*	*1.3E-07*	*6.6E-09*	*3.6E+05*	*2.7E+05*	*1.2E+03*	*1.6E+01*	*3.2E+02*	*-5.97*	*-6.34*	*-7.96*	*-1.84*	*0.61*			
97.5-p			*223*	*87*	*9.9E-03*	*1.5E+03*	*3.0E+02*	*14.0*	*3.5E-06*	*1.3E-07*	*6.6E-09*	*5.8E+07*	*2.4E+07*	*1.9E+05*	*2.5E+03*	*4.7E+04*	*-3.77*	*-4.14*	*-5.76*	*0.65*	*0.79*		
5272	68334-30-5	Fuels, diesel	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+06	1.5E+04	2.9E+05	-3.00	-3.37	-5.00	-1.68	0.58
5273	68476-33-5	Fuel oil, residual	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.4E+05	7.1E+03	1.3E+05	-3.31	-3.69	-5.31	-1.84	0.98
5274	86290-81-5	Gasoline	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.1E+05	6.8E+03	1.3E+05	-3.34	-3.71	-5.33	-1.87	0.46
5275	8008-20-6	Kerosine (petroleum)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+05	3.5E+03	7.4E+04	-3.62	-3.99	-5.61	-1.99	0.65
5276	68333-22-2	Residues (petroleum), atmospheric	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+05	2.9E+03	5.3E+04	-3.70	-4.08	-5.70	-1.84	0.98
5277	64741-45-3	Residues (petroleum), atm. tower	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+05	2.9E+03	5.4E+04	-3.71	-4.09	-5.71	-1.84	0.98
5278	68814-87-9	Distillates (petroleum), full-range straight-run middle	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.9E+05	2.6E+03	5.1E+04	-3.76	-4.13	-5.75	-1.74	0.61
5279	64741-57-7	Gas oils (petroleum), heavy vacuum	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+05	2.6E+03	4.8E+04	-3.75	-4.13	-5.75	-1.84	0.98
5280	64741-42-0	Naphtha (petroleum), full-range straight-run	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.9E+05	2.6E+03	5.0E+04	-3.76	-4.13	-5.75	-1.87	0.46
5281	64741-56-6	Residues (petroleum), vacuum	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+05	2.2E+03	4.3E+04	-3.82	-4.19	-5.81	-1.84	0.64
5282	64742-81-0	Kerosine (petroleum), hydrodesulfurized	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+05	2.2E+03	4.1E+04	-3.83	-4.21	-5.83	-1.99	0.65
5283	64742-80-9	Distillates (petroleum), hydrodesulfurized middle	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+05	2.1E+03	4.2E+04	-3.84	-4.21	-5.83	-1.75	0.61
5284	70592-78-8	Distillates (petroleum), vacuum	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.7E+04	1.2E+03	2.1E+04	-4.11	-4.48	-6.10	-1.84	0.98
5285	91770-15-9	Kerosine (petroleum), sweetened	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.6E+04	1.1E+03	1.9E+04	-4.11	-4.49	-6.11	-1.99	0.65
5286	64741-58-8	Gas oils (petroleum), light vacuum	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.0E+04	1.1E+03	1.9E+04	-4.14	-4.52	-6.14	-1.72	0.58
5287	68955-35-1	Naphtha (petroleum), catalytic reformed	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.3E+04	9.7E+02	1.9E+04	-4.18	-4.55	-6.18	-1.87	0.46
5288	68955-27-1	Distillates (petroleum), petroleum residues vacuum	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.1E+04	9.5E+02	1.8E+04	-4.19	-4.56	-6.19	-1.84	0.98
5289	64741-43-1	Gas oils (petroleum), straight-run	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.0E+04	9.2E+02	1.8E+04	-4.20	-4.57	-6.20	-1.74	0.60
5290	8052-42-4	Asphalt	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.6E+04	8.7E+02	1.8E+04	-4.23	-4.59	-6.22	-1.84	0.64
5291	64741-59-9	Distillates (petroleum), light catalytic cracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.6E+04	8.7E+02	1.7E+04	-4.23	-4.60	-6.22	-3.32	0.62
5292	64741-80-6	Residues (petroleum), thermal cracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.5E+04	8.7E+02	1.6E+04	-4.23	-4.60	-6.23	-1.84	0.98
5293	68919-37-9	Naphtha (petroleum), full-range reformed	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.9E+04	7.8E+02	1.7E+04	-4.27	-4.64	-6.26	-1.87	0.46
5294	64741-55-5	Naphtha (petroleum), light catalytic cracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.9E+04	7.9E+02	1.5E+04	-4.27	-4.64	-6.27	-1.87	0.46
5295	64741-46-4	Naphtha (petroleum), light straight-run	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.9E+04	7.8E+02	1.4E+04	-4.28	-4.65	-6.28	-1.91	0.45
5296	64742-73-0	Naphtha (petroleum), hydrodesulfurized light	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+04	7.3E+02	1.3E+04	-4.31	-4.68	-6.31	-1.87	0.46
5297	68476-34-6	Fuels, diesel, no. 2	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.2E+04	6.8E+02	1.4E+04	-4.33	-4.70	-6.32	-1.72	0.58
5298	64741-41-9	Naphtha (petroleum), heavy straight-run	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.9E+04	6.5E+02	1.4E+04	-4.35	-4.72	-6.34	-1.87	0.46
5299	64741-75-9	Residues (petroleum), hydrocracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.7E+04	6.2E+02	1.1E+04	-4.37	-4.75	-6.37	-1.84	0.97
5300	74869-22-0	Lubricating oils	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.3E+04	5.6E+02	1.1E+04	-4.41	-4.78	-6.41	0.29	1.09
5301	64742-86-5	Gas oils (petroleum), hydrodesulfurized heavy vacuum	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.2E+04	5.6E+02	1.0E+04	-4.42	-4.80	-6.42	-1.84	0.98
5302	64742-48-9	Naphtha (petroleum), hydrotreated heavy	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.2E+04	5.5E+02	1.0E+04	-4.43	-4.80	-6.43	-1.87	0.46
5303	64742-46-7	Distillates (petroleum), hydrotreated middle	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.1E+04	5.5E+02	9.9E+03	-4.43	-4.81	-6.43	-1.75	0.61
5304	64742-79-6	Gas oils (petroleum), hydrodesulfurized	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.6E+04	4.8E+02	9.2E+03	-4.49	-4.86	-6.48	-1.75	0.61
5305	64741-70-4	Naphtha (petroleum), isomerization	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.5E+04	4.6E+02	9.4E+03	-4.50	-4.87	-6.50	-1.87	0.46
5306	92045-59-5	Naphtha (petroleum), light catalytic cracked sweetened	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.1E+04	4.1E+02	7.5E+03	-4.56	-4.93	-6.55	-1.87	0.46
5307	64741-54-4	Naphtha (petroleum), heavy catalytic cracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E+04	3.7E+02	8.1E+03	-4.59	-4.96	-6.58	-1.87	0.46
5308	64741-77-1	Distillates (petroleum), light hydrocracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E+04	3.7E+02	7.1E+03	-4.60	-4.97	-6.60	-1.72	0.58
5309	64741-68-0	Naphtha (petroleum), heavy catalytic reformed	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+04	3.4E+02	7.0E+03	-4.64	-5.00	-6.63	-1.87	0.46
5310	92062-05-0	Residues (petroleum), thermal cracked vacuum	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+04	3.3E+02	7.1E+03	-4.65	-5.01	-6.64	-1.84	0.64
5311	64741-63-5	Naphtha (petroleum), light catalytic reformed	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.5E+04	3.4E+02	6.5E+03	-4.64	-5.01	-6.64	-1.87	0.46
5312	68915-96-8	Distillates (petroleum), heavy straight-run	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.5E+04	3.3E+02	6.1E+03	-4.65	-5.02	-6.64	-1.74	0.61
5313	64741-44-2	Distillates (petroleum), straight-run middle	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+04	3.2E+02	6.7E+03	-4.66	-5.03	-6.66	-1.74	0.61
5314	64741-82-8	Distillates (petroleum), light thermal cracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+04	3.2E+02	6.4E+03	-4.66	-5.03	-6.66	-3.32	0.62
5315	64742-49-0	Naphtha (petroleum), hydrotreated light	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+04	3.2E+02	5.4E+03	-4.66	-5.04	-6.66	-1.88	0.44
5316	92061-97-7	Residues (petroleum), catalytic cracking	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+04	3.0E+02	5.7E+03	-4.69	-5.07	-6.69	-1.84	0.98
5317	68783-12-0	Naphtha (petroleum), unsweetened	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.2E+04	2.9E+02	5.4E+03	-4.71	-5.08	-6.70	-1.87	0.46
5318	64741-87-3	Naphtha (petroleum), sweetened	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+04	2.7E+02	5.3E+03	-4.74	-5.11	-6.73	-1.87	0.46
5319	64741-51-1	Distillates (petroleum), heavy paraffinic	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+04	2.7E+02	4.7E+03	-4.74	-5.12	-6.74	-1.17	0.64
5320	68553-00-4	Fuel oil, no. 6	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.0E+04	2.6E+02	4.9E+03	-4.75	-5.12	-6.75	-1.84	0.98
5321	68527-27-5	Naphtha (petroleum), full-range alkylate, butane-contg.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+04	2.3E+02	4.4E+03	-4.80	-5.17	-6.79	-1.87	0.46
5322	92045-52-8	Naphtha (petroleum), hydrodesulfurized full-range	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+04	2.3E+02	4.3E+03	-4.80	-5.17	-6.80	-1.87	0.46
5323	64741-76-0	Distillates (petroleum), heavy hydrocracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+04	2.3E+02	4.9E+03	-4.81	-5.17	-6.80	0.29	1.09
5324	64742-93-4	Asphalt, oxidized	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.7E+04	2.3E+02	4.1E+03	-4.81	-5.18	-6.81	-1.84	0.64
5325	68476-30-2	Fuel oil, no. 2	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+04	2.1E+02	4.3E+03	-4.83	-5.20	-6.83	-1.72	0.58
5326	68333-25-5	Distillates (petroleum), hydrodesulfurized light catalytic cracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+04	2.1E+02	4.2E+03	-4.84	-5.21	-6.84	-3.32	0.61
5327	64742-59-2	Gas oils (petroleum), hydrotreated vacuum	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+04	2.1E+02	4.1E+03	-4.85	-5.22	-6.85	-1.84	0.98
5328	70592-77-7	Distillates (petroleum), light vacuum	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+04	2.0E+02	4.2E+03	-4.86	-5.23	-6.85	-1.84	0.98
5329	101795-01-1	Naphtha (petroleum), sweetened light	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.5E+04	2.0E+02	4.0E+03	-4.87	-5.24	-6.87	-1.87	0.46
5330	64742-65-0	Distillates (petroleum), solvent-dewaxed heavy paraffinic	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+04	1.9E+02	3.6E+03	-4.89	-5.26	-6.88	0.29	1.07
5331	64742-82-1	Naphtha (petroleum), hydrodesulfurized heavy	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+04	1.9E+02	3.7E+03	-4.89	-5.26	-6.89	-1.87	0.46
5332	90669-76-4	Residues (petroleum), vacuum, light	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+04	1.8E+02	3.9E+03	-4.92	-5.28	-6.91	-1.84	0.98
5333	68476-52-8	Hydrocarbons, C4, ethylene-manuf.-by-product	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+04	1.7E+02	3.5E+03	-4.92	-5.29	-6.92	-1.81	0.23
5334	68476-26-6	Fuel gases	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+04	1.7E+02	3.4E+03	-4.93	-5.30	-6.92	-1.59	0.39
5335	1330-20-7	xylene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+04	1.7E+02	3.2E+03	-4.94	-5.31	-6.94	-1.41	0.70
5336	68606-10-0	Gasoline, pyrolysis, debutanizer bottoms	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+04	1.7E+02	3.2E+03	-4.94	-5.31	-6.94	-2.70	0.22
5337	70592-76-6	Distillates (petroleum), intermediate vacuum	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+04	1.6E+02	3.6E+03	-4.95	-5.32	-6.94	-1.84	0.98
5338	64741-81-7	Distillates (petroleum), heavy thermal cracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+04	1.7E+02	3.2E+03	-4.95	-5.32	-6.94	-1.84	0.98
5339	64741-64-6	Naphtha (petroleum), full-range alkylate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+04	1.6E+02	3.2E+03	-4.95	-5.32	-6.95	-1.87	0.46
5340	64741-69-1	Naphtha (petroleum), light hydrocracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+04	1.6E+02	3.1E+03	-4.95	-5.33	-6.95	-1.87	0.46
5341	68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+04	1.6E+02	2.7E+03	-4.96	-5.34	-6.96	-2.70	0.22
5342	64741-78-2	Naphtha (petroleum), heavy hydrocracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+04	1.6E+02	2.7E+03	-4.96	-5.34	-6.96	-1.87	0.46
5343	64741-84-0	Naphtha (petroleum), solvent-refined light	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+04	1.6E+02	2.9E+03	-4.97	-5.34	-6.97	-2.09	0.55
5344	68607-30-7	Residues (petroleum), topping plant, low-sulfur	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+04	1.5E+02	3.3E+03	-4.98	-5.35	-6.98	-1.84	0.98
5345	92045-23-3	Hydrocarbons, C4, steam-cracker distillate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+04	1.6E+02	2.9E+03	-4.97	-5.35	-6.97	-1.83	0.21
5346	64741-88-4	Distillates (petroleum), solvent-refined heavy paraffinic	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+04	1.5E+02	2.9E+03	-4.99	-5.36	-6.99	0.29	1.09
5347	93571-75-6	Aromatic hydrocarbons, C7-12, C8-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+04	1.5E+02	2.5E+03	-5.00	-5.38	-7.00	-1.87	0.46
5348	64742-83-2	Naphtha (petroleum), light steam-cracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+04	1.4E+02	2.7E+03	-5.03	-5.41	-7.03	-2.70	0.22
5349	68783-08-4	Gas oils (petroleum), heavy atmospheric	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.5E+03	1.3E+02	2.5E+03	-5.07	-5.44	-7.06	-1.84	0.98
5350	68955-28-2	Gases (petroleum), light steam-cracked, butadiene conc.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.7E+03	1.3E+02	2.2E+03	-5.06	-5.44	-7.06	-1.81	0.23
5351	64742-47-8	Distillates (petroleum), hydrotreated light	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.7E+03	1.2E+02	2.4E+03	-5.10	-5.47	-7.10	-2.16	0.70
5352	68527-23-1	Naphtha (petroleum), light steam-cracked arom.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.8E+03	1.2E+02	2.1E+03	-5.10	-5.48	-7.10	-2.70	0.22
5353	64741-62-4	Clarified oils (petroleum), catalytic cracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.8E+03	1.2E+02	2.1E+03	-5.10	-5.48	-7.10	-1.84	0.98
5354	64741-60-2	Distillates (petroleum), intermediate catalytic cracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.8E+03	1.2E+02	2.0E+03	-5.10	-5.48	-7.10	-3.32	0.61
5355	92045-29-9	Gas oils (petroleum), thermal-cracked, hydrotreated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.6E+03	1.1E+02	2.1E+03	-5.14	-5.51	-7.14	-3.32	0.61
5356	64742-54-7	Distillates (petroleum), hydrotreated heavy paraffinic	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.0E+03	1.1E+02	2.0E+03	-5.14	-5.52	-7.14	0.29	1.09
5357	68606-11-1	Gasoline, straight-run, topping-plant	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.1E+03	1.1E+02	1.8E+03	-5.14	-5.52	-7.14	-1.87	0.46
5358	92045-14-2	Fuel oil, heavy, high-sulfur	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.6E+03	1.0E+02	1.9E+03	-5.16	-5.54	-7.16	-1.84

5442	64742-05-8	Extracts (petroleum), light paraffinic distillate solvent	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+03	1.4E+01	2.7E+02	-6.01	-6.39	-8.01	-0.67	0.64								
5443	68131-75-9	Gases (petroleum), C3-4	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+03	1.4E+01	2.9E+02	-6.02	-6.39	-8.02	-1.59	0.39								
5444	93572-36-2	Hydrocarbons, C5-11, nonaroms.-rich, reforming light fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+03	1.4E+01	2.4E+02	-6.02	-6.40	-8.02	-1.87	0.46								
5445	68410-05-9	Distillates (petroleum), straight-run light	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+03	1.4E+01	2.5E+02	-6.03	-6.41	-8.03	-1.87	0.46								
5446	92045-64-2	Hydrocarbons, C6-7, naphtha-cracking, solvent-refined	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+03	1.4E+01	2.4E+02	-6.04	-6.41	-8.03	-1.87	0.46								
5447	68921-07-3	Distillates (petroleum), hydrotreated light catalytic cracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.9E+02	1.3E+01	2.5E+02	-6.05	-6.42	-8.04	-3.32	0.62								
5448	68476-29-9	Fuel gases, crude oil distillates	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.9E+02	1.3E+01	2.5E+02	-6.05	-6.42	-8.05	-1.59	0.39								
5449	92045-58-4	Naphtha (petroleum), isomerization, C6-fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.8E+02	1.3E+01	2.6E+02	-6.05	-6.42	-8.05	-1.87	0.46								
5450	68512-62-9	Residues (petroleum), light vacuum	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.9E+02	1.3E+01	2.2E+02	-6.05	-6.43	-8.05	-1.80	0.99								
5451	68513-03-1	Naphtha (petroleum), light catalytic reformed, arom.-free	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.3E+02	1.2E+01	2.5E+02	-6.08	-6.44	-8.07	-1.87	0.46								
5452	90641-13-7	Naphtha (petroleum), steam-cracked, hydrotreated, C9-10-arom.-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.3E+02	1.2E+01	2.3E+02	-6.07	-6.45	-8.07	-2.70	0.22								
5453	64741-86-2	Distillates (petroleum), sweetened middle	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.2E+02	1.2E+01	2.2E+02	-6.08	-6.46	-8.08	-1.75	0.61								
5454	68477-38-3	Distillates (petroleum), cracked steam-cracked petroleum distillates	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.0E+02	1.2E+01	2.3E+02	-6.09	-6.46	-8.09	-2.36	0.54								
5455	88072-36-7	Aromatic hydrocarbons, distn. residues, naphthalene-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	9.1E+02	1.2E+01	2.0E+02	-6.09	-6.47	-8.09	-2.36	0.54								
5456	68475-79-6	Distillates (petroleum), catalytic reformed dependanizer	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.5E+02	1.1E+01	2.3E+02	-6.12	-6.48	-8.11	-1.87	0.46								
5457	64741-66-8	Naphtha (petroleum), light alkylate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.2E+02	1.1E+01	2.1E+02	-6.13	-6.50	-8.12	-1.87	0.46								
5458	68477-39-4	Distillates (petroleum), cracked stripped steam-cracked petroleum distillates, C8-10 fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.1E+02	1.1E+01	2.2E+02	-6.13	-6.50	-8.13	-2.40	0.57								
5459	64742-57-0	Residual oils (petroleum), hydrotreated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.1E+02	1.1E+01	2.0E+02	-6.13	-6.50	-8.13	0.29	1.09								
5460	93821-66-0	Residual oils (petroleum)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.2E+02	1.1E+01	1.8E+02	-6.13	-6.51	-8.13	-1.84	0.98								
5461	68475-80-9	Distillates (petroleum), light steam-cracked naphtha	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.1E+02	1.1E+01	2.0E+02	-6.14	-6.51	-8.14	-2.35	0.54								
5462	68477-33-8	gases (petroleum), C3-4, isobutane-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.9E+02	1.1E+01	2.0E+02	-6.15	-6.52	-8.14	-1.59	0.39								
5463	64742-67-2	Foots oil (petroleum)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.2E+02	9.6E+00	1.8E+02	-6.19	-6.56	-8.18	-1.84	0.64								
5464	92045-57-3	Naphtha (petroleum), hydrotreated light steam-cracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.0E+02	9.3E+00	1.6E+02	-6.20	-6.58	-8.20	-2.70	0.22								
5465	92045-63-1	Hydrocarbons, C4-11, naphtha-cracking, arom.-free	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.0E+02	9.3E+00	1.6E+02	-6.20	-6.58	-8.20	-1.87	0.46								
5466	64741-52-2	Distillates (petroleum), light naphthenic	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.8E+02	9.1E+00	1.6E+02	-6.21	-6.59	-8.21	-1.17	0.64								
5467	64742-70-7	Paraffin oils (petroleum), catalytic dewaxed heavy	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.4E+02	8.4E+00	1.7E+02	-6.24	-6.61	-8.24	0.29	1.09								
5468	64741-53-3	Distillates (petroleum), heavy naphthenic	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.0E+02	8.0E+00	1.6E+02	-6.26	-6.63	-8.26	-1.17	0.64								
5469	8009-03-8	Petrolatum	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.9E+02	7.7E+00	1.6E+02	-6.28	-6.64	-8.27	0.17	1.10								
5470	92062-09-4	Slack wax (petroleum), hydrotreated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.9E+02	7.8E+00	1.5E+02	-6.28	-6.65	-8.27	0.42	1.02								
5471	90622-53-0	Alkanes, C12-26-branched and linear	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.7E+02	7.5E+00	1.4E+02	-6.29	-6.67	-8.29	-1.75	0.61								
5472	68783-04-0	Extracts (petroleum), solvent-refined heavy paraffinic distillate solvent	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+02	7.3E+00	1.4E+02	-6.30	-6.67	-8.30	-1.38	0.64								
5473	68956-55-8	Hydrocarbons, C5-unsatd.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.2E+02	6.9E+00	1.3E+02	-6.33	-6.70	-8.32	-1.94	0.40								
5474	92045-61-9	Hydrocarbons, C4-12, naphtha-cracking, hydrotreated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.1E+02	6.7E+00	1.4E+02	-6.34	-6.71	-8.33	-2.70	0.22								
5475	68783-65-3	Gases (petroleum), C2-4, sweetened	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.1E+02	6.7E+00	1.4E+02	-6.34	-6.71	-8.33	-1.59	0.39								
5476	86290-83-7	Hydrocarbons, steam-cracking tar middle	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.7E+02	6.2E+00	1.2E+02	-6.37	-6.75	-8.37	-2.36	0.54								
5477	68603-08-7	Naphtha (petroleum), arom	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.3E+02	5.7E+00	1.1E+02	-6.41	-6.78	-8.41	-1.87	0.46								
5478	63231-60-7	Paraffin waxes and Hydrocarbon waxes, microcryst.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.6E+02	4.8E+00	9.4E+01	-6.49	-6.86	-8.48	0.42	1.06								
5479	68783-11-9	Naphtha (petroleum), light polymn.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.6E+02	4.7E+00	9.0E+01	-6.49	-6.86	-8.49	-1.87	0.46								
5480	68527-18-4	Gas oils (petroleum), steam-cracked	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.6E+02	4.8E+00	8.8E+01	-6.49	-6.87	-8.49	-2.36	0.54								
5481	64742-66-1	Naphtha (petroleum), catalytic dewaxed	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.5E+02	4.6E+00	8.2E+01	-6.50	-6.88	-8.50	-1.87	0.46								
5482	97593-01-6	Alkenes, C8-10-branched, C9-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.4E+02	4.4E+00	9.5E+01	-6.52	-6.88	-8.51	-3.03	0.81								
5483	92045-41-5	Lubricating oils, used, vacuum distd.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.0E+02	4.0E+00	8.0E+01	-6.56	-6.93	-8.56	-2.16	0.64								
5484	93821-12-6	Alkenes, C10-14-branched and linear, C12-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	3.0E+02	4.0E+00	6.8E+01	-6.57	-6.95	-8.57	-3.04	0.82								
5485	68476-49-3	Hydrocarbons, C2-4, C3-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.9E+02	3.8E+00	6.8E+01	-6.59	-6.97	-8.59	-1.59	0.39								
5486	94733-07-0	Distillates (petroleum), cracked, ethylene manuf. by-product, C9-10 fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E+02	3.6E+00	7.4E+01	-6.60	-6.97	-8.60	-2.64	0.51								
5487	64742-43-4	Paraffin waxes (petroleum), clay-treated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.8E+02	3.7E+00	7.1E+01	-6.60	-6.97	-8.60	0.42	1.02								
5488	68410-71-9	Raffinates (petroleum), catalytic reformer ethylene glycol-water countercurrent exts.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.6E+02	3.5E+00	6.3E+01	-6.63	-7.00	-8.63	-1.87	0.46								
5489	95465-90-0	Hydrocarbons, C4, n-butene conc.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.5E+02	3.4E+00	6.1E+01	-6.64	-7.02	-8.64	-1.85	0.21								
5490	102110-14-5	Hydrocarbons, C3-6, C5-rich, steam-cracked naphtha	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.5E+02	3.3E+00	6.2E+01	-6.65	-7.02	-8.65	-1.94	0.40								
5491	68477-71-4	Gases (petroleum), catalytic-cracked gas oil depropanizer bottoms, C4-rich acid-free	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+02	3.2E+00	5.6E+01	-6.66	-7.04	-8.66	-1.59	0.39								
5492	92045-77-7	Petrolatum (petroleum), hydrotreated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+02	3.2E+00	6.0E+01	-6.67	-7.04	-8.67	0.17	1.10								
5493	64741-67-9	Residues (petroleum), catalytic reformer fractionator	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.4E+02	3.1E+00	5.4E+01	-6.67	-7.05	-8.67	-1.84	0.98								
5494	72623-86-0	Lubricating oils (petroleum), C15-30, hydrotreated neutral oil-based	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+02	2.7E+00	5.9E+01	-6.73	-7.09	-8.72	0.29	1.09								
5495	68526-56-7	Alkenes, C9-11, C10-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+02	2.7E+00	5.9E+01	-6.73	-7.10	-8.72	-2.64	0.51								
5496	68814-67-5	Gases (petroleum), refinery	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+02	2.8E+00	5.1E+01	-6.72	-7.10	-8.72	-1.59	0.39								
5497	91995-70-9	Extracts (petroleum), deasphalted vacuum residue solvent	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	2.1E+02	2.7E+00	5.8E+01	-6.73	-7.10	-8.72	-0.32	0.75								
5498	101316-69-2	Lubricating oils (petroleum), C>25, solvent-extd., deasphalted, dewaxed, hydrogenated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.4E+00	4.2E+01	-6.80	-7.17	-8.80	0.29	1.09								
5499	68477-87-2	Gases (petroleum), deisobutanizer tower overheads	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.8E+02	2.3E+00	4.5E+01	-6.80	-7.17	-8.80	-1.59	0.39								
5500	157707-86-3	Dec-1-ene, trimers, hydrogenated	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.6E+02	2.1E+00	3.8E+01	-6.84	-7.22	-8.84	0.46	0.64								
5501	101316-66-9	Hydrocarbons, C6-8, hydrogenated sorption-dearomatized, toluene raffination	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.4E+02	1.9E+00	3.7E+01	-6.90	-7.27	-8.89	-1.86	0.45								
5502	64741-99-7	Extracts (petroleum), light naphtha solvent	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.8E+00	3.7E+01	-6.92	-7.29	-8.91	-2.70	0.22								
5503	64742-96-7	Solvent naphtha (petroleum), heavy aliph.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.7E+00	3.5E+01	-6.93	-7.30	-8.92	-1.99	0.65								
5504	64741-98-6	Extracts (petroleum), heavy naphtha solvent	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.7E+00	3.4E+01	-6.95	-7.31	-8.94	-1.94	0.40								
5505	68477-40-7	Distillates (petroleum), cracked stripped steam-cracked petroleum distillates, C10-12 fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.3E+02	1.7E+00	3.1E+01	-6.94	-7.32	-8.94	-2.64	0.52								
5506	68526-55-6	Alkenes, C8-10, C9-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.6E+00	3.1E+01	-6.96	-7.33	-8.96	-2.68	1.28								
5507	25378-22-7	dodecene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.2E+02	1.5E+00	2.7E+01	-6.98	-7.36	-8.98	-2.62	1.23								
5508	85681-75-0	Alkenes, C10-14	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.1E+02	1.5E+00	2.8E+01	-6.99	-7.37	-8.99	-2.68	1.28								
5509	91995-41-4	Distillates (petroleum), heat-soaked steam-cracked naphtha, C5-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+02	1.4E+00	2.5E+01	-7.03	-7.40	-9.03	-1.93	0.39								
5510	64742-60-5	Hydrocarbon waxes (petroleum), hydrotreated microcryst.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	1.0E+02	1.3E+00	2.8E+01	-7.04	-7.41	-9.03	0.42	1.06								
5511	91053-01-9	Hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	8.2E+01	1.1E+00	2.2E+01	-7.13	-7.50	-9.13	-4.28	0.64								
5512	64742-42-3	Hydrocarbon waxes (petroleum), clay-treated microcryst.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.9E+01	1.1E+00	2.0E+01	-7.14	-7.52	-9.14	0.42	1.06								
5513	68477-50-9	Distillates (petroleum), polymd. steam-cracked petroleum distillates, C5-12 fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.9E+01	1.0E+00	2.1E+01	-7.15	-7.52	-9.14	-2.33	0.58								
5514	64742-71-8	Paraffin oils (petroleum), catalytic dewaxed light	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.8E+01	1.0E+00	2.0E+01	-7.15	-7.52	-9.15	0.29	1.09								
5515	90622-47-2	Alkanes, C14-17	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.7E+01	1.0E+00	2.0E+01	-7.16	-7.53	-9.16	-5.33	0.64								
5516	91052-99-2	Hydrocarbons, C4, 1,3-butadiene-free, polymd., dibutylene fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.2E+01	9.5E-01	1.9E+01	-7.19	-7.56	-9.18	-4.28	0.64								
5517	68477-69-0	Gases (petroleum), butane splitter overheads	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	7.0E+01	9.3E-01	1.7E+01	-7.20	-7.57	-9.20	-1.59	0.39								
5518	64741-96-4	Distillates (petroleum), solvent-refined heavy naphthenic	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.8E+01	8.9E-01	2.0E+01	-7.21	-7.58	-9.21	0.29	1.09								
5519	95465-91-1	Hydrocarbons, C4, butane conc., n-butene-contg.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.8E+01	9.0E-01	1.7E+01	-7.21	-7.59	-9.21	-1.85	0.21								
5520	94733-15-0	Lubricating oils (petroleum), C18-40, solvent-dewaxed hydrocracked distillate-based	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.7E+01	8.9E-01	1.7E+01	-7.22	-7.59	-9.21	0.29	1.09								
5521	64741-48-6	Natural gas (petroleum), raw liq. mix	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.6E+01	8.7E-01	1.7E+01	-7.23	-7.60	-9.22	-1.87	0.46								
5522	68476-43-7	Hydrocarbons, C4-6, C5-rich	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.6E+01	8.7E-01	1.7E+01	-7.23	-7.60	-9.22	-1.93	0.39								
5523	85116-53-6	Distillates (petroleum), hydrodesulfurized thermal cracked middle	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	6.2E+01	8.2E-01	1.7E+01	-7.25	-7.62	-9.25	-3.32	0.62								
5524	25377-82-6	tridecene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.9E+01	7.8E-01	1.6E+01	-7.27	-7.64	-9.27	-0.63	0.64								
5525	85116-58-1	Distillates (petroleum), catalytic reformed hydrotreated light, C8-12 arom. fraction	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.6E+01	7.4E-01	1.4E+01	-7.30	-7.67	-9.29	-1.87	0.46								
5526	68919-10-8	Gases (petroleum), straight-run stabilizer off	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.6E+01	7.5E-01	1.3E+01	-7.29	-7.67	-9.29	-1.59	0.39								
5527	64742-88-7	Solvent naphtha (petroleum), medium aliph.	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.5E+01	7.3E-01	1.3E+01	-7.31	-7.68	-9.30	-1.99	0.65								
5528	26952-13-6	tetradecene	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	5.0E+01	6.6E-01	1.2E+01	-7.35	-7.72	-9.35	-0.63	0.64								
5529	92045-24-4	Gas oils (petroleum), hydrotreated light vacuum	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.9E+01	6.5E-01	1.2E+01	-7.35	-7.73	-9.35	-1.72	0.58								
5530	68514-34-1	Hydrocarbons, C9-14, ethylene-manuf. by-product	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	conf	conf	4.7E+01	6.2E-01	1.1E+01	-7.38	-7.75	-9.37	-1.84	0.64								
5531	93763-35-0	Hydrocarbons, C9-16, hydrot

5688	139264-17-8	MYCOPHENOLATE	287	202	1.9E-07	1.5E+03	8.3E+01	8.7	3.5E-06	3.5E-07	1.1E-07	4.5E+01	2.6E+01	3.7E-01	5.8E-02	3.1E+00	-9.03	-9.21	-11.35	-3.09	0.60	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5693	657-24-9	Metformin Hydrochloride (Metformin)	129	74	1.0E-02	4.4E+04	2.3E-03	11.9	3.5E-06	1.3E-07	3.5E-07	4.2E+03	2.4E+03	3.0E+01	5.4E+00	3.1E+02	-6.76	-6.75	-8.54	-0.63	0.58	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5659	23593-75-1	Clotrimazole	345	207	2.8E-07	9.4E-02	1.8E+06	7.0	3.5E-06	2.0E-08	3.5E-08	3.8E+00	2.2E+00	5.0E-02	5.1E-03	1.4E-01	-10.47	-10.68	-11.81	-4.42	0.69	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5609	169590-42-5	Celecoxib	381	213	1.6E-07	2.4E+00	3.0E+03	1.0	3.5E-06	3.1E-09	3.5E-08	4.4E+01	8.3E+00	2.4E-01	2.0E-02	2.5E-01	-8.97	-8.98	-10.00	-2.67	1.13	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5871	42399-41-7	Diltiazem Hydrochloride (Diltiazem)	415	232	4.0E-09	6.6E+00	6.2E+02	8.0	3.5E-06	1.9E-07	3.5E-07	1.1E+02	6.3E+01	1.4E+00	1.5E-01	4.8E+00	-8.70	-8.77	-10.64	-2.46	0.37	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5883	97-77-8	Disulfiram	297	139	8.8E-04	9.7E+00	4.7E+03	-2.0	3.5E-06	2.7E-08	1.1E-06	2.3E+00	1.3E+00	2.3E-02	3.0E-03	1.2E-01	-10.17	-9.97	-11.29	-3.65	0.36	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5678	61-68-7	Mefenamic Acid	241	153	7.8E-06	1.1E+01	1.9E+05	-2.0	3.5E-06	1.3E-08	3.5E-07	5.3E+01	3.1E+01	8.0E-01	7.2E-02	1.4E+00	-8.68	-8.52	-9.69	-2.18	0.17	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5684	15307-86-5	Diclofenac	296	175	8.2E-06	1.6E+01	1.0E+04	4.4	3.5E-06	2.2E-09	1.1E-07	1.3E+02	7.6E+01	1.3E+00	1.7E-01	6.8E+00	-8.29	-8.04	-9.07	-1.69	0.63	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5681	87-08-01	Phenoxymethylpenicillin (Penicillin V)	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	1.5E+02	8.6E+01	1.4E+00	1.9E-01	8.8E+00	-8.41	-8.23	-10.02	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5682	11041-12-6	Cholestyramine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	1.3E+02	7.4E+01	6.0E-01	1.6E-01	1.1E+01	-8.49	-8.23	-10.03	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5795	57-27-2	MORPHINE	285	174	5.6E-08	1.3E+04	5.2E+02	8.2	3.5E-06	1.7E-08	3.5E-07	1.8E+01	1.0E+01	5.2E-02	2.3E-02	1.0E+00	-8.92	-8.95	-10.16	-2.51	0.45	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5685	91161-71-6	TERBINAFINE	291	147	7.8E-05	2.0E+00	6.5E+05	14.0	3.5E-06	1.1E-06	1.1E-07	2.9E+01	1.7E+01	3.8E-01	3.9E-02	2.2E+00	-10.76	-10.71	-12.69	-4.22	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5834	298-46-4	Carbamazepine	236	162	1.2E-05	1.5E+01	1.8E+02	0.1	3.5E-06	2.5E-08	1.1E-07	1.9E+02	1.1E+02	1.7E+00	2.5E-01	1.2E+01	-8.05	-7.92	-9.21	-1.41	0.41	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5600	723-46-6	Sulfamethoxazol	253	172	1.7E-05	1.3E+03	3.0E+00	1.8	3.5E-06	1.3E-07	1.1E-06	1.1E+02	6.5E+01	5.1E-01	1.4E-01	9.6E+00	-8.63	-8.55	-10.34	-2.02	1.36	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5644	88150-42-9	Amlodipine	409	201	1.6E-07	1.5E+03	1.2E+02	9.0	3.5E-06	1.9E-07	3.5E-07	2.4E+01	1.4E+01	8.9E-02	3.6E-02	2.2E+00	-9.48	-9.37	-11.30	-2.84	0.81	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5630	198904-31-3	Docusate Sodium	705	350	1.4E-24	1.1E-02	7.6E+02	3.9	3.5E-06	3.5E-07	3.5E-07	3.7E+01	2.2E+01	6.0E-01	5.1E-02	1.1E+00	-9.29	-9.41	-11.47	-2.87	0.89	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5738	76-57-3	Codeine Phosphate (Codeine)	299	169	2.5E-08	8.8E+02	1.9E+01	8.2	3.5E-06	1.1E-06	3.5E-07	2.4E+02	1.4E+02	8.2E-01	3.0E-01	2.3E+01	-8.95	-8.99	-11.60	-2.44	0.54	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5601	81103-11-9	Clarithromycin	748	350	1.E-23	7.7E-01	1.5E+03	8.6	3.5E-06	2.3E-07	1.1E-06	6.9E+01	4.0E+01	3.1E-01	6.0E-02	9.2E-01	-9.25	-9.13	-11.13	-2.55	1.29	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5690	2753-45-9	Mebeverine Hydrochloride	466	87	9.9E-03	3.2E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	1.0E+02	5.9E+01	1.3E+00	1.4E-01	4.8E+00	-8.56	-8.42	-10.21	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5602	83905-01-5	Azithromycin	749	350	3.5E-22	7.4E-01	1.7E+03	14.0	3.5E-06	2.6E-07	1.1E-06	6.7E+00	3.9E+00	1.1E-01	9.3E-03	1.8E-01	-10.05	-10.19	-12.13	-3.60	1.29	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5691	315-30-0	Allopurinol	136	164	5.0E-05	8.7E-04	7.2E-02	9.3	3.5E-06	3.5E-07	3.5E-07	1.6E+02	9.3E+01	2.4E+00	2.2E-01	6.0E+00	-8.14	-8.60	-10.71	-1.99	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5931	143322-58-1	Quetiapine	383	234	1.4E-09	1.2E+01	5.2E+03	9.2	3.5E-06	1.1E-06	1.1E-07	4.5E+01	2.6E+01	6.1E-01	6.1E-02	2.0E+00	-9.64	-10.07	-12.33	-3.42	0.30	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5898	65277-42-1	Ketoconazole	531	292	8.5E-12	2.6E-01	2.8E+04	6.4	3.5E-06	2.3E-08	1.1E-07	9.5E+00	5.5E+00	1.0E-01	1.3E-02	4.7E-01	-9.54	-9.43	-10.70	-2.77	0.35	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5934	1400-61-9	Nystatin	276	132	1.2E-04	7.0E-01	1.2E+07	4.9	3.5E-06	1.1E-06	3.5E-07	8.0E+00	4.6E+00	8.1E-02	1.0E-02	4.8E-01	-10.86	-11.00	-13.25	-4.33	0.30	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5694	65807-02-5	Theophylline	180	193	2.4E-08	9.3E+04	4.2E+01	4.7	3.5E-06	7.0E-09	3.5E-07	3.8E+01	2.2E+01	3.8E-01	4.9E-02	2.0E+00	-8.47	-8.55	-9.64	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5725	599-79-1	Sulfasalazine	398	265	3.0E-12	8.2E-03	6.5E+03	1.8	3.5E-06	1.1E-06	1.1E-06	2.7E+02	1.6E+02	3.0E+00	3.5E-01	1.5E+01	-9.13	-9.27	-11.60	-2.52	0.58	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5618	165800-03-3	STRONTIUM	337	222	9.2E-09	1.4E+03	1.8E+01	3.0	3.5E-06	4.4E-08	3.5E-07	4.7E+01	2.7E+01	7.5E-01	6.4E-02	1.2E+00	-8.52	-8.66	-10.08	-1.87	1.06	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5963	3546-03-0	Crotamiton	204	94	5.6E-02	1.1E+02	5.4E+02	-0.4	3.5E-06	3.5E-07	3.5E-07	6.7E+00	3.9E+00	7.5E-02	8.9E-03	3.7E-01	-10.21	-10.12	-12.23	-3.28	0.22	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5787	137-58-6	Lidocaine	234	144	9.0E-04	6.8E+02	4.6E+01	7.9	3.5E-06	3.9E-08	1.1E-07	8.5E+00	4.9E+00	7.7E-02	1.1E-02	5.0E-01	-9.44	-9.35	-10.75	-2.45	0.50	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5702	119478-56-7	VERAPAMIL HYDROCHLORIDE	438	87	9.9E-03	3.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	4.4E+01	2.6E+01	3.9E-01	5.7E-02	2.8E+00	-8.93	-8.75	-10.54	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5961	202409-33-4	Etoricoxib	359	221	1.0E-08	1.6E+00	8.1E+02	2.8	3.5E-06	3.5E-08	1.1E-08	1.1E+00	6.6E-01	1.3E-02	1.5E-03	5.4E-02	-10.06	-10.13	-11.50	-3.21	0.23	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5696	53123-88-9	Isosorbide	914	350	1.4E-34	2.4E-05	5.5E+04	10.4	3.5E-06	3.6E-01	2.1E-01	5.6E+01	4.9E+02	9.8E-01	9.8E-01	1.0E+01	-10.45	-12.52	-13.51	-3.51	0.65	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5704	144701-48-4	Telmisartan	515	350	1.2E-17	8.6E-07	2.6E+08	3.3	3.5E-06	3.5E-07	1.1E-07	4.8E+00	2.8E+00	1.8E-02	6.0E-03	4.4E-01	-10.49	-10.35	-12.50	-3.41	1.76	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5705	67018-85-3	Nortriptyline	263	130	2.9E-04	6.2E+00	5.5E+04	9.9	3.5E-06	3.5E-07	3.5E-08	2.1E+00	1.2E+00	2.6E-02	2.8E-03	9.4E-02	-11.12	-10.90	-12.94	-3.96	1.54	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5706	486460-32-6	Sitagliptin	407	182	1.8E-06	5.6E+00	2.5E+03	0.0	3.5E-06	1.1E-07	1.1E-07	2.3E+01	1.3E+01	3.8E-01	1.2E-02	5.9E-01	-8.85	-9.13	-10.84	-2.18	1.81	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5640	29110-47-2	Gliclazide	323	207	1.6E-07	2.3E+02	1.3E+02	3.4	3.5E-06	1.1E-06	3.5E-07	1.7E+02	9.8E+01	2.6E+00	2.3E-01	6.1E+00	-8.94	-9.31	-11.65	-2.36	0.87	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5762	93957-54-1	FLUVASTATIN	411	256	2.5E-14	7.3E-01	7.1E+04	4.3	3.5E-06	1.1E-07	3.5E-08	9.8E-01	5.7E-01	4.3E-03	1.2E-03	8.4E-02	-10.81	-10.39	-12.13	-3.43	0.54	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5707	16679-58-6	Hydroxychloroquine Sulphate	1069	87	9.9E-03	7.4E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	3.9E+01	2.3E+01	3.6E-01	5.1E-02	2.4E+00	-8.98	-8.81	-10.60	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5604	21829-25-4	Nifedipine	346	176	3.5E-06	1.1E+01	1.6E+02	2.0	3.5E-06	1.1E-07	3.5E-07	1.6E+01	9.1E+00	1.2E-01	2.0E-02	1.1E+00	-9.53	-9.32	-11.04	-2.34	1.34	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5708	26807-65-8	Indapamide	366	241	4.2E-09	7.3E+01	4.6E+02	9.7	3.5E-06	1.1E-07	1.1E-07	4.1E-01	2.4E-01	2.1E-03	5.2E-04	3.4E-02	-11.03	-10.95	-12.69	-3.97	2.81	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5710	10540-29-1	TAMOXIFEN	372	181	4.6E-06	8.6E-03	2.0E+06	8.0	3.5E-06	1.6E-08	1.1E-07	2.2E+00	1.3E+00	1.3E-02	2.7E-03	1.6E-01	-11.00	-11.23	-12.55	-4.24	0.13	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5676	7722-84-1	PROPRANOLOL HYDROCHLORIDE	34	87	9.9E-03	2.3E+02	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	7.0E+01	4.1E+01	6.4E-01	9.1E-02	4.4E+00	-8.75	-8.55	-10.34	-1.56	0.72	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5606	26787-78-0	Amoxicillin	365	330	6.3E-15	2.1E+04	9.3E+00	14.0	3.5E-06	2.1E-07	1.1E-06	4.7E+02	2.7E+02	8.2E+00	6.6E-01	1.1E+01	-7.88	-8.13	-10.03	-1.13	1.29	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5605	114-07-8	Erythromycin	734	350	2.8E-23	2.2E+00	3.0E+02	9.0	3.5E-06	2.7E-07	3.5E-07	1.2E+02	6.8E+01	2.0E+00	1.6E-01	3.0E+00	-8.65	-8.87	-10.83	-1.81	1.35	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5616	79-57-2	Oxytetracycline	460	344	1.2E-20	6.6E+03	1.3E-03	3.3	3.5E-06	1.7E-07	1.1E-06	8.6E+01	5.0E+01	8.8E-01	1.1E-01	5.0E+00	-8.40	-8.72	-10.58	-1.66	1.13	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5957	27262-47-1	Levetiracetam	170	141	2.4E-04	1.5E+02	2.6E-01	-1.3	3.5E-06	3.5E-06	3.5E-06	1.9E+02	1.1E+02	3.1E+00	2.6E-01	6.2E+00	-9.22	-10.15	-12.26	-3.07	0.26	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5713	50-28-2	Estradiol	272	152	2.7E-07	8.8E+00	8.7E+03	10.0	3.5E-06	9.5E-08	1.1E-06	1.2E-01	6.8E-02	6.5E-04	1.5E-04	9.3E-03	-11.78	-11.73	-13.43	-4.64	1.61	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5808	22071-15-4	Ketoprofen	254	149	1.9E-04	1.3E+01	1.0E+03	4.1	3.5E-06	3.6E-09	3.5E-07	1.0E+01	6.0E+00	1.2E-01	1.4E-02	4.3E-01	-9.38	-9.17	-10.22	-2.07	0.48	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5615	84625-61-6	Itraconazole	706	350	1.5E-18	1.5E-04	1.4E+06	5.5	3.5E-06	1.1E-07	1.1E-07	2.0E+00	1.2E+00	2.6E-02	2.7E-03	1.1E-01	-10.51	-10.46	-12.16	-3.36	1.15	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5729	130-95-0	Quinine	324	190	1.3E-08	4.1E+02	1.9E+03	8.6	3.5E-06	1.1E-06	3.5E-07	1.5E+02	8.8E+01	1.6E+00	2.0E-01	8.9E+00	-9.30	-9.61	-11.89	-2.50	0.60	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5714	214766-78-6	Ursodeoxycholic Acid	1632	87	9.9E-03	1.1E+04	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	2.7E+01	1.5E+01	2.4E-01	3.5E-02	1.7E+00	-9.15	-8.97	-10.76	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5715	102625-70-7	Pantoprazole	383	253	1.6E-13	8.6E+00	1.4E+02	3.9	3.5E-06	1.1E-06	3.5E-07	4.4E+00	2.6E+00	3.8E-02	5.7E-03	3.1E-01	-10.69	-10.79	-13.29	-3.66	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5646	66357-35-5	RANITIDINE	314	168	1.9E-04	8.0E+03	1.9E+00	8.0	3.5E-06	6.2E-08	3.5E-07	1.7E+02	9.8E+01	2.8E+00	2.3E-01	3.8E+00	-7.96	-8.14	-9.66	-1.00	0.88	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5890	43200-80-2	Zopiclone	389	228	1.3E-08	8.4E+02	3.5E+01	6.8	3.5E-06	3.5E-07	1.1E-07	5.3E+00	3.1E+00	7.8E-02	7.2E-03	2.0E-01	-9.71	-10.15	-12.24	-2.99	0.40	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5716	39474-58-3	Sucralfate	1559	87	9.9E-03	1.1E+04	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	2.1E+01	1.2E+01	1.2E-01	2.7E-02	1.7E+00	-9.26	-9.03	-10.83	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5955	50-06-6	Phenobarbital	232	245	1.8E-09	2.1E+03	2.6E+01	7.5	3.5E-06	3.5E-07	3.5E-07	3.7E+01	2.0E+01	4.0E+01	4.9E+02	2.1E+02	-7.11	-7.36	-9.47	-0.16	0.28	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5657	13311-84-7	Flutamide	276	155	1.5E-04	3.1E+00	3.2E+03	12.3	3.5E-06	2.2E-09	1.1E-07	8.5E+00	4.9E+00	1.1E-01	1.1E-02	3.1E-01	-9.61	-9.36	-10.42	-2.15	0.80	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5718	120287-85-6	Etodolac	1431	87	9.9E-03	9.9E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	2.4E+01	1.4E+01	3.0E-01	3.2E-02	1.1E+00	-9.19	-9.07	-10.85	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5719	84057-84-1	Lamotrigine	256	189	1.8E-06	4.4E+02	9.8E+00	5.5	3.5E-06	2.2E-09	1.1E-07	4.2E+01	2.5E+01	5.2E-01	5.6E-02	1.8E+00	-8.44	-8.49	-9.51	-1.24	0.17	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5721	73590-58-6	Omeprazole	345	254	1.3E-13	1.4E+01	2.9E+03	4.0	3.5E-06	3.5E-08	3.5E-07	9.9E+01	5.8E+01	2.2E+00	1.3E-01	4.6E+00	-8.49	-8.32	-9.69	-1.06	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5624	41859-67-0	Bezafibrate	362	230	8.2E-09	6.5E+01	1.8E+04	-0.9	3.5E-06	9.2E-08	1.1E-06	8.1E+01	4.7E+01	9.8E-01	1.1E-01	3.8E+00	-8.77	-8.63	-10.28	-1.36	1.04	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5775	98319-26-7	Finasteride	373	236	6.4E-10	1.2E-02	1.6E+03	0.0	3.5E-06	8.2E-08	3.5E-07	1.8E+00	1.1E+00	2.3E-02	2.5E-03	8.0E-02	-10.32	-10.20	-11.81	-2.92	0.54	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5814	58-46-8	Venlafaxine	317	158	7.1E-05	1.7E+01	4.6E+02	7.0	3.5E-06	1.1E-06	3.5E-07	5.3E+01	3.1E+01	8.6E-01	7.3E-02	1.7E+00	-9.84	-10.00	-12.25	-2.72	0.48	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5722	61337-67-5	Mirtazapine	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	1.6E+01	9.5E+00	6.8E-02	2.0E-02	1.4E+00	-9.38	-9.12	-10.92	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5663	604-75-1	Oxazepam	287	209	5.5E-10	8.8E+01	2.1E+02	3.8	3.5E-06	2.2E-08	3.5E-08	2.7E+00	1.5E+00	3.5E-02	3.6E-03	1.0E-01	-9.63	-9.74	-11.00	-2.45	0.80	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5717	18321-74-6	Aminophylline	393	222	2.4E-09	1.2E+00	6.2E+02	5.9	3.5E-06	1.1E-06	3.5E-07	2.6E+01	1.5E+01	1.3E-01	3.3E-02	2.3E+00	-10.24	-10.14	-12.69	-2.83	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5938	439-14-5	Diazepam	285	182	1.4E-05	3.2E+01	5.0E+02	3.0	3.5E-06	3.5E-08	3.5E-08	3.8E+00	2.2E+00	2.1E-02	4.8E-03	2.9E-01	-9.80	-9.58	-10.96	-2.26	0.32	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5843	745-65-3	Carbidopa	354	218	3.1E-11	3.1E+00	5.4E+03	4.9	3.5E-06	1.1E-06	3.5E-07	2.7E+01	1.6E+01	3.2E-01	3.6E-02	1.5E+00	-10.06	-10.17	-12.53	-2.84	0.45	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5720	18321-74-6	Aminophylline	393	222	9.4E-09	1.2E+00	6.2E+02	5.9	3.5E-06	1.1E-06	3.5E-07	2.6E+01	1.5E+01	2.1E-01	3.4E-02	1.9E+00	-10.13	-10.17	-12.63	-2.83	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5746	70458-96-7	Norflox	319	315	1.1E-09	5.4E+02	4.9E+01	6.2	3.5E-06	3.0E-08	3.5E-07	5.2E-01	3.0E-01	4.7E-03	6.8E-04	3.1E-02	-10.40	-10.51	-11.85	-3.17	0.60	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5627	72956-09-3	Carvedilol	406	252	7.9E-12	1.8E+00	1.1E+03	8.0	3.5E-06	1.6E-07	1.1E-07	2.1E+00	1.2E+00	8.5E-03	2.6E-03	1.9E-01	-10.49	-10.38	-12.23	-3.00	1.04	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5885	298-46-4	Atenolol	266	184	1.0E-07	1.5E+04	9.3E-01	0.1	3.5E-06	2.9E-07	3.5E-07	1.2E+02	6.8E+01	2.1E+00	1.6E-01	2.6E+00	-8.20	-8.79	-10.80	-1.41	0.41	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5728	53772-83-1	ZUCLOPENTHIXOL	401	223	3.9E-11	6.4E-01	5.8E+03	7.7	3.5E-06	1.1E-08	1.1E-08	2.6E-01	1.5E-01	2.8E-03	3.4E-04	1.3E-02	-10.75	-10.81	-11.96	-3.34	0.08	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5916	86386-73-4	Ciprofloxacin	331	317	3.8E-11	1.2E+03	3.0E+02	2.0	3.5E-06	6.3E-09	3.5E-07	2.9E+01	1.7E+01	4.6E-01	4.0E-02	6.5E-01	-8.81	-8.73	-9.81	-1.21	0.37	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5612	60-54-8	Tetracycline	444	327	2.8E-19	2.6E+03	4.7E-02	3.4	3.5E-06	1.7E-07	1.1E-06	5.9E+00	3.4E+00	9.3E-02	8.1E-03	1.9E-01	-9.48	-9.92	-11.75	-2.37	1.29	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5884	5633-20-5	Losartan Potassium	358	186	2.8E-08	1.4E+01	5.1E+03	8.3	3.5E-06	1.1E-06	3.5E-07	7.0E+01	4.1E+01	6.3E-01	9.1E-02	4.7E+00	-9.77	-10.02	-12.30	-2.44	0.43	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5731	641571-10-0	Nilotinib	530	331	2.7E-16	3.5E-05	1.0E+05	5.9	3.5E-06	1.1E-06	3.5E-07	3.7E+00	2.1E+00	1.6E-02	4.6E-03	3.3E-01	-11.28	-11.30	-13.74	-3.71	0.17	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5709	125-28-0	Dihydrocodeine	301	168	2.7E-07	4.5E+02	3.1E+01	8.2	3.5E-06	1.1E-06	3.5E-07	5.2E+01	3.0E+01	2.6E-01	6.6E-02	4.6E+00	-9.61	-9.73	-12.29	-2.11	0.69	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5607	54910-89-3	F

5645	55-98-1	Acamprosate Calcium	246	130	1.2E-05	1.5E+04	2.1E-01	14.0	3.5E-06	1.1E-06	1.1E-06	2.5E+01	1.4E+01	2.4E-01	3.3E-02	1.6E+00	-9.63	-9.95	-12.47	-0.90	1.12	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5794	72559-06-9	Citalopram Hydrobromide (Citalopram)	847	350	1.2E-31	1.1E-04	3.2E+07	7.2	3.5E-06	1.1E-06	3.5E-07	4.5E+01	2.6E+01	3.3E-01	5.7E-02	3.0E+00	-10.59	-10.89	-12.44	-6.90	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5796	106266-06-2	Risperidone	411	236	6.2E-09	8.4E-01	3.1E+03	8.0	3.5E-06	1.2E-08	3.5E-07	1.2E-01	6.8E-02	9.1E-04	1.5E-04	7.5E-03	-11.44	-11.31	-12.51	-2.22	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5699	15676-16-1	Sulpiride	341	227	1.6E-08	2.0E+03	4.5E+00	9.2	3.5E-06	1.1E-06	3.5E-07	9.8E+00	5.7E+00	1.6E-01	1.3E-02	1.2E-01	-9.89	-10.47	-12.84	-1.33	0.85	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5799	29094-61-9	Glipizide	446	301	3.6E-14	2.2E+01	2.2E+03	0.5	3.5E-06	1.1E-06	3.5E-07	9.0E-01	5.2E-01	8.6E-03	1.2E-03	5.9E-02	-11.56	-11.54	-13.99	-2.40	1.82	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5800	135062-02-1	Repaglinide	453	274	2.6E-12	5.9E-02	1.5E+06	3.6	3.5E-06	1.1E-06	3.5E-07	5.8E-02	3.4E-02	2.2E-04	7.3E-05	5.5E-03	-13.09	-12.85	-15.39	-3.70	0.19	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5823	139264-17-8	Zolmitriptan	287	202	1.9E-07	1.5E+03	8.3E+01	8.7	3.5E-06	3.5E-07	1.1E-07	4.3E-02	2.5E-02	4.0E-04	5.6E-05	2.8E-03	-12.01	-12.24	-14.37	-3.09	0.60	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5892	54965-21-8	Albendazole	265	192	2.0E-07	6.5E+00	1.4E+03	4.0	3.5E-06	7.5E-09	1.1E-07	2.8E-02	1.6E-02	4.5E-04	3.8E-05	5.9E-04	-11.84	-11.73	-12.82	-2.52	0.51	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5928	5633-20-5	Oxybutynin	358	186	2.3E-08	1.4E+01	9.1E+03	8.3	3.5E-06	1.1E-06	3.5E-07	1.6E+00	9.3E-01	2.0E-02	2.1E-03	8.1E-02	-11.31	-11.66	-13.85	-2.44	0.43	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5632	100986-85-4	Levofloxacin	361	318	1.3E-10	6.3E+01	6.3E-01	6.1	3.5E-06	5.2E-09	3.5E-07	2.2E-01	1.3E-01	2.8E-03	2.9E-04	8.4E-03	-10.65	-10.81	-11.88	-1.58	1.24	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5642	638-23-3	Carbocisteine	179	259	2.0E-05	3.3E+04	5.8E-05	1.9	3.5E-06	3.5E-06	1.1E-06	2.7E+00	1.5E+00	5.3E-03	3.5E-01	1.5E+01	-8.83	-9.57	-12.18	-0.30	1.15	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5641	64-86-8	Colchicine	399	242	4.2E-09	1.4E+01	7.2E+01	-1.0	3.5E-06	2.1E-07	3.5E-07	3.2E-02	1.9E-02	2.8E-04	4.2E-05	2.1E-03	-12.21	-12.20	-14.16	-2.93	1.16	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5979	51333-22-3	Fluorouracil	431	234	1.5E-12	2.2E+00	4.1E+02	13.3	3.5E-06	4.0E-08	1.1E-06	2.6E-01	1.5E-01	2.9E-03	3.4E-04	1.3E-02	-11.11	-11.02	-12.44	-1.73	0.25	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5831	1977-10-2	Lormetazepam	335	208	6.4E-10	1.0E+01	1.7E+02	1.0	3.5E-06	1.1E-08	1.1E-06	6.1E-03	7.2E-05	1.3E-05	7.3E-04	-12.06	-12.04	-13.20	-2.75	0.60	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5818	59-67-6	Nicotinic Acid	123	63	2.2E-02	4.1E+04	4.9E+00	2.0	3.5E-06	3.5E-07	1.1E-07	8.7E-02	5.1E-02	2.0E-02	7.2E-01	-9.64	-10.00	-12.29	-0.71	0.61	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5911	52-86-8	Haloperidol	376	194	2.0E-08	9.4E+00	1.6E+04	8.7	3.5E-06	3.5E-08	3.5E-08	2.5E-02	1.5E-02	3.3E-04	3.4E-05	9.6E-04	-12.03	-12.06	-13.43	-2.76	0.47	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5803	354812-41-2	Moxifloxacin	401	325	9.7E-13	1.3E+02	8.9E+00	6.1	3.5E-06	1.1E-06	3.5E-07	1.7E-01	9.8E-02	2.5E-03	2.3E-04	6.8E-03	-11.65	-12.25	-14.63	-2.94	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5917	33005-95-7	Tiaprofenic Acid	260	163	1.3E-04	1.3E+01	6.6E+02	3.8	3.5E-06	1.1E-06	3.5E-07	4.8E-01	2.8E-01	6.2E-03	6.0E-04	4.2E-02	-11.75	-14.33	-14.33	-2.43	0.45	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5673	58-25-3	Chlordiazepoxide	300	234	1.3E-09	1.5E+05	2.6E+02	5.0	3.5E-06	3.4E-08	1.1E-08	5.2E-01	3.0E-01	7.5E-03	7.0E-04	1.7E-02	-10.26	-10.49	-11.85	-1.17	0.97	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5636	154-21-2	Isotretinoin	300	148	1.4E-05	2.8E-01	7.1E+07	4.4	3.5E-06	3.6E-08	1.1E-06	8.5E-02	4.9E-02	1.0E-03	1.1E-04	3.8E-03	-11.71	-11.65	-13.04	-2.31	1.21	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5637	59467-70-8	Midazolam	326	201	6.8E-07	6.7E+01	2.1E+04	6.0	3.5E-06	3.4E-08	1.1E-08	1.7E-02	1.0E-02	1.4E-04	2.2E-05	1.1E-03	-12.14	-12.02	-13.39	-2.67	0.92	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5658	62571-86-2	Captopril	217	134	9.7E-04	1.4E+04	6.9E+00	3.3	3.5E-06	1.2E-07	1.1E-06	2.0E-00	1.1E-00	2.9E-02	2.7E-03	6.8E-02	-10.26	-10.30	-12.04	-0.94	1.04	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5980	51333-22-3	Budesonide	431	234	1.5E-12	2.2E+00	4.1E+02	13.3	3.5E-06	4.0E-08	1.1E-06	2.1E-01	1.2E-01	3.6E-03	2.9E-04	3.7E-03	-11.13	-11.10	-12.51	-1.73	0.25	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5712	53-03-2	PRAVASTATIN	425	243	8.1E-14	5.1E+01	1.3E+03	4.3	3.5E-06	1.1E-06	3.5E-07	1.3E+01	7.5E+00	1.5E-01	1.7E-02	7.0E-01	-10.31	-10.42	-12.81	-1.02	0.84	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5749	93-14-1	Fenofenadine Hydrochloride	198	100	2.4E-04	1.2E+05	2.6E+00	14.0	3.5E-06	1.1E-06	3.5E-07	4.9E-01	2.5E-01	5.8E-02	1.8E-03	9.2E-01	-9.77	-9.77	-12.21	-0.35	0.76	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5786	123-99-9	Azelaic Acid	188	127	3.1E-03	3.8E+03	5.0E+01	4.6	3.5E-06	1.1E-06	1.1E-06	2.2E+00	1.3E+00	4.1E-02	3.1E-03	4.4E-02	-11.00	-11.37	-13.58	-1.95	0.68	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5809	404-86-4	Capsaicin	305	196	1.8E-06	4.8E+00	1.0E+04	0.0	3.5E-06	3.1E-07	3.5E-07	2.9E-02	1.7E-02	2.9E-04	3.8E-05	1.7E-03	-12.61	-12.46	-14.53	-3.01	0.11	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5827	469-21-6	Doxepin	279	133	1.6E-03	6.2E+00	9.0E+03	8.8	3.5E-06	1.1E-06	3.5E-07	7.8E-01	4.5E-01	1.1E-02	1.1E-03	3.1E-02	-12.26	-12.01	-14.19	-2.55	0.61	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5748	63590-64-7	TERAZOSIN	387	240	2.2E-10	4.4E+02	3.0E+01	7.4	3.5E-06	1.1E-06	3.5E-07	1.1E-01	6.4E-02	2.2E-04	1.4E-04	1.0E-02	-12.32	-12.38	-14.97	-2.91	0.77	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5811	37332-99-3	VANCOMYCIN	1449	87	9.9E-03	1.0E+04	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	1.0E-01	6.1E-02	3.9E-04	1.3E-04	9.4E-03	-11.57	-11.31	-13.11	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5810	6740-88-1	Ketamine	238	110	6.9E-03	1.6E+03	1.3E+03	7.1	3.5E-06	3.5E-07	1.1E-07	1.2E-01	7.1E-02	2.1E-03	1.7E-04	3.0E-03	-11.95	-11.96	-14.01	-2.48	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5733	19767-45-4	Sevelamer	141	72	1.0E-02	1.3E+05	1.1E-02	1.2	3.5E-06	1.1E-05	3.5E-06	4.0E+01	2.3E+01	6.1E-01	5.5E-02	1.0E+00	-11.48	-11.48	-13.49	-1.98	0.79	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5776	56-75-7	Chloramphenicol	323	216	2.3E-10	3.5E+03	8.3E+00	9.3	3.5E-06	1.1E-07	1.1E-07	9.1E-02	5.3E-02	1.0E-03	1.2E-04	4.6E-03	-11.24	-11.47	-13.20	-1.97	0.70	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5680	31218-83-4	Praziquantel	312	202	9.9E-07	1.6E+02	2.6E+02	-2.0	3.5E-06	5.9E-08	3.5E-07	4.5E-03	2.6E-03	2.2E-05	5.6E-06	3.6E-04	-12.95	-12.72	-14.25	-3.21	0.95	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5665	19395-41-6	Rifaximin	787	350	1.4E-33	6.7E-06	6.5E+02	2.5	3.5E-06	3.5E-07	3.5E-07	1.5E-01	8.9E-02	1.6E-03	2.0E-04	9.1E-03	-12.17	-11.87	-13.98	-2.36	1.03	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5689	224785-90-4	Vardenafil	489	342	4.6E-17	2.9E+01	6.2E+02	8.1	3.5E-06	3.5E-07	3.5E-07	1.1E-01	6.6E-02	1.6E-03	1.5E-04	4.7E-03	-11.84	-12.02	-14.07	-2.50	0.93	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5828	177036-94-1	Almotriptan	335	207	8.5E-08	9.7E+02	1.3E+02	8.6	3.5E-06	3.5E-07	1.1E-07	4.5E-02	2.6E-02	4.6E-04	6.0E-05	2.7E-03	-12.01	-12.25	-14.37	-2.69	0.62	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5812	50-18-0	Cyclophosphamide	261	86	5.9E-03	6.2E+03	9.3E+00	14.0	3.5E-06	6.5E-09	1.1E-07	4.2E-02	2.4E-02	3.2E-04	5.4E-05	2.7E-03	-11.61	-11.49	-12.58	-1.92	0.15	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5805	68-22-4	Norethisterone	298	161	3.1E-07	4.7E+00	9.8E+02	13.6	3.5E-06	3.0E-07	1.1E-07	2.4E-01	8.1E-02	2.5E-03	1.9E-04	3.1E-03	-11.62	-11.84	-13.85	-2.23	0.65	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5970	152459-95-5	IMATINIB	494	313	4.8E-15	5.1E-01	1.0E+03	7.6	3.5E-06	1.1E-06	1.1E-06	3.1E-01	1.8E-01	1.9E-03	3.9E-04	2.5E-02	-12.22	-12.35	-14.74	-2.73	0.29	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5662	165800-03-3	Linezolid	337	222	9.2E-09	1.4E+03	1.8E+01	3.0	3.5E-06	4.4E-08	3.5E-07	6.5E-02	3.7E-02	6.3E-04	8.4E-05	3.7E-03	-11.50	-11.50	-12.94	-1.87	1.06	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5966	143322-58-1	Eletriptan	383	234	1.4E-09	1.2E+01	3.2E+03	9.2	3.5E-06	1.1E-06	1.1E-07	4.4E-02	2.5E-02	3.4E-04	5.6E-05	3.2E-03	-12.82	-13.06	-15.46	-3.42	0.30	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5974	201530-41-8	Dasatinib	488	305	1.2E-17	4.4E-01	1.3E+01	7.7	3.5E-06	3.5E-07	3.5E-07	6.6E-02	3.8E-02	9.4E-04	8.9E-05	2.6E-03	-11.73	-12.12	-14.20	-2.46	0.28	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5815	126544-47-6	Mupirocin	501	273	2.1E-16	4.8E+00	9.1E+02	4.9	3.5E-06	1.1E-06	3.5E-07	4.3E-01	2.5E-01	7.7E-03	5.9E-04	9.5E-03	-11.62	-12.01	-14.24	-2.33	0.20	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5816	69-53-4	Ampicillin	349	325	3.8E-11	3.5E+03	2.8E+01	7.0	3.5E-06	5.5E-08	3.5E-07	3.3E-01	1.9E-01	3.4E-03	4.3E-04	1.8E-02	-10.84	-10.86	-12.35	-1.16	2.09	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5817	193-91-8	Tinidazole	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	7.6E-02	4.4E-02	8.6E-04	1.0E-04	4.0E-03	-11.69	-11.54	-13.32	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5819	50-63-5	Chloroquine Phosphate	516	87	9.9E-03	3.6E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	8.6E-02	5.0E-02	1.4E-03	1.2E-04	2.2E-03	-11.62	-11.56	-13.33	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5984	58-39-9	Perphenazine	404	223	1.0E-09	5.7E+00	6.6E+03	7.9	3.5E-06	1.1E-06	1.1E-07	9.8E-02	5.7E-02	1.4E-03	1.3E-04	3.9E-03	-12.34	-12.77	-14.99	-3.05	0.26	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5730	1404-04-2	Nadolol	309	181	1.8E-08	1.0E+03	1.5E+01	10.0	3.5E-06	3.7E-08	3.5E-07	1.8E-01	1.0E-01	1.8E-03	2.8E-04	9.9E-03	-11.02	-11.04	-12.43	-1.31	0.82	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5821	50-02-2	Dexamethasone	392	217	7.7E-12	6.5E+01	5.2E+01	13.0	3.5E-06	1.0E-07	1.1E-06	1.1E-01	6.1E-02	7.9E-04	1.4E-04	7.4E-03	-11.66	-11.57	-13.27	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5942	13992-18-2	Fenoprofen	242	136	3.1E-03	2.2E+01	7.9E+03	4.3	3.5E-06	1.1E-06	3.5E-07	3.1E-01	1.8E-01	3.4E-03	4.1E-04	1.8E-02	-12.11	-12.08	-14.51	-2.31	0.42	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5856	58306-30-2	Famciclovir	321	202	3.6E-07	2.6E+02	4.4E+00	3.9	3.5E-06	3.5E-06	1.1E-06	1.0E+00	5.9E-01	8.4E-03	1.3E-03	7.4E-02	-11.72	-12.16	-14.77	-2.36	0.59	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5824	7491-74-9	Piracetam	142	132	8.5E-04	9.2E+05	4.0E-02	-1.3	3.5E-06	3.5E-06	1.1E-06	5.6E+00	3.2E+00	9.0E-02	7.6E-03	1.8E-01	-10.44	-11.47	-13.78	-1.66	1.54	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5975	54024-22-5	Desogestrel	310	149	8.3E-06	3.8E-02	4.5E+05	9.0	3.5E-06	3.5E-07	1.1E-07	5.9E-02	3.4E-02	4.6E-04	7.6E-05	4.0E-03	-12.91	-12.87	-14.85	-3.04	0.28	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5829	99200-09-6	Nebivolol	405	214	5.7E-11	6.3E+00	5.1E+03	8.2	3.5E-06	1.1E-06	1.1E-07	3.0E-01	1.7E-01	4.7E-03	4.1E-04	9.6E-03	-11.80	-12.28	-14.47	-2.45	0.63	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5914	83-43-2	Methylprednisolone	374	219	5.9E-12	8.9E+00	6.6E+02	13.2	3.5E-06	1.1E-06	1.1E-06	6.8E+00	3.9E+00	2.8E-02	8.5E-03	6.3E-01	-10.88	-11.39	-13.09	-1.04	0.49	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5977	175591-23-8	TAPENTADOL	221	82	1.6E-02	3.1E+02	3.7E+03	9.2	3.5E-06	1.1E-06	3.5E-07	1.2E-01	7.2E-02	1.9E-03	1.7E-04	4.4E-03	-12.95	-12.73	-14.92	-2.87	0.27	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5742	80-08-0	Dapsone	248	183	3.6E-06	2.1E+03	5.9E+00	1.8	3.5E-06	1.1E-06	1.1E-06	6.3E-01	3.7E-01	1.0E-02	8.7E-04	2.1E-02	-11.27	-11.86	-14.11	-2.00	0.81	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5830	38821-53-3	Cefradine	349	326	3.8E-11	2.6E+03	9.8E-01	2.8	3.5E-06	3.5E-06	1.1E-06	4.4E+00	2.5E+00	6.3E-02	5.9E-03	1.8E-01	-10.73	-11.60	-13.93	-1.68	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5982	52485-79-7	Buprenorphine	468	226	2.3E-11	1.2E-01	7.9E+04	8.3	3.5E-06	1.1E-06	3.5E-07	9.6E-02	5.6E-02	4.7E-04	1.2E-04	8.2E-03	-12.91	-13.07	-15.40	-3.14	0.21	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5674	144-83-2	Sulfapyridine	249	176	5.5E-06	2.5E+03	3.4E+00	3.1	3.5E-06	4.3E-09	1.1E-06	3.7E-02	2.2E-02	5.5E-04	5.1E-05	1.1E-03	-11.65	-11.62	-12.67	-1.68	1.03	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5920	58-46-8	Tetrabenazine	317	158	7.1E-05	1.7E+01	4.6E+02	7.0	3.5E-06	1.1E-06	3.5E-07	1.0E-01	5.9E-02	9.5E-04	1.3E-04	6.7E-03	-12.68	-12.69	-15.09	-2.72	0.48	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5922	532-32-1	Sodium Benzoate	144	87	9.9E-03	1.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	3.2E-01	1.8E-01	1.6E-03	4.0E-04	2.2E-02	-11.09	-10.85	-12.64	-0.87	0.48	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5833	119478-56-7	Meropenem	438	87	9.9E-03	3.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	4.0E-02	2.3E-02	4.5E-04	5.3E-05	2.1E-03	-11.97	-11.82	-13.60	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5771	51-52-5	Propylthiouracil	170	165	9.2E-06	9.6E+02	9.5E+00	7.5	3.5E-06	1.1E-06	1.1E-06	8.2E-01	4.8E-01	7.2E-03	1.1E-03	5.6E-02	-11.48	-11.69	-14.13	-1.64	0.75	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5813	471-34-1	Calcium Gluconate	430	87	9.9E-03	3.0E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	1.8E-01	1.1E-01	8.5E-04	2.3E-04	1.5E-02	-11.33	-11.08	-12.88	-1.03	0.67	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5807	2098-66-0	Digoxin	781	350	4.4E-28	6.9E-02	3.2E+00	13.3	3.5E-06	1.6E-07	3.5E-07	8.5E-02	4.9E-02	9.0E-04	1.1E-04	4.7E-03	-11.42	-11.63	-13.47	-1.54	0.68	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5727	82834-16-0	Perindopril	368	310	7.5E-10	8.3E+00	3.9E+02	3.1	3.5E-06	3.5E-06	1.1E-06	4.8E+00	2.8E+00	2.5E-02	6.0E-03	4.1E-01	-11.54	-11.56	-14.23	-1.45	0.87	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5629	274901-16-5	VILDAGLIPTIN	303	190	1.3E-08	1.1E+02	6.2E+00	7.6	3.5E-06	1.1E-06	3.5E-07	3.9E-01	2.3E-01	4.6E-03	5.2E-04	2.1E-02	-11.34	-11.80	-14.26	-1.68	1.39	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5837	108736-35-2	Telmisartan	1804	87	9.9E-03	1.2E+04	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	2.8E-02	1.6E-02	3.0E-04	3.7E-05	1.5E-03	-12.12	-11.96	-13.75	-1.84	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5838	68693-11-8	Modafinil	273	202	1.0E-09	9.7E+01	2.8E+02	12.5	3.5E-06	1.1E-06	3.5E-07	2.8E+00	1.6E+00	4.3E-02	3.8E-03	9.5E-02	-10.77	-11.27	-13.49	-1.13	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5839	25614-03-3	Bromocriptine	655	350	8.7E-24	6.8E-03	1.1E+04	5.2	3.5E-06	1.1E-06	3.5E-07	1.4E-02	8.1E-03	1.4E-04	1.8E-05	8.7E-04	-13.42	-13.50	-15.88	-3.34	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5635	56211-40-6	Torasemide	348	225	5.8E-09	1.0E+01	8.9E+01	6.7	3.5E-06	3.5E-07	3.5E-07	3.3E-02	1.9E-02	5.7E-04	4.5E-05	7.7E-04	-12.18	-12.50	-14.55	-2.29	1.33	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5840	10238-21-8	Glibenclamide	494	310	4.2E-13	4.0E-01	6.2E+04	-1.0	3.5E-06	1.1E-07	3.5E-07	2.2E-01	1.3E-01	2.5E-03	2.9E-04	1.1E-02	-11.38	-11.22	-12.92	-1.00	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5919	137-58-6	Pindolol	248	146	8.5E-07	6.7E+03	3.0E+01	7.9	3.5E-06	1.8E-07	3.5E-07	9.6E-03	5.6E-03	4.1E-05	1.2E-05	8.5E-04	-12.75	-12.68	-14.60	-2.45	0.50	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5654	104227-87-4	Exemestane	296	155	1.6E-04	4.6E+01	8.9E+02	14.0	3.5E-06	1.1E-06	3.5E-07	6.2E-01	3.6E-01	1.1E-02	8.6E-04	1.6E-02	-11.86	-11.98	-14.18	-1.74	1.18	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5841	30652-11-0	Deferasirox	373	272	2.2E-14	1.5E+00	2.8E+03	0.2	3.5E-06	3.5E-07	1.1E-07	6.0E-02	3.5E-02	6.2E-04	7.9E-05	3.6E-03	-12.16	-12.04	-14.17	-1.80	0.64	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5842	142217-69-4	Diethylamine Salicylate (Diethylamine)	277	266	4.0E-15	1.3E+05	6.2E-02	3.1	3.5E-06	3.5E-06	3.5E-06	2.5E+01	1.5E+01	3.5E-01	3.4E-02	1.1E+00	-10.07	-10.99	-13.20	-0.75	1.49	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
5983	104987-11-3	Tacrolimus	804	350	1.1E-29	3.4E-03	1.1E+03	10.1	3.5E-06	1.1E-06	3.5E-07

5992	16846-24-5	Ivermectin	875	350	1.6E-28	2.6E-04	4.1E+04	12.8	3.5E-06	1.1E-06	3.5E-07	4.5E-05	2.6E-05	5.4E-07	6.0E-08	2.3E-06	-16.53	-16.32	-18.51	-1.87	0.29	0.0%	0.0%	0.0%
5937	83150-76-9	NAFARELIN	1323	87	9.9E-03	9.1E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	1.1E-06	6.2E-07	9.0E-09	1.4E-09	7.1E-08	-16.55	-16.36	-18.15	-1.84	0.64	0.0%	0.0%	0.0%
5763	55-98-1	Busulfan	246	130	1.2E-05	1.5E+04	2.1E-01	14.0	3.5E-06	1.1E-06	1.1E-06	8.6E-05	5.0E-05	1.1E-06	1.2E-07	4.2E-06	-15.01	-15.48	-17.92	-0.90	1.12	0.0%	0.0%	0.0%
5994	124-94-7	Triamcinolone	394	230	1.2E-13	3.4E+02	9.1E+01	12.4	3.5E-06	1.1E-06	1.1E-06	7.9E-06	4.6E-06	7.5E-08	1.0E-08	3.1E-07	-16.37	-16.70	-19.11	-1.84	0.33	0.0%	0.0%	0.0%
5991	3385-03-3	Flunisolide	435	225	8.7E-12	3.0E+01	4.6E+02	13.3	3.5E-06	1.1E-06	3.5E-07	1.2E-04	7.2E-05	2.2E-06	1.7E-07	3.1E-06	-15.12	-15.65	-17.82	-0.68	0.26	0.0%	0.0%	0.0%
5962	10596-23-3	KETOTIFEN	309	185	2.4E-06	8.8E+00	7.1E+03	8.6	3.5E-06	1.1E-06	3.5E-07	3.1E-03	1.8E-03	2.4E-05	4.0E-06	2.2E-04	-14.24	-14.37	-16.72	0.61	0.50	0.0%	0.0%	0.0%
5836	110-17-8	Fumaric Acid	116	84	1.3E-09	5.5E+04	1.1E+00	3.0	3.5E-06	4.7E-06	1.1E-06	2.0E-04	1.2E-04	2.1E-06	2.6E-07	1.2E-05	-15.30	-16.02	-18.53	-0.97	0.95	0.0%	0.0%	0.0%
5945	120287-85-6	Cetronexa	1431	87	9.9E-03	9.9E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	2.1E-07	1.2E-07	1.6E-09	2.7E-10	1.4E-08	-17.26	-17.06	-18.85	-1.84	0.64	0.0%	0.0%	0.0%
5946	142217-69-4	Entecavir	277	266	4.0E-15	1.3E+05	6.2E-02	3.1	3.5E-06	3.5E-06	3.5E-06	2.3E-04	1.3E-04	1.9E-06	2.9E-07	1.6E-05	-15.28	-15.98	-18.43	-0.75	1.49	0.0%	0.0%	0.0%
5948	50-35-1	Taflupirost	453	205	5.1E-11	1.0E-01	3.2E+06	14.0	3.5E-06	1.1E-06	3.5E-07	9.3E-05	5.4E-05	9.8E-07	1.2E-07	4.9E-06	-16.20	-16.53	-18.21	-0.94	1.51	0.0%	0.0%	0.0%
5902	78755-81-4	Flumazenil	303	205	3E-07	2.6E+01	1.1E+01	2.0	3.5E-06	1.1E-06	3.5E-07	9.3E-07	5.4E-07	1.5E-08	1.3E-09	2.9E-08	-16.94	-17.56	-19.90	-1.83	0.83	0.0%	0.0%	0.0%
5995	437-38-7	NANDROLONE	336	187	8.7E-06	1.8E+02	7.8E+03	8.1	3.5E-06	1.1E-06	3.5E-07	6.5E-08	3.7E-08	4.3E-10	8.2E-11	5.1E-09	-18.92	-19.06	-21.42	-2.97	0.27	0.0%	0.0%	0.0%
5954	139110-80-8	Zanamivir	332	268	5.8E-16	1.1E+04	2.2E-05	3.5	3.5E-06	3.5E-06	1.1E-06	7.9E-05	4.6E-05	7.2E-07	1.0E-07	5.3E-06	-15.42	-16.04	-18.75	0.43	1.96	0.0%	0.0%	0.0%
Pesticides																						*0.2%*	*0.1%*	*0.0%*
n			*420*	*420*	*420*	*420*	*420*	*420*	*420*	*420*	*420*	*420*	*420*	*420*	*420*	*420*	*420*	*420*	*420*	*420*	*420*	*420*	*420*	*420*
sum												***1.8E+05***		***2.7E+04***	***2.5E+01***	***1.5E+05***								
av												*4.2E+02*	*2.4E+02*	*6.4E+01*	*6.0E-02*	*3.5E+02*				*-2.76*	*0.91*			
std												*2.8E+03*	*1.6E+03*	*4.2E+02*	*4.0E-01*	*2.3E+03*				*1.24*	*0.43*			
2.5-p			*152*	*5*	*1.5E-10*	*1.3E-03*	*1.5E-01*		*3.5E-06*	*2.2E-09*	*6.6E-09*	*6.9E-01*	*4.0E-01*	*1.0E-01*	*9.9E-05*	*5.7E-01*	*-10.45*	*-11.01*	*-12.71*	*-5.99*	*0.62*	*8.8E-34*	*2.0E-36*	*2.5E-54*
50-p			*295*	*140*	*2.3E-04*	*2.6E+01*	*1.4E+03*	*0*	*3.5E-06*	*6.3E-08*	*3.5E-07*	*5.8E+01*	*3.4E+01*	*8.8E+00*	*8.3E-03*	*4.8E+01*	*-8.20*	*-8.42*	*-9.72*	*-2.65*	*0.85*	*6.4E-15*	*9.0E-16*	*7.6E-24*
97.5-p			*481*	*264*	*2.1E+00*	*7.2E+04*	*5.6E+06*	*14.0*	*3.5E-06*	*3.5E-06*	*1.1E-06*	*2.4E+03*	*1.4E+03*	*3.6E+02*	*3.4E-01*	*2.0E+03*	*-6.42*	*-6.50*	*-7.92*	*1.00*	*1.19*	*3.0E-06*	*2.3E-06*	*2.4E-11*
6027	2921-88-2	Chlorpyrifos	351	83	2.7E-03	2.4E-01	1.3E+05	0.0	3.5E-06	1.3E-08	3.5E-07	5.7E+02	3.3E+02	8.6E+01	8.2E-02	4.8E+02	-7.33	-7.40	-8.44	-4.95	1.40	0.03%	0.02%	0.0%
6000	34123-59-6	Isoproturon	206	109	1.0E-03	7.7E+01	6.9E+02	0.1	3.5E-06	1.1E-08	1.1E-07	1.3E+04	7.4E+03	1.9E+03	1.8E+00	1.1E+04	-5.52	-5.57	-6.67	-3.06	1.40	0.02%	0.02%	0.0%
5999	8018-01-7	Mancozeb	541	87	9.9E-03	3.7E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	1.3E+04	7.6E+03	2.0E+03	1.9E+00	1.1E+04	-5.08	-5.41	-7.18	-2.88	0.63	0.08%	0.01%	0.0%
6004	1582-09-8	Trifluralin	335	140	1.8E-03	2.8E-01	2.0E+05	0.0	3.5E-06	1.8E-08	1.1E-07	3.1E+03	1.8E+03	4.6E+02	4.4E-01	2.5E+03	-6.58	-6.34	-7.51	-3.49	0.88	0.00%	0.00%	0.0%
6054	175013-18-0	Pyraclostrobin	388	205	1.1E-07	1.3E+00	2.8E+05	0.0	3.5E-06	2.0E-07	1.1E-07	2.7E+02	1.6E+02	4.2E+01	3.9E-02	2.3E+02	-7.67	-7.58	-9.41	-4.68	0.73	0.00%	0.00%	0.0%
6025	1897-45-6	Chlorothalonil	266	132	6.3E-05	7.4E-01	4.6E+03	0.0	3.5E-06	2.2E-09	1.1E-07	6.3E+02	3.7E+02	9.6E+01	9.1E-02	5.3E+02	-7.03	-6.90	-7.88	-3.99	0.74	0.00%	0.00%	0.0%
6285	900-95-8	Fentin acetate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	2.4E+01	1.4E+01	3.7E+00	3.5E-03	2.0E+01	-8.26	-8.22	-9.97	-5.19	1.05	0.00%	0.00%	0.0%
6007	9006-42-2	Metiram	276	87	9.9E-03	1.9E+03	3.0E+02	0.0	3.5E-06	1.3E-07	6.6E-09	2.4E+03	1.4E+03	3.7E+02	3.5E-01	2.0E+03	-5.82	-6.15	-7.91	-3.08	1.39	0.00%	0.00%	0.0%
6019	137-26-8	Thiram	240	107	1.5E-03	3.9E+02	5.0E+01	-2.0	3.5E-06	2.4E-08	3.5E-07	9.3E+02	5.4E+02	1.4E+02	1.3E-01	7.8E+02	-6.48	-6.93	-8.13	-3.82	1.10	0.01%	0.00%	0.0%
6287	668-34-8	Fentin	350	94	7.9E-03	2.5E-02	3.8E+06	0.0	3.5E-06	2.6E-08	1.1E-08	2.4E+01	1.4E+01	3.7E+00	3.5E-03	2.0E+01	-6.10	-8.12	-9.40	-4.96	1.43	0.00%	0.00%	0.0%
6032	7440-50-8	Copper	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	4.8E+02	2.8E+02	7.3E+01	7.0E-02	4.0E+02	-6.96	-6.92	-8.67	-3.74	0.70	0.00%	0.00%	0.0%
6020	137-30-4	Ziram	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	7.7E+02	4.5E+02	1.2E+02	1.1E-01	6.5E+02	-6.76	-6.71	-8.47	-3.45	0.75	0.00%	0.00%	0.0%
6028	74070-46-5	Aclonifen	265	160	3.8E-04	2.4E+01	7.6E+03	0.0	3.5E-06	4.2E-09	1.1E-07	5.5E+02	3.2E+02	8.4E+01	7.9E-02	4.6E+02	-7.13	-6.98	-7.98	-3.71	1.03	0.00%	0.00%	0.0%
6291	13121-70-5	Cyhexatin	385	141	2.7E-07	2.4E-02	4.3E+06	0.0	3.5E-06	5.2E-09	3.5E-07	2.4E+01	1.4E+01	3.6E+00	3.4E-03	2.0E+01	-8.59	-8.88	-9.77	-5.55	0.68	0.00%	0.00%	0.0%
6310	115-29-7	Endosulfan	407	166	1.7E-04	7.6E-02	3.2E+03	0.0	3.5E-06	3.5E-08	3.5E-08	1.5E+01	8.5E+00	2.2E+00	1.2E-01	8.3E+00	-8.39	-8.37	-9.72	-5.04	1.24	0.00%	0.00%	0.0%
6062	82-68-8	Quintozene	295	119	3.6E-03	4.1E-01	1.1E+05	0.0	3.5E-06	3.5E-08	1.1E-08	2.6E+02	1.5E+02	3.9E+01	3.7E-02	2.1E+02	-7.32	-7.06	-8.42	-3.70	0.84	0.00%	0.00%	0.0%
6290	13356-08-6	Fenbutatin-oxide	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	2.4E+01	1.4E+01	3.6E+00	3.4E-03	2.0E+01	-8.27	-8.22	-9.98	-4.81	0.80	0.00%	0.00%	0.0%
6350	66230-04-4	Esfenvalerate	420	84	5.5E-06	3.6E-04	5.8E+06	0.0	3.5E-06	2.6E-08	3.5E-07	7.3E+00	4.2E+00	1.1E+00	1.0E-03	6.1E+00	-9.24	-9.45	-10.57	-5.97	1.33	0.00%	0.00%	0.0%
6035	133-06-2	Captan	301	183	3.4E-06	1.2E+02	5.5E+02	-2.0	3.5E-06	8.7E-08	3.5E-08	4.1E+02	2.4E+02	6.3E+01	5.9E-02	3.4E+02	-6.66	-6.95	-8.56	-3.47	0.74	0.00%	0.00%	0.0%
6011	40487-42-1	Pendimethalin	281	148	1.7E-02	1.7E+01	6.6E+04	0.0	3.5E-06	3.1E-09	1.1E-07	1.8E+03	1.0E+03	2.7E+02	2.6E-01	1.5E+03	-6.76	-6.52	-7.50	-3.02	1.07	0.00%	0.00%	0.0%
6059	7758-98-7	Copper sulphate	160	87	9.9E-03	1.1E+03	3.0E+02	0.0	3.5E-06	1.3E-07	6.6E-09	2.6E+02	1.5E+02	3.9E+01	3.7E-02	2.2E+02	-6.80	-7.12	-8.88	-3.59	0.82	0.00%	0.00%	0.0%
6005	542-75-6	1,3-Dichloropropene	111	-73	3.0E+03	4.9E+03	1.9E+02	0.0	3.5E-06	1.2E-07	3.5E-08	2.8E+03	1.6E+03	4.2E+02	4.0E-01	2.3E+03	-5.76	-6.17	-7.90	-2.61	0.51	0.00%	0.00%	0.0%
6157	5598-13-0	Chlorpyrifos-Methyl	323	84	9.6E-03	1.5E+00	1.3E+04	0.0	3.5E-06	1.5E-08	3.5E-07	7.9E+01	4.6E+01	1.2E+01	1.1E-02	6.6E+01	-8.15	-8.17	-9.25	-4.58	1.59	0.00%	0.00%	0.0%
6014	1332-40-7	Copper oxychloride	249	87	9.9E-03	1.7E+03	3.0E+02	0.0	3.5E-06	1.3E-07	6.6E-09	1.3E+03	7.3E+02	1.9E+02	1.8E-01	1.1E+03	-6.11	-6.43	-8.20	-2.84	1.17	0.00%	0.00%	0.0%
6274	131807-57-3	Famoxadone	374	254	1.3E-09	2.1E+00	7.8E+04	0.0	3.5E-06	8.6E-09	3.5E-07	3.0E+01	1.7E+01	4.6E+00	4.3E-03	2.5E+01	-8.44	-8.63	-9.61	-4.99	0.49	0.00%	0.00%	0.0%
6220	86-50-0	Azinphos-methyl	317	88	1.8E-05	1.6E+01	3.4E+02	0.0	3.5E-06	1.1E-08	3.5E-07	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-7.97	-8.19	-9.25	-4.50	1.30	0.00%	0.00%	0.0%
6010	34256-82-1	Acetochlor	270	128	3.7E-03	8.7E+02	2.3E+03	0.0	3.5E-06	5.0E-08	1.1E-07	1.9E+01	1.1E+01	2.8E+00	2.7E-03	1.6E+01	-6.53	-6.48	-7.90	-2.78	0.68	0.00%	0.00%	0.0%
6077	55283-68-6	Ethalfluralin	333	142	2.0E-03	6.4E-01	1.7E+05	0.0	3.5E-06	3.0E-08	1.1E-07	1.8E+02	1.1E+02	2.8E+01	2.6E-02	1.5E+02	-7.82	-7.58	-8.85	-3.88	0.91	0.00%	0.00%	0.0%
6351	52918-63-5	Deltamethrin	505	140	1.2E-06	9.8E-03	1.5E+06	0.0	3.5E-06	3.9E-08	3.5E-07	7.3E+00	4.2E+00	1.1E+00	1.0E-03	6.1E+00	-9.25	-9.41	-10.65	-5.71	1.59	0.00%	0.00%	0.0%
6161	13071-79-9	Terbufos	288	14	2E-02	2.3E+00	3.1E+04	0.0	3.5E-06	1.1E-08	1.1E-06	7.4E+01	4.3E+01	1.1E+01	1.1E-02	6.2E+01	-8.22	-8.61	-9.51	-4.90	1.09	0.00%	0.00%	0.0%
6039	91315-15-0	Aldimorph	284	103	4.9E-03	2.7E-03	7.8E+05	0.0	3.5E-06	3.5E-07	1.1E-07	4.0E+02	2.3E+02	6.0E+01	5.7E-02	3.3E+02	-7.49	-7.58	-9.64	-3.86	0.36	0.00%	0.00%	0.0%
6356	28434-01-7	Bioresmethrin	338	146	7.1E-04	2.8E-01	1.3E+07	0.0	3.5E-06	5.2E-08	3.5E-07	7.3E+00	4.2E+00	1.1E+00	1.0E-03	6.1E+00	-9.28	-9.51	-10.79	-5.78	1.35	0.00%	0.00%	0.0%
6198	22224-92-6	Fenamiphos	303	85	1.2E-03	2.2E+01	1.9E+03	0.0	3.5E-06	7.7E-08	1.1E-07	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-8.06	-8.01	-9.57	-4.27	0.97	0.00%	0.00%	0.0%
6353	67375-30-8	Alpha-cypermethrin	416	82	1.7E-05	5.9E-02	2.4E+06	0.0	3.5E-06	3.9E-08	3.5E-07	7.3E+00	4.2E+00	1.1E+00	1.0E-03	6.1E+00	-9.26	-9.43	-10.66	-5.68	1.35	0.00%	0.00%	0.0%
6033	79622-59-6	Fluazinam	465	191	7.3E-06	1.4E-01	1.0E+04	6.2	3.5E-06	1.5E-08	1.1E-07	4.5E+02	2.6E+02	6.8E+01	6.4E-02	3.7E+02	-7.79	-7.74	-8.71	-3.96	0.75	0.00%	0.00%	0.0%
6343	82657-04-3	Bifenthrin	423	167	5.2E-05	7.1E-03	1.4E+08	0.0	3.5E-06	2.0E-07	3.5E-07	7.3E+00	4.2E+00	1.1E+00	1.1E-03	6.1E+00	-9.33	-9.76	-11.38	-5.98	1.26	0.00%	0.00%	0.0%
6333	68359-37-5	Beta-Cyfluthrin	434	93	5.6E-05	1.2E-02	5.5E+05	0.0	3.5E-06	1.1E-06	1.1E-07	9.3E+00	5.4E+00	1.4E+00	1.4E-03	7.8E+00	-9.74	-9.52	-11.92	-5.70	1.15	0.00%	0.00%	0.0%
6289	41083-11-8	Azocyclotin	436	154	5.2E-06	8.8E-01	2.5E+05	0.0	3.5E-06	4.8E-09	3.5E-07	2.4E+01	1.4E+01	3.6E+00	3.4E-03	2.0E+01	-8.65	-8.78	-9.71	-4.96	1.06	0.00%	0.00%	0.0%
6200	944-22-9	Fonofos	246	1	7.3E-02	1.1E+01	1.0E+04	0.0	3.5E-06	1.0E-08	1.1E-07	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-8.15	-7.97	-9.06	-4.15	1.09	0.00%	0.00%	0.0%
6013	1912-24-9	Atrazine	216	114	3.8E-03	1.5E+01	6.6E+02	1.7	3.5E-06	2.2E-09	1.1E-07	1.3E+03	7.6E+02	2.0E+02	1.9E-01	1.1E+03	-6.49	-6.55	-7.54	-2.72	1.13	0.00%	0.00%	0.0%
6282	76-87-9	Fentin hydroxide	367	131	1E-06	1.6E+02	3.0E+03	0.0	3.5E-06	3.4E-09	1.1E-08	2.4E+01	1.4E+01	3.7E+00	3.5E-03	2.0E+01	-7.75	-8.02	-9.03	-4.18	1.20	0.00%	0.00%	0.0%
6081	33629-47-9	Butralin	295	148	7.4E-04	2.5E+00	1.4E+05	0.0	3.5E-06	2.2E-09	1.1E-07	1.8E+02	1.1E+02	2.8E+01	2.6E-02	1.5E+02	-7.78	-7.53	-8.50	-3.70	0.91	0.00%	0.00%	0.0%
6209	298-02-2	Phorate	260	-2	9.4E-02	1.6E+01	4.2E+03	0.0	3.5E-06	1.1E-08	1.1E-06	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-8.31	-8.65	-9.57	-4.81	1.15	0.00%	0.00%	0.0%
6042	731-27-1	Tolylfluanid	347	151	2.4E-04	2.2E+00	1.9E+03	0.0	3.5E-06	2.2E-08	3.5E-07	3.8E+02	2.2E+02	5.8E+01	5.5E-02	3.2E+02	-7.38	-7.44	-8.61	-3.60	0.65	0.00%	0.00%	0.0%
6049	131860-33-8	Azoxystrobin	403	228	6.6E-08	2.3E+00	3.8E+01	0.0	3.5E-06	1.0E-07	1.1E-07	2.8E+02	1.6E+02	4.3E+01	4.1E-02	2.4E+02	-6.81	-7.26	-8.92	-3.35	0.47	0.00%	0.00%	0.0%
6193	2642-71-9	Azinphos-ethyl	345	90	7.3E-06	2.5E+00	3.2E+03	-0.4	3.5E-06	1.0E-08	1.1E-06	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-8.24	-8.63	-9.54	-4.69	1.38	0.00%	0.00%	0.0%
6204	56-38-2	Parathion	291	89	4.5E-03	1.5E+01	5.4E+03	0.0	3.5E-06	1.1E-08	3.5E-07	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-8.25	-8.28	-9.33	-4.33	1.49	0.00%	0.00%	0.0%
6143	29232-93-7	Pirimiphos-Methyl	305	90	5.0E-03	1.1E+01	1.6E+04	0.0	3.5E-06	2.6E-08	3.5E-07	1.1E+02	6.3E+01	1.6E+01	1.6E-02	9.0E+01	-8.02	-8.05	-9.24	-4.10	1.47	0.00%	0.00%	0.0%
6017	5915-41-3	Terbuthylazine	230	123	2.1E-03	9.2E-01	1.9E+03	0.0	3.5E-06	2.5E-09	1.1E-07	1.1E+03	6.4E+02	1.7E+02	1.6E-01	9.2E+02	-6.70	-6.64	-7.62	-2.68	1.16	0.00%	0.00%	0.0%
6118	10380-28-6	Oxine-copper	352	87	9.9E-03	2.4E+03	3.0E+02	0.0	3.5E-06	1.3E-07	6.6E-09	1.3E+02	7.8E+01	2.0E+01	1.9E-02	1.1E+02	-7.08	-7.40	-9.17	-3.43	1.06	0.00%	0.00%	0.0%
6184	10311-84-9	Dialifos	394	90	4.6E-06	1.8E+00	1.4E+04	-1.0	3.5E-06	1.1E-06	3.5E-07	5.8E+01	3.4E+01	8.8E+00	8.4E-03	4.8E+01	-8.80	-8.95	-11.20	-4.96	1.38	0.00%	0.00%	0.0%
6008	133-07-3	Folpet	297	189	1.9E-06	3.0E+00	6.9E+02	-2.0	3.5E-06	2.6E-07	1.1E-06	2.3E+03	1.3E+03	3.5E+02	3.3E-01	1.9E+03	-6.74	-7.25	-8.93	-3.25	1.00	0.00%	0.00%	0.0%
6208	3689-24-5	Sulfotep	322	-32	1.9E-02	6.1E+00	9.5E+03	0.0	3.5E-06	3.5E-07	3.5E-07	5.8E+01	3.4E+01	8.8E+00	8.4E-03	4.8E+01	-8.57	-8.61	-10.57	-4.60	1.38	0.00%	0.00%	0.0%
6044	13181-17-4	Bromofenoxim	461	221	3E-09	8.1E-01	3.5E+03	5.1	3.5E-06	6.5E-08	1.1E-07	3.6E+02	2.1E+02	5.5E+01	5.2E-02	3.0E+02	-7.19	-7.31	-8.78	-3.27	0.52	0.00%	0.00%	0.0%
6196	23560-59-0	Heptenophos	251	72	1.2E-01	1.7E+03	2.6E+01	0.0	3.5E-06	5.9E-08	1.1E-07	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-7.55	-7.91	-9.38	-3.85	1.01	0.00%	0.00%	0.0%
6347	39515-41-8	Fenpropathrin	349	64	4.2E-04	5.7E-01	4.2E+05	0.0	3.5E-06	3.8E-08	3.5E-07	7.3E+00	4.2E+00	1.1E+00	1.0E-03	6.1E+00	-9.27	-9.37	-10.60	-5.31	1.16	0.00%	0.00%	0.0%
6213	300-76-5	Naled	381	76	5.6E-02	4.1E+01	4.0E+01	0.0	3.5E-06	2.6E-08	1.1E-07	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-7.54	-7.87	-9.14	-3.80	1.29	0.00%	0.00%	0.0%
6052	117428-22-5	Picoxystrobine	367	150	6.0E-05	4.9E+00	4.7E+03	-1.1	3.5E-06	1.1E-06	3.5E-07	2.7E+02	1.6E+02	4.2E+01	3.9E-02	2.3E+02	-8.24	-10.53	-11.53	-4.16	0.42	0.00%	0.00%	0.0%
6344	51630-58-1	Fenvalerate	420	84	5.5E-06	3.6E-04	5.8E+06	0.0	3.5E-06	2.6E-08	3.5E-07	7.3E+00	4.2E+00	1.1E+00	1.0E-03	6.1E+00	-9.24	-9.45	-10.57	-5.36	1.20	0.00%	0.00%	0.0%
6354	10453-86-8	Resmethrin	338	146	7.1E-04	2.8E-01	1.3E+07	0.0	3.5E-06	5.2E-08	3.5E-07	7.3E+00	4.2E+00	1.1E+00	1.0E-03	6.1E+00	-9.28	-9.51	-10.79	-5.42	0.92	0.00%	0.00%	0.0%
6178	470-90-6	Chlorfenvinphos	360	86	1.3E-03	1.8E+00	1.4E+04	0.0	3.5E-06	1.3E-08	1.1E-07	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-8.18	-7.98	-9.11	-3.88	1.52	0.00%	0.00%	0.0%
6341	91465-08-6	Lambda-Cyhalothrin	450	69	8.5E-05	1.4E-02	7.1E+06	0.0	3.5E-06	1.1E-06	3.5E-07	7.6E+00	4.4E+00	1.2E+00	1.1E-03	6.4E+00	-9.82	-10.07	-12.20	-5.96	1.34	0.00%	0.00%	0.0%
6015	52888-80-9	Prosulfocarb	251	117	6.4E-03	1.4E+01	1.7E+04	-0.6	3.5E-06	2.1E-07	3.5E-07	1.2E+03	6.9E+02	1.8E+02	1.7E-01	1.0E+03	-7.18	-7.21	-9.00	-3.09	0.50	0.00%	0.00%	0.0%
6101	136426-54-5	Fluquinconazole	376	218	3.8E-08	7.5E-02	5.4E+03	0.0	3.5E-06	2.4E-08	3.5E-08	1.5E+02	8.6E+01	2.2E+01	2.1E-02	1.2E+02	-7.35	-7.35	-8.60	-3.18	0.69	0.00%	0.00%	0.0%
6016	15972-60-8	Alachlor	270	128	2.7E-03	1.7E+02	2.3E+03	0.0	3.5E-06	7.1E-08	1.1E-07	1.2E+03	6.8E+02	1.8E+02	1.7E-01	9.8E+02	-6.77	-6.70	-8.23	-2.49	0.72	0.00%	0.00%	0.0%
6012	87392-12-9	S-Metolachlor	284	136	6.7E-01	2.2E+02	1.7E+03	-1.0	3.5E-06	6.8E-08	1.1E-07	1.6E+03	9.1E+02	2.4E+02	2.2E-01	1.3E+03	-6.61	-6.57	-8.08	-2.34	1.04	0.00%	0.00%	0.0%
6009	67129-08-2	Metazachlor	278	164	1.5E-04	8.7E+01	2.4E+02	0.0	3.5E-06	6.3E-08	1.1E-07	1.9E+03	1.1E+03	2.9E+02	2.7E-01	1.6E+03	-6.24	-6.44	-7.93	-2.20	1.04	0.00%	0.00%	0.0%
6072	138261-41-3	Imidacloprid	256	162	2.4E-04	2.1E+03	3.6E+03	1.0	3.5E-06	6.3E-08	1.1E-07	2.2E+02	1.3E+02	3.4E+01	3.2E-02	1.9E+02	-6.80	-7.29	-8.79	-3.05	1.78	0.00%	0.00%	0.0%
6038	24602-86-6

6235	18691-97-9	Methabenthiazuron	221	165	1.4E-04	3.1E+02	4.5E+02	0.0	3.5E-06	5.7E-08	1.1E-07	5.8E+01	3.3E+01	8.8E+00	8.3E-03	4.8E+01	-7.77	-7.95	-9.41	-2.78	1.42	0.00%	0.00%	0.0%
6229	1929-88-0	Benzthiazuron	207	160	8.9E-05	7.4E+02	1.3E+02	0.0	3.5E-06	5.0E-09	1.1E-07	5.8E+01	3.3E+01	8.8E+00	8.3E-03	4.8E+01	-7.52	-7.86	-8.88	-2.68	0.93	0.00%	0.00%	0.0%
6060	87674-68-8	Dimethenamid	276	139	4.0E-03	7.1E+03	3.7E+02	0.0	3.5E-06	1.2E-07	3.5E-07	2.6E+02	1.5E+02	3.9E+01	3.7E-02	2.2E+02	-7.44	-7.67	-9.32	-2.48	0.63	0.00%	0.00%	0.0%
6058	57018-04-9	Tolclofos-methyl	301	33	8.5E-03	1.5E+00	5.9E+04	0.0	3.5E-06	1.3E-08	3.5E-07	2.2E+02	1.5E+02	3.9E+01	3.7E-02	2.2E+02	-7.67	-7.71	-8.77	-2.52	1.01	0.00%	0.00%	0.0%
6003	94-75-7	2,4-D	221	109	3.7E-03	5.0E+02	4.2E+02	3.0	3.5E-06	7.5E-08	3.5E-07	3.3E+03	1.9E+03	5.1E+02	4.8E-01	2.8E+03	-6.37	-6.52	-8.01	-1.29	0.93	0.00%	0.00%	0.0%
6194	7786-34-7	Mevinphos	224	28	4.7E-01	1.6E+04	5.8E+00	0.0	3.5E-06	3.5E-06	1.1E-06	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-8.88	-9.52	-11.85	-4.29	1.04	0.00%	0.00%	0.0%
6133	23135-22-0	Oxamyl	219	95	7.8E-03	1.9E+04	6.3E-02	-2.0	3.5E-06	1.7E-07	3.5E-07	1.2E+02	6.8E+01	1.8E+01	1.7E-02	9.7E+01	-7.09	-7.82	-9.63	-2.59	0.62	0.00%	0.00%	0.0%
6134	17804-35-2	Benomyl	290	222	8.1E-08	3.8E+02	1.7E+02	3.0	3.5E-06	7.1E-08	3.5E-07	1.1E+02	6.6E+01	1.7E+01	1.6E-02	9.5E+01	-7.59	-7.94	-9.41	-2.70	0.96	0.00%	0.00%	0.0%
6083	60207-90-1	Propiconazole	342	173	4.8E-04	3.7E+00	1.3E+04	0.0	3.5E-06	5.6E-09	3.5E-07	1.8E+02	1.0E+02	2.7E+01	2.5E-02	1.5E+02	-7.79	-7.82	-8.79	-2.57	0.76	0.00%	0.00%	0.0%
6195	298-04-4	Disulfoton	274	7	4.7E-02	1.3E+01	1.2E+04	0.0	3.5E-06	9.9E-09	1.1E-06	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-8.33	-8.68	-9.57	-3.42	1.18	0.00%	0.00%	0.0%
6255	63-25-2	Carbaryl	201	91	7.1E-03	9.0E+01	2.2E+02	12.2	3.5E-06	3.8E-08	1.1E-07	4.3E+01	2.5E+01	6.1E-03	5.8E-02	3.5E+01	-8.62	-8.42	-9.68	-3.14	1.21	0.00%	0.00%	0.0%
6192	24934-91-6	Chlormephos	235	-25	5.1E-01	8.3E+01	1.1E+03	0.0	3.5E-06	1.7E-08	1.1E-06	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-8.28	-8.61	-9.61	-3.32	0.85	0.00%	0.00%	0.0%
6342	886-50-0	Terbutryn	241	140	3.1E-03	1.6E+01	5.9E+03	0.0	3.5E-06	2.2E-09	1.1E-07	7.5E+00	4.4E+00	1.1E+00	1.1E-03	6.3E+00	-8.98	-8.84	-9.81	-3.53	1.12	0.00%	0.00%	0.0%
6128	7287-36-7	Monalide	240	139	1.4E-03	6.9E+00	1.2E+04	-0.1	3.5E-06	1.1E-06	3.5E-07	1.2E+02	7.1E+01	1.9E+01	1.8E-02	1.0E+02	-8.60	-8.63	-10.90	-3.32	0.44	0.00%	0.00%	0.0%
6328	1420-07-1	Dinoterb	240	139	1.4E-04	2.1E+02	4.4E+03	4.2	3.5E-06	1.1E-07	3.5E-07	1.2E+01	7.0E+00	1.8E+00	1.8E-03	1.0E+01	-8.38	-9.29	-11.74	-3.99	1.29	0.00%	0.00%	0.0%
6320	58138-08-2	Tridiphane	320	107	5.2E-02	6.1E-01	1.5E+05	0.0	3.5E-06	3.5E-08	1.1E-08	1.2E+01	7.0E+00	1.8E+00	1.7E-03	1.0E+01	-8.58	-8.39	-9.75	-3.07	0.81	0.00%	0.00%	0.0%
6168	111479-05-1	Propaquizafop	444	228	2.2E-07	2.1E-01	3.9E+04	0.0	3.5E-06	1.2E-07	3.5E-07	6.3E+01	3.7E+01	9.6E+00	9.1E-03	5.3E+01	-8.31	-8.43	-10.01	-3.10	0.84	0.00%	0.00%	0.0%
6139	21725-46-2	Cyanazine	241	152	2.0E-04	6.8E+00	3.2E+02	0.0	3.5E-06	2.2E-09	1.1E-07	6.5E+01	1.7E+01	1.6E-02	9.4E+01	-7.65	-7.60	-8.59	-2.27	0.99	0.00%	0.00%	0.0%
6140	1912-26-1	Trietazine	230	120	1.4E-02	1.2E+01	2.8E+03	0.0	3.5E-06	1.4E-08	3.5E-07	1.1E+02	6.5E+01	1.7E+01	1.6E-02	9.4E+01	-7.93	-7.97	-9.06	-2.64	1.16	0.00%	0.00%	0.0%
6094	66246-88-6	Penconazole	284	132	4.8E-03	2.8E+00	4.7E+04	0.0	3.5E-06	1.2E-07	1.1E-07	1.5E+02	8.6E+01	2.3E+01	2.1E-02	1.2E+02	-7.96	-7.73	-9.42	-2.40	0.69	0.00%	0.00%	0.0%
6189	95465-99-9	Cadusafos	270	33	4.5E-02	5.5E+00	9.5E+03	0.0	3.5E-06	5.7E-09	1.1E-06	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-8.32	-8.68	-9.54	-3.34	1.36	0.00%	0.00%	0.0%
6245	50594-66-6	Acifluorfen	362	186	5.3E-06	1.0E+00	1.5E+04	2.2	3.5E-06	3.5E-07	1.1E-07	5.2E+01	3.0E+01	7.9E+00	7.5E-03	4.3E+01	-8.52	-8.34	-10.40	-2.99	1.01	0.00%	0.00%	0.0%
6097	83657-24-3	Diniconazole	326	170	6.0E-07	7.7E+00	8.3E+03	1.0	3.5E-06	8.4E-09	1.1E-07	1.5E+02	8.6E+01	2.2E+01	2.1E-02	1.2E+02	-7.61	-7.55	-8.61	-2.17	0.69	0.00%	0.00%	0.0%
6228	1746-81-2	Monolinuron	215	118	5.9E-03	2.1E+02	1.8E+02	0.0	3.5E-06	2.2E-09	1.1E-07	5.8E+01	3.3E+01	8.8E+00	8.3E-03	4.8E+01	-7.69	-7.87	-8.85	-2.49	1.02	0.00%	0.00%	0.0%
6301	67564-91-4	Fenpropimorph	303	121	5.9E-03	6.1E+00	3.2E+05	0.0	3.5E-06	1.1E-06	3.5E-07	5.3E+02	3.1E+02	8.3E+01	7.7E-02	4.5E+02	-8.01	-8.11	-10.31	-2.72	0.71	0.00%	0.00%	0.0%
6311	156-29-74	Tetradifon	356	174	1.3E-05	2.4E-02	1.5E+05	0.0	3.5E-06	2.2E-09	3.5E-09	1.5E+01	8.5E+00	2.2E+00	2.1E-03	1.2E+01	-8.30	-8.22	-9.22	-2.83	0.81	0.00%	0.00%	0.0%
6318	68049-83-2	Azafenidin	338	188	2.6E-06	5.8E+00	6.5E+04	0.0	3.5E-06	1.1E-06	3.5E-07	1.2E+01	7.0E+00	1.8E+00	1.7E-03	1.0E+01	-9.51	-9.68	-11.89	-4.28	2.62	0.00%	0.00%	0.0%
6137	101463-69-8	Flufenoxuron	489	258	1.7E-10	6.5E-05	9.3E+05	7.7	3.5E-06	1.9E-08	3.5E-07	8.1E+01	4.7E+01	1.2E+01	1.2E-03	6.7E+01	-8.79	-11.06	-11.01	-5.65	1.70	0.00%	0.00%	0.0%
6084	709-98-8	Propanil	218	131	3.8E-03	3.6E+01	7.6E+02	-1.0	3.5E-06	1.0E-07	1.1E-07	1.6E+02	9.4E+01	2.5E+01	2.3E-02	1.4E+02	-7.53	-7.57	-9.22	-2.14	0.44	0.00%	0.00%	0.0%
6066	3347-22-6	Dithianon	296	219	1.2E-08	2.1E+02	4.4E+02	0.0	3.5E-06	1.1E-08	1.1E-06	2.3E+02	1.4E+02	3.5E+01	3.3E-02	1.9E+02	-7.47	-7.96	-8.90	-2.53	1.36	0.00%	0.00%	0.0%
6241	2303-17-5	Tri-allate	305	96	2.4E-02	4.5E+00	3.7E+04	-1.0	3.5E-06	3.0E-07	3.5E-07	5.7E+01	3.3E+01	8.7E+00	8.2E-03	4.8E+01	-8.59	-8.63	-10.52	-3.19	0.65	0.00%	0.00%	0.0%
6114	60-51-5	Dimethoate	229	86	5.5E-03	4.0E+03	5.2E+00	0.0	3.5E-06	6.9E-08	1.1E-06	1.3E+02	7.8E+01	2.0E+01	1.9E-02	1.1E+02	-7.49	-8.14	-9.53	-2.69	1.35	0.00%	0.00%	0.0%
6211	41198-08-7	Profenofos	374	86	1.0E-03	4.1E-01	6.6E+04	14.0	3.5E-06	3.9E-09	3.5E-07	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-9.98	-9.92	-10.37	-4.45	1.09	0.00%	0.00%	0.0%
6264	114-26-1	Propoxur	209	69	1.1E-01	7.8E+02	7.9E+01	12.2	3.5E-06	9.7E-09	3.5E-07	4.3E+01	2.5E+01	6.5E+00	6.1E-03	3.5E+01	-8.79	-8.60	-9.55	-3.12	1.08	0.00%	0.00%	0.0%
6265	121552-61-2	Cyprodinil	225	127	3.2E-03	2.2E+01	9.8E+02	0.0	3.5E-06	6.4E-09	3.5E-07	3.8E+01	2.2E+01	5.8E+00	5.5E-03	3.2E+01	-8.45	-8.47	-9.45	-2.98	0.71	0.00%	0.00%	0.0%
6309	1085-98-9	Dichlofluanid	333	141	4.0E-04	6.7E+00	5.2E+02	0.0	3.5E-06	2.3E-08	3.5E-07	1.6E+01	9.1E+00	2.4E+00	2.2E-03	1.3E+01	-8.65	-8.79	-9.97	-3.29	1.07	0.00%	0.00%	0.0%
6075	122-34-9	Simazine	202	112	1.2E-03	3.4E+01	2.5E+02	0.0	3.5E-06	2.7E-09	3.5E-07	2.0E+02	1.2E+02	3.1E+01	2.9E-02	1.7E+02	-7.44	-7.62	-8.57	-2.12	1.16	0.00%	0.00%	0.0%
6064	2764-72-9	Diquat	184	95	2.0E-02	9.2E+03	2.1E-01	0.0	3.5E-06	1.1E-06	3.5E-07	2.4E+02	1.4E+02	3.7E+01	3.5E-02	2.0E+02	-7.37	-8.01	-10.44	-2.50	1.22	0.00%	0.00%	0.0%
6270	41483-43-6	Bupirimate	316	179	1.3E-04	5.1E+01	1.4E+02	0.0	3.5E-06	6.7E-08	1.1E-07	3.7E+01	2.1E+01	5.6E+00	5.3E-03	3.1E+01	-8.05	-8.17	-9.68	-2.65	0.36	0.00%	0.00%	0.0%
6236	13360-45-7	Chlorbromuron	294	141	7.8E-04	6.1E+01	1.4E+03	0.0	3.5E-06	2.2E-09	1.1E-07	5.8E+01	3.3E+01	8.8E+00	8.3E-03	4.8E+01	-7.93	-7.92	-8.89	-2.40	0.63	0.00%	0.00%	0.0%
6099	76674-21-0	Flutriafol	301	164	2.7E-06	2.7E+02	3.3E+02	1.0	3.5E-06	2.2E-09	1.1E-07	1.5E+02	8.6E+01	2.2E+01	2.1E-02	1.2E+02	-7.22	-7.46	-8.44	-1.94	0.74	0.00%	0.00%	0.0%
6155	82558-50-7	Isoxaben	332	198	5.7E-07	2.6E+00	9.5E+03	-1.0	3.5E-06	2.3E-07	3.5E-07	8.1E+01	4.7E+01	1.2E+01	1.2E-02	6.7E+01	-8.19	-8.36	-10.16	-2.83	0.65	0.00%	0.00%	0.0%
6057	21087-64-9	Metribuzin	214	150	6.9E-04	2.7E+03	3.1E+01	0.0	3.5E-06	2.7E-08	3.5E-07	2.6E+02	1.5E+02	3.9E+01	3.7E-02	2.2E+02	-7.01	-7.48	-8.71	-1.95	1.03	0.00%	0.00%	0.0%
6244	33089-61-1	Amitraz	293	132	3.5E-04	6.5E-01	3.5E+05	0.0	3.5E-06	3.3E-08	1.1E-07	5.4E+01	3.1E+01	8.2E+00	7.7E-03	4.5E+01	-8.37	-8.13	-9.42	-2.59	0.98	0.00%	0.00%	0.0%
6240	28249-77-6	Thiobencarb	258	122	8.3E-03	1.6E+01	7.9E+03	-1.0	3.5E-06	1.6E-07	3.5E-07	5.7E+01	3.3E+01	8.7E+00	8.2E-03	4.8E+01	-8.43	-8.46	-10.16	-2.92	0.58	0.00%	0.00%	0.0%
6152	35256-85-0	Tebutam	233	96	1.6E-02	2.2E+01	3.1E+03	-0.8	3.5E-06	3.5E-07	3.5E-07	8.1E+01	4.7E+01	1.2E+01	1.2E-02	6.7E+01	-8.38	-8.43	-10.40	-2.89	0.64	0.00%	0.00%	0.0%
6207	121-75-5	Malathion	330	-24	1.7E-02	3.2E+02	1.9E+02	0.0	3.5E-06	1.4E-07	3.5E-06	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-8.43	-9.10	-10.43	-3.55	1.32	0.00%	0.00%	0.0%
6223	555-37-3	Neburon	275	143	3.7E-04	9.3E+00	1.4E+04	-1.6	3.5E-06	3.5E-07	3.5E-07	5.8E+01	3.3E+01	8.8E+00	8.3E-03	4.8E+01	-8.53	-8.62	-10.57	-3.06	1.02	0.00%	0.00%	0.0%
6117	1184-64-1	Copper carbonate	124	87	9.9E-03	5.5E+02	3.0E+02	0.0	3.5E-06	1.3E-07	6.6E-09	1.3E+02	7.8E+01	2.0E+01	1.9E-02	1.1E+02	-7.09	-7.40	-9.17	-1.84	0.64	0.00%	0.00%	0.0%
6300	58810-48-3	Ofurace	282	165	7.3E-06	5.1E+01	2.5E+01	0.0	3.5E-06	3.5E-07	1.1E-07	1.6E+01	9.1E+00	2.4E+00	2.3E-03	1.3E+01	-8.23	-8.71	-10.79	-3.14	0.47	0.00%	0.00%	0.0%
6130	115-32-2	Dicofol	370	148	9.2E-06	9.3E-03	6.5E+05	9.7	3.5E-06	4.4E-09	1.1E-08	1.2E+02	6.8E+01	1.8E+01	1.7E-02	9.8E+01	-9.05	-8.95	-9.59	-3.35	0.61	0.00%	0.00%	0.0%
6119	4685-14-7	Paraquat	186	85	1.3E-02	1.4E+04	2.8E-01	0.0	3.5E-06	3.5E-07	1.1E-07	1.3E+02	7.5E+01	2.0E+01	1.9E-02	1.1E+02	-7.23	-7.73	-9.84	-2.14	1.08	0.00%	0.00%	0.0%
6267	63284-71-9	Nuarimol	315	173	8.2E-07	5.7E+01	1.5E+03	2.0	3.5E-06	2.2E-09	1.1E-08	3.7E+01	2.1E+01	5.6E+00	5.3E-03	3.1E+01	-7.55	-7.83	-8.83	-2.22	0.24	0.00%	0.00%	0.0%
6297	161326-34-7	Fenamidone	311	200	2.5E-07	7.7E-01	2.8E+03	0.0	3.5E-06	2.5E-09	1.1E-06	2.1E+01	1.2E+01	3.1E+00	2.9E-03	1.7E+01	-8.62	-9.07	-9.88	-3.46	0.66	0.00%	0.00%	0.0%
6258	65907-30-4	Furathiocarb	382	155	2.3E-04	3.8E+01	2.7E+04	0.0	3.5E-06	1.1E-06	3.5E-07	4.3E+01	2.5E+01	6.5E+00	6.1E-03	3.6E+01	-9.05	-9.12	-11.37	-3.50	1.48	0.00%	0.00%	0.0%
6112	36734-19-7	Iprodione	330	234	2.8E-08	8.9E+01	7.1E+02	13.0	3.5E-06	9.5E-08	1.1E-06	1.4E+02	8.0E+01	2.1E+01	2.0E-02	1.1E+02	-8.44	-8.14	-9.61	-2.52	0.45	0.00%	0.00%	0.0%
6070	12122-67-7	Zineb	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	2.2E+02	1.3E+02	3.4E+01	3.2E-02	1.9E+02	-7.29	-7.25	-9.01	-1.63	0.92	0.00%	0.00%	0.0%
6095	43121-43-3	Triadimefon	294	149	1.2E-03	8.9E+01	8.7E+02	-1.0	3.5E-06	2.2E-09	3.5E-07	1.5E+02	8.6E+01	2.2E+01	2.1E-02	1.2E+02	-7.66	-7.79	-8.73	-2.17	0.69	0.00%	0.00%	0.0%
6023	26225-79-6	Ethofumesate	286	142	2.8E-03	1.6E+01	7.8E+02	0.0	3.5E-06	1.1E-07	3.5E-07	5.7E+01	3.3E+01	8.7E+00	8.2E-03	4.8E+01	-8.43	-8.46	-10.16	-2.92	0.58	0.00%	0.00%	0.0%
6063	23950-58-5	Propyzamide	256	153	1.4E-04	1.6E+01	3.7E+03	-2.0	3.5E-06	2.4E-08	3.5E-08	2.4E+02	1.4E+02	3.7E+01	3.5E-02	2.0E+02	-7.06	-7.13	-8.38	-1.50	0.74	0.00%	0.00%	0.0%
6141	139-40-2	Propazine	230	116	9.7E-04	6.4E+00	1.7E+03	2.0	3.5E-06	2.2E-09	1.1E-07	1.1E+02	6.5E+01	1.7E+01	1.6E-02	9.4E+01	-7.67	-7.63	-8.61	-2.00	1.05	0.00%	0.00%	0.0%
6137	3878-19-1	Fuberidazole	184	149	6.2E-07	4.5E+02	2.2E+02	3.0	3.5E-06	3.5E-09	3.5E-07	1.1E+02	6.6E+01	1.7E+01	1.6E-02	9.5E+01	-7.56	-7.86	-8.82	-2.21	0.41	0.00%	0.00%	0.0%
6146	15545-48-9	Chlorotoluron	213	119	1.2E-03	2.3E+02	3.8E+02	-1.0	3.5E-06	8.5E-09	1.1E-07	9.4E+01	5.4E+01	1.4E+01	1.3E-02	7.8E+01	-7.49	-7.68	-8.75	-1.99	1.31	0.00%	0.00%	0.0%
6086	85509-19-9	Flusilazole	315	144	2.5E-03	1.7E+00	7.8E+04	0.0	3.5E-06	2.2E-09	3.5E-07	1.5E+02	8.6E+01	2.3E+01	2.1E-02	1.2E+02	-7.90	-7.94	-8.85	-2.25	0.69	0.00%	0.00%	0.0%
6305	55814-41-0	Mepronil	269	171	4.6E-05	3.0E+00	1.7E+04	0.9	3.5E-06	3.5E-07	1.1E-07	1.6E+01	9.1E+00	2.4E+00	2.3E-03	1.3E+01	-9.06	-8.86	-10.92	-3.16	0.49	0.00%	0.00%	0.0%
6246	77501-60-1	Fluorodylcofen	420	209	2.4E-08	2.6E+00	5.2E+03	2.7	3.5E-06	3.5E-07	1.1E-07	5.2E+01	3.0E+01	7.9E+00	7.5E-03	4.3E+01	-8.33	-8.30	-10.37	-2.60	0.97	0.00%	0.00%	0.0%
6037	94-81-5	MCPB	229	118	4.1E-03	1.2E+02	3.2E+03	4.7	3.5E-06	1.1E-06	1.1E-06	4.0E+02	2.3E+02	6.1E+01	5.8E-02	3.3E+02	-8.12	-8.56	-10.51	-2.85	1.17	0.00%	0.00%	0.0%
6262	22259-30-9	Formetanate	221	88	1.3E-03	1.0E+03	7.6E+00	7.6	3.5E-06	1.1E-06	3.5E-07	4.3E+01	2.5E+01	6.5E+00	6.1E-03	3.6E+01	-8.46	-8.83	-11.24	-3.11	1.63	0.00%	0.00%	0.0%
6227	2164-17-2	Fluometuron	232	96	3.8E-03	1.2E+02	2.2E+02	-1.0	3.5E-06	8.8E-09	1.1E-07	5.8E+01	3.3E+01	8.8E+00	8.3E-03	4.8E+01	-7.70	-7.88	-8.96	-2.15	0.80	0.00%	0.00%	0.0%
6041	15299-99-7	Napropamide	271	140	3.9E-04	4.2E+01	3.1E+03	-1.6	3.5E-06	1.1E-06	1.1E-07	3.8E+02	2.2E+02	5.8E+01	5.5E-02	3.2E+02	-7.70	-7.75	-10.19	-2.00	0.39	0.00%	0.00%	0.0%
6174	67747-09-5	Prochloraz	377	213	2.1E-06	1.2E+00	1.3E+04	0.0	3.5E-06	1.8E-07	3.5E-07	6.1E+01	3.5E+01	9.3E+00	8.8E-03	5.1E+01	-8.39	-8.47	-10.21	-2.72	0.69	0.00%	0.00%	0.0%
6187	6923-22-4	Monocrotophos	223	88	3.7E-03	3.5E+04	4.9E-01	11.0	3.5E-06	5.7E-08	1.1E-06	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-7.68	-8.14	-9.57	-2.37	1.06	0.00%	0.00%	0.0%
6026	1698-60-8	Chloridazon	222	155	1.5E-04	1.0E+02	5.8E+00	0.0	3.5E-06	5.2E-08	1.1E-06	6.1E+02	3.5E+02	9.3E+01	8.8E-03	5.1E+02	-6.81	-7.47	-8.78	-1.70	1.04	0.00%	0.00%	0.0%
6043	99105-77-8	Sulcotrione	329	200	1.2E-06	2.8E+02	2.0E+02	3.1	3.5E-06	2.6E-07	3.5E-07	3.7E+02	2.1E+02	5.6E+01	5.3E-02	3.1E+02	-7.33	-7.61	-9.51	-1.84	1.52	0.00%	0.00%	0.0%
6142	49866-87-7	Difenzoquat	249	144	6.5E-05	1.6E-01	5.1E+00	0.0	3.5E-06	1.1E-07	3.5E-08	1.1E+02	6.5E+01	1.7E+01	1.6E-02	9.3E+01	-7.14	-7.52	-9.23	-1.74	1.50	0.00%	0.00%	0.0%
6135	23564-05-8	Thiophanate-methyl	342	185	1.8E-06	1.0E+02	1.3E+01	1.0	3.5E-06	1.4E-08	3.5E-07	1.1E+02	6.6E+01	1.7E+01	1.6E-02	9.5E+01	-7.23	-7.79	-8.90	-2.00	0.72	0.00%	0.00%	0.0%
6205	298-00-0	Parathion-Methyl	263	80	1.5E-02	9.4E+01	5.6E+02	0.0	3.5E-06	1.1E-06	3.5E-07	5.8E+01	3.4E+01	8.8E+00	8.4E-03	4.8E+01	-8.72	-8.85	-11.18	-3.05	1.40	0.00%	0.00%	0.0%
6181	13171-21-6	Phosphamidon	300	83	4.4E-03	1.6E+03	2.4E+01	0.0	3.5E-06	3.5E-07	3.5E-07	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-7.99	-8.42	-10.45	-2.59	1.43	0.00%	0.00%	0.0%
6113	163515-14-8	Dimethenamid-P	276	139	4.0E-03	7.1E+03	3.7E+02	0.0	3.5E-06	1.2E-07	3.5E-07	1.4E+02	7.9E+01	2.1E+01	2.0E-02	1.1E+02	-7.72	-7.95	-9.59	-2.11	0.63	0.00%	0.00%	0.0%
6092	55219-65-3	Triadimenol	296	153	4.4E-06	5.2E+02	8.9E+02	0.0	3.5E-06	4.7E-09	3.5E-07	1.5E+02	8.6E+01	2.2E+01	2.1E-02	1.2E+02	-7.56	-7.79	-8.75	-1.92	0.69	0.00%	0.00%	0.0%
6197	13194-48-4	Ethoprophos	242	42	7.8E-02	5.0E+01	1.4E+03	0.0	3.5E-06	1.1E-06	1.1E-06	5.8E+01	3.4E+01	8.8E+00	8.3E-03	4.8E+01	-8.92	-9.29	-11.33	-3.42	1.22	0.00%	0.00%	0.0%
6022	13684-63-4	Phenmedipham	300	126	8.9E-05	4.1E+00	1.9E+03	12.9	3.5E-06	3.3E-08	3.5E-07	6.7E+02	3.9E+02	1.0E+02	9.6E-02	5.6E+02	-7.87	-7.96	-8.91	-2.07	0.56	0.00%	0.00%	0.0%
6307	156052-68-5	Zoxamide	337	192	3.7E-07	1.5E+00	2.2E+04	12.8	3.5E-06	4.5E-08	3.5E-07	1.6E+01	9.1E+00	2.4E+00	2.3E-03	1.3E+01	-8.65	-9.36	-10.53	-3.44	0.61	0.00%	0.00%	0.0%
6283	2439-01-2	Quinomethionate	234	163	5.1E-05	3.3E+00	2.3E+03	-0.5	3.5E-06	1.1E-06	3.5E-07	2.4E+01	1.4E+01	3.7E+00	3.5E-03	2.0E+01	-9.19	-9.28	-11.57	-3.35	1.38	0.00%	0.00%	0.0%
6138	33693-04-8	Terbumeton	225	127	6.5E-03	8.3E+01	4.0E+03	0.0	3.5E-06	2.2E-09	1.1E-07	1.1E+02	6.5E+01	1.7E+01	1.6E-02	9.4E+01	-7.77	-7.66	-8.64	-1.72	0.27	0.00%	0.00%	0.0%
6093	94361-06-5	Cyproconazole	292	158	7.6E-06	1.2E+02	1.1E+03	1.0	3.5E-06	2.7E-08	3.5E-07	1.5E+02	8.6E+01	2.2E+01	2.1E-02	1.2E+02	-7.79	-7.84	-9.04	-1.90	0.69	0.00%	0.00%	0.0%
6252	13516-27-3	Guazatine	356	216	2.2E-08	1.6E+01	5.1E+02	0.0	3.5E-06	1.1E-

6153	72178-02-0	Fomesafen	439	242	7.8E-10	2.0E+00	2.6E+03	3.0	3.5E-06	4.1E-08	1.1E-07	8.1E+01	4.7E+01	1.2E+01	1.2E-02	6.7E+01	-7.77	-7.82	-9.18	-0.60	0.66	0.00%	0.00%	0.0%
6322	2797-51-5	Quinoclamine	208	126	2.3E-04	4.2E+01	3.2E+01	0.0	3.5E-06	1.1E-06	1.1E-06	1.2E+01	7.0E+00	1.8E+00	1.7E-03	1.0E+01	-9.32	-9.84	-11.96	-2.60	0.14	0.00%	0.00%	0.0%
6191	98886-44-3	Phosthiazate	283	87	7.7E-04	9.5E+01	3.0E+02	0.0	3.5E-06	1.1E-06	1.1E-06	5.8E+01	3.4E+01	8.8E+00	8.4E-03	4.8E+01	-8.83	-9.24	-11.31	-1.98	1.38	0.00%	0.00%	0.0%
6361	841-06-5	Methoprotryne	271	155	1.8E-04	1.6E+02	1.1E+03	0.0	3.5E-06	3.7E-08	1.1E-07	5.4E+00	3.1E+00	8.2E-01	7.8E-04	4.5E+00	-8.93	-8.99	-10.33	-1.73	0.24	0.00%	0.00%	0.0%
6380	824-78-2	Sodium paranitrophenolate	223	87	9.9E-03	1.5E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	3.1E+00	1.8E+00	4.7E-01	4.4E-04	2.6E+00	-9.16	-9.11	-10.87	-1.84	0.64	0.00%	0.00%	0.0%
6232	34014-18-1	Tebuthiuron	228	163	5.8E-05	1.8E+02	6.0E+01	1.0	3.5E-06	5.7E-08	3.5E-07	5.8E+01	3.3E+01	8.8E+00	8.3E-03	4.8E+01	-7.86	-8.20	-9.61	-0.89	0.25	0.00%	0.00%	0.0%
6370	80-33-1	Chlorfenson	303	149	2.5E-04	5.0E+00	1.6E+04	0.0	3.5E-06	2.2E-09	3.5E-08	3.1E+00	1.8E+00	4.8E-01	4.5E-04	2.6E+00	-9.23	-9.02	-10.01	-1.70	0.55	0.00%	0.00%	0.0%
6278	70630-17-0	Metalaxyl-M	279	130	3.8E-03	1.0E+04	5.0E+01	0.0	3.5E-06	9.8E-08	3.5E-07	2.5E+01	1.4E+01	3.7E+00	3.5E-03	2.1E+01	-8.19	-8.60	-10.19	-1.26	0.46	0.00%	0.00%	0.0%
6387	131341-86-1	Fludioxonil	248	143	4.2E-05	1.4E+01	6.8E+03	14.0	3.5E-06	2.9E-09	3.5E-07	2.1E+00	1.2E+00	3.2E-01	3.1E-04	1.8E+00	-9.93	-10.61	-11.19	-3.27	0.24	0.00%	0.00%	0.0%
6250	5902-51-2	Terbacil	217	164	3.7E-05	3.9E+02	5.6E+01	5.0	3.5E-06	3.5E-07	3.5E-07	4.6E+01	2.7E+01	7.0E+00	6.7E-03	3.9E+01	-8.22	-8.56	-10.57	-1.16	0.45	0.00%	0.00%	0.0%
6331	126833-17-8	Fenhexamid	302	188	2.6E-07	1.3E+00	5.2E+03	7.7	3.5E-06	9.8E-09	3.5E-07	1.1E+01	6.5E+00	1.7E+00	1.6E-03	9.4E+00	-8.93	-9.84	-10.50	-2.43	0.80	0.00%	0.00%	0.0%
6332	52315-07-8	Cypermethrin	416	82	1.7E-05	5.9E-02	2.4E+06	0.0	3.5E-06	3.9E-08	3.5E-07	1.1E+01	6.4E+00	1.7E+00	1.6E-03	9.2E+00	-9.08	-9.25	-10.48	-6.11	1.19	0.00%	0.00%	0.0%
6284	126448-41-7	Acidenzolar	196	140	3.1E-04	3.7E+02	2.0E+01	3.4	3.5E-06	3.5E-06	1.1E-06	2.4E+01	1.4E+01	3.7E+00	3.5E-03	2.0E+01	-9.41	-9.94	-12.23	-2.51	0.60	0.00%	0.00%	0.0%
6313	74051-80-2	Sethoxydim	327	161	1.5E-06	4.8E+00	9.8E+03	4.4	3.5E-06	6.4E-08	1.1E-06	1.4E+01	8.0E+00	2.1E+00	2.0E-03	1.2E+01	-8.96	-9.45	-10.68	-1.99	0.97	0.00%	0.00%	0.0%
6271	10004-44-1	Hymexazol	99	67	8.9E-01	3.2E+04	5.8E-01	7.0	3.5E-06	3.5E-07	1.1E-06	3.4E+01	2.0E+01	5.2E+00	4.9E-03	2.8E+01	-8.56	-8.72	-10.70	-1.25	0.88	0.00%	0.00%	0.0%
6371	113136-77-9	Cyclanilide	274	187	1.8E-06	4.8E+01	6.9E+01	3.4	3.5E-06	2.2E-09	3.5E-07	3.1E+00	1.8E+00	4.6E-01	4.4E-04	2.6E+00	-9.10	-9.41	-10.36	-1.88	0.32	0.00%	0.00%	0.0%
6166	76578-12-6	Quizalofop	345	210	5.7E-08	1.6E+01	3.7E+03	-0.3	3.5E-06	1.1E-06	3.5E-07	6.3E+01	3.7E+01	9.6E+00	9.1E-03	5.3E+01	-8.67	-8.86	-11.12	-1.31	0.84	0.00%	0.00%	0.0%
6292	101-21-3	Chlorpropham	214	65	4.5E-01	1.5E+02	2.0E+03	13.2	3.5E-06	1.2E-08	3.5E-07	2.2E+01	1.3E+01	3.4E+00	3.2E-03	1.9E+01	-10.03	-9.89	-10.49	-2.32	0.17	0.00%	0.00%	0.0%
6346	70124-77-5	Flucythrinate	451	75	1.1E-05	3.3E-03	3.6E+06	0.0	3.5E-06	2.6E-08	3.5E-07	7.3E+00	4.2E+00	1.1E+00	1.0E-03	6.1E+00	-9.25	-9.43	-10.56	-6.04	0.77	0.00%	0.00%	0.0%
6352	102851-06-9	Tau-fluvalinate	503	156	2.7E-06	1.1E-03	6.5E+06	0.0	3.5E-06	1.7E-08	3.5E-07	7.3E+00	4.2E+00	1.1E+00	1.0E-03	6.1E+00	-9.24	-9.44	-10.48	-6.05	1.35	0.00%	0.00%	0.0%
6319	39807-15-3	Oxadiargyl	341	186	8.8E-06	8.5E-01	1.3E+04	0.0	3.5E-06	7.8E-09	3.5E-07	1.2E+01	7.0E+00	1.8E+00	1.7E-03	1.0E+01	-8.94	-8.98	-9.98	-1.37	0.81	0.00%	0.00%	0.0%
6349	79538-32-2	Tefluthrin	419	106	4.0E-02	3.4E-02	1.5E+07	0.0	3.5E-06	1.3E-08	3.5E-07	7.3E+00	4.2E+00	1.1E+00	1.0E-03	6.1E+00	-8.97	-9.48	-10.52	-6.39	1.35	0.00%	0.00%	0.0%
6388	78587-05-0	Hexythiazox	353	231	5.8E-08	2.9E+00	3.7E+05	-0.2	3.5E-06	1.1E-06	3.5E-07	1.9E+00	1.1E+00	2.9E-01	2.8E-04	1.6E+00	-10.29	-10.54	-12.70	-2.89	0.90	0.00%	0.00%	0.0%
6408	104040-78-0	Flazasulfuron	407	226	1.8E-08	7.4E+00	1.2E+01	1.7	3.5E-06	1.4E-08	1.1E-07	6.9E-01	4.0E-01	1.0E-01	9.8E-05	5.7E-01	-9.25	-9.75	-10.90	-2.09	1.98	0.00%	0.00%	0.0%
6377	127277-53-6	Prohexadione-calcium	462	87	9.9E-03	3.2E+03	3.0E+02	0.0	3.5E-06	1.3E-07	6.6E-09	3.1E+00	1.8E+00	4.7E-01	4.4E-04	2.6E+00	-8.71	-9.04	-10.81	-1.37	0.77	0.00%	0.00%	0.0%
6359	5234-68-4	Carboxin	235	166	1.7E-04	4.9E+02	3.1E+01	0.0	3.5E-06	2.1E-07	1.1E-06	6.7E+00	3.9E+00	1.0E+00	9.6E-04	5.6E+00	-9.05	-9.64	-11.33	-1.95	0.81	0.00%	0.00%	0.0%
6414	80060-09-9	Diafenthiuron	385	196	1.4E-06	4.2E-02	5.6E+07	1.4	3.5E-06	1.1E-06	1.1E-07	4.0E-02	2.3E-02	6.1E-03	5.8E-06	3.3E-02	-11.89	-12.03	-14.31	-4.30	0.77	0.00%	0.00%	0.0%
6302	57837-19-1	Metalaxyl	279	130	3.8E-03	1.0E+04	5.0E+01	0.0	3.5E-06	9.8E-08	3.5E-07	1.6E+01	9.1E+00	2.4E+00	2.3E-03	1.3E+01	-8.38	-8.80	-10.38	-1.07	0.80	0.00%	0.00%	0.0%
6030	15165-67-0	Dichlorprop-P	235	110	4.5E-03	6.9E+02	1.1E+03	3.0	3.5E-06	1.1E-06	1.1E-06	5.4E+02	3.1E+02	8.1E+01	7.7E-02	4.5E+02	-7.95	-8.32	-10.36	-0.58	0.38	0.00%	0.00%	0.0%
6293	122-42-9	Propham	179	36	6.3E-01	8.5E+02	4.6E+02	13.2	3.5E-06	3.5E-07	3.5E-07	2.2E+01	1.3E+01	3.4E+00	3.2E-03	1.9E+01	-9.77	-9.61	-11.10	-1.84	0.49	0.00%	0.00%	0.0%
6315	55635-13-7	Alloxydim-sodium	345	87	9.9E-03	2.4E+03	3.0E+02	0.0	3.5E-06	1.3E-07	6.6E-09	1.4E+01	8.0E+00	2.1E+00	2.0E-03	1.2E+01	-8.06	-8.39	-10.16	-0.60	0.20	0.00%	0.00%	0.0%
6401	74223-64-6	Metsulfuron-methyl	381	241	3.8E-09	2.6E+01	1.0E+02	4.1	3.5E-06	8.8E-08	3.5E-07	6.9E-01	4.0E-01	1.0E-01	9.9E-05	5.7E-01	-9.77	-10.17	-11.70	-2.36	1.82	0.00%	0.00%	0.0%
6363	123312-89-0	Pymetrozine	217	179	1.8E-06	8.2E+03	7.8E+00	0.0	3.5E-06	2.6E-07	1.1E-07	5.3E+00	3.1E+00	8.1E-01	7.7E-04	4.4E+00	-8.55	-9.10	-11.08	-1.20	0.59	0.00%	0.00%	0.0%
6325	3813-05-6	Benazolin	244	175	6.3E-06	1.1E+03	1.2E+02	2.9	3.5E-06	1.0E-08	3.5E-07	1.2E+01	7.0E+00	1.8E+00	1.7E-03	1.0E+01	-8.53	-8.83	-9.89	-0.90	0.81	0.00%	0.00%	0.0%
6251	314-40-9	Bromacil	261	176	1.5E-05	6.8E+02	4.8E+01	5.1	3.5E-06	1.1E-06	1.1E-06	4.6E+01	2.7E+01	7.0E+00	6.7E-03	3.9E+01	-8.78	-9.29	-11.40	-1.30	0.73	0.00%	0.00%	0.0%
6162	69806-34-4	Haloxyfop	362	176	5.3E-05	8.8E+00	2.4E+03	0.0	3.5E-06	2.2E-09	1.1E-06	7.1E+01	4.1E+01	1.1E+01	1.0E-02	5.9E+01	-8.18	-8.52	-9.33	-0.50	0.84	0.00%	0.00%	0.0%
6404	120923-37-7	Amidosulfuron	369	237	7.1E-09	8.3E+02	5.1E-02	2.0	3.5E-06	4.5E-08	3.5E-07	6.9E-01	4.0E-01	1.0E-01	9.8E-05	5.7E-01	-9.19	-9.92	-11.29	-1.82	2.39	0.00%	0.00%	0.0%
6314	99129-21-2	Clethodim	360	178	3.5E-07	2.1E+00	1.6E+04	4.3	3.5E-06	2.6E-08	1.1E-06	1.4E+01	8.0E+00	2.1E+00	2.0E-03	1.2E+01	-8.88	-9.41	-10.41	-1.31	0.36	0.00%	0.00%	0.0%
6275	77732-09-3	Oxadiyl	278	173	2.3E-05	1.6E+04	2.5E+01	0.0	3.5E-06	3.5E-07	3.5E-07	3.0E+01	1.7E+01	4.6E+00	4.3E-03	2.5E+01	-8.16	-8.69	-10.70	-0.57	0.32	0.00%	0.00%	0.0%
6006	15845-66-6	Fosetyl	110	-11	7.4E+00	5.7E+05	2.0E-01	2.4	3.5E-06	3.5E-06	1.1E-06	2.5E+03	1.4E+03	3.8E+02	3.6E-01	2.1E+03	-7.00	-7.78	-10.18	0.36	1.01	0.00%	0.00%	0.0%
6406	173159-57-4	Foramsulfuron	452	315	4.0E-15	9.8E+02	1.5E-01	0.0	3.5E-06	5.6E-08	1.1E-07	6.9E-01	4.0E-01	1.0E-01	9.8E-05	5.7E-01	-9.15	-9.74	-11.21	-1.59	1.83	0.00%	0.00%	0.0%
6413	126801-58-9	Ethoxysulfuron	398	244	4.5E-09	5.3E+00	1.0E+02	2.0	3.5E-06	2.7E-07	3.5E-07	6.9E-01	4.0E-01	1.0E-01	9.9E-05	5.7E-01	-9.93	-10.32	-12.24	-2.15	1.64	0.00%	0.00%	0.0%
6378	76738-62-0	Paclobutrazol	294	150	2.2E-06	3.9E+01	2.3E+03	1.5	3.5E-06	3.5E-07	3.5E-07	3.1E+00	1.8E+00	4.7E-01	4.4E-04	2.6E+00	-9.69	-9.83	-11.80	-1.65	0.38	0.00%	0.00%	0.0%
6376	16672-87-0	Ethephon	144	35	2.1E-03	2.0E+05	5.6E-01	2.1	3.5E-06	6.4E-09	3.5E-08	3.1E+00	1.8E+00	4.6E-01	4.4E-04	2.6E+00	-8.49	-8.94	-10.00	-0.73	0.33	0.00%	0.00%	0.0%
6288	101205-02-1	Cycloxydim	325	172	5.1E-07	1.4E+01	7.6E+03	4.4	3.5E-06	6.6E-08	1.1E-06	2.4E+01	1.4E+01	3.7E+00	3.5E-03	2.0E+01	-8.65	-9.19	-10.42	-0.97	0.35	0.00%	0.00%	0.0%
6298	68505-69-1	Benfuresate	256	134	8.7E-03	1.7E+02	6.3E+02	0.0	3.5E-06	3.5E-06	1.1E-06	1.9E+01	1.1E+01	2.9E+00	2.8E-03	1.6E+01	-9.78	-10.17	-12.35	-1.94	0.79	0.00%	0.00%	0.0%
6074	24579-73-5	Propamocarb	188	37	3.6E+00	7.0E+04	1.3E+01	9.8	3.5E-06	3.5E-06	1.1E-06	2.2E+02	1.3E+02	3.3E+01	3.1E-02	1.8E+02	-9.15	-9.02	-11.24	-0.76	0.27	0.00%	0.00%	0.0%
6316	149979-41-9	Tepraloxydim	342	173	1.6E-08	3.3E+01	1.8E+03	4.3	3.5E-06	1.1E-06	1.1E-06	1.4E+01	8.0E+00	2.1E+00	2.0E-03	1.2E+01	-9.39	-9.95	-11.90	-1.68	0.79	0.00%	0.00%	0.0%
6364	95266-40-3	Trinexapac-Ethyl	252	147	1.7E-05	4.8E+02	4.3E+00	4.8	3.5E-06	8.6E-08	1.1E-06	3.4E+00	2.0E+00	5.1E-01	4.8E-04	2.8E+00	-9.12	-9.76	-11.23	-1.36	0.92	0.00%	0.00%	0.0%
6399	150315-10-9	Flupyrsulfuron	451	264	1.3E-11	6.7E+00	4.2E+00	-1.3	3.5E-06	1.1E-06	3.5E-07	6.9E-01	4.0E-01	1.0E-01	9.9E-05	5.7E-01	-9.95	-10.62	-13.00	-2.19	1.99	0.00%	0.00%	0.0%
6326	650-51-1	TCA	185	87	9.9E-03	1.3E+03	3.0E+02	14.0	3.5E-06	1.3E-07	6.6E-09	1.2E+01	7.0E+00	1.8E+00	1.7E-03	1.0E+01	-8.56	-8.52	-10.27	-0.07	1.02	0.00%	0.00%	0.0%
6334	83121-18-0	Teflubenzuron	381	219	1.3E-08	1.3E-02	4.4E+04	8.7	3.5E-06	3.5E-07	1.1E-07	8.1E+00	4.7E+00	1.2E+00	1.2E-03	6.8E+00	-9.48	-10.43	-11.74	-1.86	1.70	0.00%	0.00%	0.0%
6367	29104-30-1	Benzoximate	364	163	5.4E-05	8.8E-01	1.6E+04	0.0	3.5E-06	1.1E-06	3.5E-07	3.1E+00	1.8E+00	4.8E-01	4.5E-04	2.6E+00	-10.19	-10.23	-12.50	-1.61	0.21	0.00%	0.00%	0.0%
6397	82097-50-5	Triasulfuron	402	249	7.4E-10	5.1E+00	2.8E+02	4.6	3.5E-06	2.6E-08	3.5E-07	6.9E-01	4.0E-01	1.0E-01	9.8E-05	5.7E-01	-9.81	-10.14	-11.33	-1.51	1.32	0.00%	0.00%	0.0%
6412	101200-48-0	Tribenuron-methyl	395	246	3.5E-09	9.0E+00	3.5E+02	4.1	3.5E-06	7.1E-08	3.5E-07	6.9E-01	4.0E-01	1.0E-01	9.9E-05	5.7E-01	-9.89	-10.19	-11.65	-1.55	0.95	0.00%	0.00%	0.0%
6400	113036-87-6	Primisulfuron	454	256	4.9E-11	2.6E-01	3.6E+01	2.0	3.5E-06	3.5E-06	1.1E-06	6.9E-01	4.0E-01	1.0E-01	1.0E-04	5.7E-01	-10.86	-11.49	-13.73	-2.82	1.50	0.00%	0.00%	0.0%
6330	27314-13-2	Norflurazon	304	159	9.5E-05	2.0E+01	1.5E+02	0.0	3.5E-06	3.5E-06	3.5E-06	1.2E+01	6.8E+00	1.8E+00	1.7E-03	9.9E+00	-10.01	-10.74	-12.59	-2.06	0.20	0.00%	0.00%	0.0%
6391	66215-27-8	Cyromazine	166	141	1.5E-04	7.9E+04	9.1E+00	0.0	3.5E-06	1.1E-07	3.5E-07	1.9E+00	1.1E+00	2.9E-01	2.8E-04	1.6E+00	-9.06	-9.67	-11.31	-0.97	1.70	0.00%	0.00%	0.0%
6407	111991-09-4	Nicosulfuron	410	266	2.6E-10	1.8E+03	7.1E-02	1.7	3.5E-06	1.3E-07	1.1E-07	6.9E-01	4.0E-01	1.0E-01	9.9E-05	5.7E-01	-9.22	-9.81	-11.55	-1.10	1.32	0.00%	0.00%	0.0%
6323	75-99-0	Dalapon	143	23	8.9E+01	7.5E+04	4.8E+01	1.6	3.5E-06	3.5E-07	3.5E-07	1.2E+01	7.0E+00	1.8E+00	1.7E-03	1.0E+01	-8.77	-9.12	-11.14	-0.40	0.89	0.00%	0.00%	0.0%
6368	18181-80-1	Bromopropylate	428	170	9.0E-07	5.4E-01	7.9E+04	9.9	3.5E-06	1.1E-06	3.5E-07	3.1E+00	1.8E+00	4.8E-01	4.5E-04	2.6E+00	-10.46	-11.58	-12.68	-2.84	0.60	0.00%	0.00%	0.0%
6411	141776-32-1	Sulfosulfuron	470	318	6.5E-14	7.3E-01	9.8E+00	-1.0	3.5E-06	1.3E-08	1.1E-07	6.9E-01	4.0E-01	1.0E-01	9.8E-05	5.7E-01	-9.21	-9.75	-10.88	-0.99	1.32	0.00%	0.00%	0.0%
6382	122-88-3	4-CPA	187	89	6.5E-03	2.2E+03	9.3E+01	3.1	3.5E-06	1.1E-06	3.5E-07	3.1E+00	1.8E+00	4.7E-01	4.4E-04	2.6E+00	-9.79	-10.07	-12.43	-1.32	0.62	0.00%	0.00%	0.0%
6339	103055-07-8	Lufenuron	511	232	1.1E-08	3.4E-05	4.1E+06	7.5	3.5E-06	2.5E-08	1.1E-07	8.1E+00	4.7E+00	1.2E+00	1.2E-03	6.7E+00	-10.65	-11.18	-11.12	-2.42	1.70	0.00%	0.00%	0.0%
6415	71751-41-2	Abamectin	873	350	1.4E-28	3.3E-04	2.5E+04	12.8	3.5E-06	1.5E-07	1.1E-06	1.9E-02	1.1E-02	2.9E-03	2.8E-06	1.6E-02	-13.37	-13.34	-14.11	-4.57	1.69	0.00%	0.00%	0.0%
6294	1967-16-4	Chlorbufam	224	88	1.4E-01	9.5E+00	1.0E+03	13.2	3.5E-06	1.1E-06	3.5E-07	2.2E+01	1.3E+01	3.4E+00	3.2E-03	1.9E+01	-10.60	-10.58	-11.55	-1.77	0.18	0.00%	0.00%	0.0%
6375	15302-91-7	Mepiquat	114	123	1.7E-03	2.8E+05	1.5E-01	0.0	3.5E-06	1.1E-06	1.1E-07	3.1E+00	1.8E+00	4.7E-01	4.4E-04	2.6E+00	-9.07	-9.67	-12.18	-0.73	0.96	0.00%	0.00%	0.0%
6395	135990-29-3	Trifloxsulphuron	478	275	5.5E-11	8.1E+00	1.3E+03	2.0	3.5E-06	3.5E-06	1.1E-06	8.1E-01	4.7E-01	1.2E-01	1.2E-04	6.8E-01	-11.02	-11.55	-13.67	-2.61	1.45	0.00%	0.00%	0.0%
6381	123-33-1	Maleic hydrazide	112	150	4.9E-06	2.0E+05	1.3E-01	5.7	3.5E-06	2.2E-09	1.1E-06	3.1E+00	1.8E+00	4.6E-01	4.4E-04	2.6E+00	-8.67	-9.53	-10.44	-0.51	0.44	0.00%	0.00%	0.0%
6402	122931-48-0	Rimsulfuron	431	273	4.3E-11	2.4E+00	1.1E+00	1.0	3.5E-06	1.4E-08	3.5E-07	6.9E-01	4.0E-01	1.0E-01	9.8E-05	5.7E-01	-9.24	-9.95	-11.06	-0.82	1.32	0.00%	0.00%	0.0%
6403	208465-21-8	Mesosulfuron-methyl	504	304	2.3E-14	1.2E+01	6.3E+00	3.7	3.5E-06	1.1E-06	3.5E-07	6.9E-01	4.0E-01	1.0E-01	9.9E-05	5.7E-01	-9.99	-10.63	-13.00	-1.45	0.93	0.00%	0.00%	0.0%
6409	83055-99-6	Bensulfuron-methyl	410	250	6.7E-10	8.4E+00	2.6E+01	5.2	3.5E-06	2.3E-07	3.5E-07	6.9E-01	4.0E-01	1.0E-01	9.9E-05	5.7E-01	-9.73	-10.26	-12.12	-0.98	0.37	0.00%	0.00%	0.0%
6398	185119-76-0	Iodosulfuron	493	280	1.1E-12	2.0E+00	2.1E+02	1.8	3.5E-06	1.1E-06	1.1E-06	6.9E-01	4.0E-01	1.0E-01	9.9E-05	5.7E-01	-10.59	-11.14	-13.18	-1.76	1.35	0.00%	0.00%	0.0%
6405	79277-27-3	Thifensulfuron-methyl	387	244	1.9E-09	2.4E+01	1.9E+01	4.1	3.5E-06	1.5E-07	3.5E-07	6.9E-01	4.0E-01	1.0E-01	9.9E-05	5.7E-01	-9.62	-10.17	-11.89	-0.79	0.95	0.00%	0.00%	0.0%
6372	81335-37-7	Imazaquin	311	264	4.5E-11	4.4E+00	7.9E+02	1.8	3.5E-06	3.5E-06	1.1E-06	3.1E+00	1.8E+00	4.7E-01	4.4E-04	2.6E+00	-10.43	-10.95	-13.09	-0.49	0.08	0.00%	0.00%	0.0%
6416	88805-35-0	Prohexadione	212	142	2.3E-04	1.9E+05	1.1E+01	4.2	3.5E-06	3.5E-06	1.1E-06	1.9E-02	1.1E-02	2.9E-03	2.8E-06	1.6E-02	-12.37	-13.01	-15.30	-0.04	1.83	0.00%	0.00%	0.0%