

**Table S1.** The detailed data list of the collected chemicals, which includes the SMILES format and the environmental impact values (GWP, HTP, MDP, FETP, PMFP and TAP).

	Name	SMILES	Environmental Impacts					
			GWP	HTP	MDP	FETP	PMFP	TAP
			kg CO2-Eq	kg 1,4-DCB-Eq	kg Fe-Eq	kg 1,4-DCB-Eq	kg PM10-Eq	kg SO2-Eq
1	1-propanol	CCCO	4.44E+00	1.56E+00	1.54E-01	4.07E-02	8.66E-03	2.04E-02
2	1,1-difluoroethane	CC(F)F	6.40E+00	2.68E+00	3.14E-01	7.39E-02	1.45E-02	2.93E-02
3	1-butanol	CCCCO	2.90E+00	8.21E-01	8.78E-02	2.19E-02	4.89E-03	1.19E-02
4	2-butanol	CCC(C)O	4.29E+00	7.60E-01	7.61E-02	1.76E-02	5.22E-03	1.45E-02
5	isobutanol	CC(C)CO	2.90E+00	8.21E-01	8.78E-02	2.19E-02	4.89E-03	1.19E-02
6	2-methyl-2-butanol	CCC(C)(C)O	3.16E+00	8.30E-01	7.23E-02	1.99E-02	5.20E-03	1.48E-02
7	2-nitroaniline	C1=CC=C(C(=C1)N)[N+](=O)[O-]	6.86E+00	2.53E+00	3.72E-01	1.21E-01	1.23E-02	2.81E-02
8	2, 4-dichlorophenol	C1=CC(=C(C=C1Cl)Cl)O	4.48E+00	2.34E+00	2.13E-01	5.25E-02	9.67E-03	1.78E-02
9	2, 4-dichlorotoluene	CC1=C(C=C(C=C1)Cl)C1	3.33E+00	1.74E+00	1.52E-01	3.61E-02	6.70E-03	1.30E-02
10	3-methyl-1-butyl acetate	CC(C)CCOC(=O)C	5.38E+00	1.62E+00	1.58E-01	4.07E-02	9.14E-03	2.36E-02
11	4-methyl-2-pentanone	CC(C)CC(=O)C	4.28E+00	7.91E-01	9.22E-02	3.74E-02	6.77E-03	1.80E-02
12	4-tert-butylbenzaldehyde	CC(C)(C)C1=CC=C(C=C1)C=O	4.60E+00	1.20E+00	1.79E-01	3.26E-02	6.01E-03	1.35E-02
13	4-tert-butyltoluene	CC1=CC=C(C=C1)C(C)(C)C	2.37E+00	3.50E-01	5.77E-02	9.81E-03	2.60E-03	6.51E-03
14	acetaldehyde	CC=O	1.84E+00	4.63E-01	5.75E-02	1.49E-02	3.00E-03	6.83E-03
15	acetanilide	CC(=O)NC1=CC=CC=C1	5.48E+00	2.46E+00	3.57E-01	6.21E-02	1.09E-02	2.71E-02
16	acetic acid	CC(=O)O	1.72E+00	7.29E-01	9.86E-02	2.29E-02	3.57E-03	7.66E-03
17	acetic anhydride	CC(=O)OC(=O)C	3.53E+00	1.27E+00	1.70E-01	4.44E-02	5.46E-03	1.28E-02

18	acetoacetic acid	<chem>CC(=O)CC(=O)O</chem>	8.35E+00	2.62E+00	4.09E-01	7.82E-02	1.16E-02	2.75E-02
19	acetone	<chem>CC(=O)C</chem>	2.27E+00	2.02E-01	2.36E-02	1.70E-02	3.20E-03	9.35E-03
20	acetyl chloride	<chem>CC(=O)Cl</chem>	7.36E+00	2.58E+00	3.35E-01	8.39E-02	1.13E-02	2.51E-02
21	acetylene	<chem>C#C</chem>	6.46E+00	2.31E+00	1.03E-01	7.77E-02	1.69E-02	2.62E-02
22	acrolein	<chem>C=CC=O</chem>	2.43E+00	5.77E-01	6.10E-02	1.73E-02	3.63E-03	7.94E-03
23	acrylic acid	<chem>C=CC(=O)O</chem>	2.13E+00	3.44E-01	5.65E-02	9.37E-03	2.09E-03	4.66E-03
24	allyl chloride	<chem>C=CCCl</chem>	1.51E+00	6.79E-01	7.57E-02	1.68E-02	2.74E-03	6.04E-03
25	alpha-naphthol	<chem>C1=CC=C2C(=C1)C=CC=C2O</chem>	3.15E+00	1.67E+00	2.46E-01	4.27E-02	7.73E-03	2.01E-02
26	alpha-picoline	<chem>CC1=CC=CC=N1</chem>	3.86E+00	1.12E+00	1.54E-01	3.25E-02	6.27E-03	1.49E-02
27	aniline	<chem>C1=CC=C(C=C1)N</chem>	5.48E+00	2.46E+00	3.54E-01	5.62E-02	1.11E-02	2.89E-02
28	anthranilic acid	<chem>C1=CC=C(C(=C1)C(=O)O)N</chem>	8.96E+00	1.84E+00	5.05E-01	4.52E-02	1.05E-02	3.37E-02
29	benzal chloride	<chem>C1=CC=C(C=C1)C(Cl)C1</chem>	2.75E+00	1.42E+00	1.18E-01	2.62E-02	4.81E-03	1.03E-02
30	benzaldehyde	<chem>C1=CC=C(C=C1)C=O</chem>	5.12E+00	2.57E+00	2.42E-01	4.82E-02	8.75E-03	1.93E-02
31	benzyl alcohol	<chem>C1=CC=C(C=C1)CO</chem>	4.34E+00	1.89E+00	2.34E-01	3.98E-02	7.27E-03	1.80E-02
32	benzyl chloride	<chem>C1=CC=C(C=C1)CCl</chem>	2.63E+00	1.04E+00	9.66E-02	2.01E-02	4.04E-03	9.12E-03
33	bisphenol A	<chem>CC(C)(C1=CC=C(C=C1)O)C2=CC=C(C=C2)O</chem>	4.12E+00	1.19E+00	1.46E-01	3.64E-02	7.21E-03	1.43E-02
34	bromopropane	<chem>CCCBBr</chem>	5.16E+00	1.50E+00	1.70E-01	3.82E-02	7.51E-03	1.90E-02
35	butane	<chem>CCCC</chem>	8.20E-01	2.24E-01	2.74E-02	1.19E-02	1.53E-03	3.77E-03
36	butane-1, 4-diol	<chem>CC(C)(CO)CO.C(CCC(=O)O)CC(=O)O.C(CCO)CO</chem>	5.29E+00	1.81E+00	1.73E-01	5.32E-02	1.05E-02	2.20E-02
37	butyl acetate	<chem>CCCCOC(=O)C</chem>	3.73E+00	1.28E+00	1.65E-01	3.41E-02	6.60E-03	1.59E-02
38	butyl acrylate	<chem>CCCCOC(=O)C=C</chem>	4.27E+00	1.17E+00	1.40E-01	2.79E-02	7.09E-03	1.88E-02

39	carbon tetrachloride	<chem>C(Cl)(Cl)(Cl)Cl</chem>	1.70E+00	3.56E-01	6.53E-03	4.71E-03	4.63E-03	1.15E-02
40	chloroacetic acid	<chem>C(C(=O)O)Cl</chem>	2.35E+00	1.62E+00	1.68E-01	3.51E-02	5.34E-03	1.09E-02
41	chloroacetyl chloride	<chem>C(C(=O)Cl)Cl</chem>	4.55E+00	3.34E+00	3.81E-01	7.20E-02	1.41E-02	3.79E-02
42	chloromethyl methyl ether	<chem>COCCl</chem>	1.66E+00	1.10E+00	1.45E-01	2.70E-02	3.28E-03	7.10E-03
43	chloronitrobenzene	<chem>C1=CC=C(C(=C1)[N+](=O)[O-])Cl</chem>	4.64E+00	1.63E+00	2.43E-01	9.10E-02	8.28E-03	1.90E-02
44	chloropropionic acid	<chem>CC(C(=O)O)Cl</chem>	3.49E+00	1.89E+00	1.87E-01	4.34E-02	7.46E-03	1.47E-02
45	cumene	<chem>CC(C)C1=CC=CC=C1</chem>	2.51E+00	6.61E-01	6.11E-02	1.75E-02	4.72E-03	8.92E-03
46	cyanogen chloride	<chem>C(#N)Cl</chem>	5.25E+00	2.38E+00	2.08E-01	5.76E-02	9.61E-03	2.09E-02
47	cyanuric chloride	<chem>C1(=NC(=NC(=N1)Cl)Cl)Cl</chem>	5.70E+00	2.73E+00	2.65E-01	6.51E-02	1.06E-02	2.27E-02
48	cyclohexane	<chem>C1CCCCC1</chem>	2.60E+00	8.13E-01	6.65E-02	2.03E-02	5.74E-03	1.08E-02
49	cyclohexanol	<chem>C1CCC(CC1)O</chem>	2.94E+00	9.89E-01	1.08E-01	2.66E-02	5.91E-03	1.09E-02
50	cyclohexanone	<chem>C1CCC(=O)CC1</chem>	4.51E+00	1.43E+00	1.29E-01	3.85E-02	8.83E-03	1.93E-02
51	dichloromethane	<chem>C(Cl)Cl</chem>	3.48E+00	5.57E-01	5.44E-03	4.38E-03	9.26E-03	2.12E-02
52	diethanolamine	<chem>C(CO)NCCO</chem>	2.89E+00	8.71E-01	1.19E-01	2.34E-02	4.45E-03	1.02E-02
53	diethyl ether	<chem>CCOCC</chem>	5.20E+00	2.43E+00	3.59E-01	5.86E-02	1.15E-02	2.95E-02
54	diethylene glycol	<chem>C(COCCO)O</chem>	2.24E+00	7.31E-01	1.04E-01	2.03E-02	3.80E-03	7.78E-03
55	dimethyl ether	<chem>COC</chem>	1.42E+00	5.93E-01	1.02E-01	2.24E-02	2.19E-03	5.11E-03
56	dimethyl malonate	<chem>COC(=O)CC(=O)OC</chem>	5.73E+00	3.12E+00	4.10E-01	8.59E-02	1.11E-02	2.40E-02
57	dimethyl sulfate	<chem>COS(=O)(=O)OC</chem>	1.42E+00	1.10E+00	1.95E-01	2.90E-02	4.26E-03	1.25E-02
58	dimethyl sulfide	<chem>CSC</chem>	1.84E+00	7.77E-01	1.27E-01	2.71E-02	3.12E-03	7.44E-03
59	dimethyl sulfoxide	<chem>CS(=O)C</chem>	1.46E+00	6.69E-01	1.13E-01	2.29E-02	2.57E-03	5.96E-03
60	dimethylacetamide	<chem>CC(=O)N(C)C</chem>	3.25E+00	1.30E+00	1.99E-01	4.07E-02	5.91E-03	1.35E-02

61	dimethylamine	CNC	2.47E+00	8.11E-01	1.33E-01	2.80E-02	3.71E-03	1.01E-02
62	dioxane	C1COCCO1	4.89E+00	1.56E+00	2.01E-01	4.10E-02	7.99E-03	1.78E-02
63	dipropyl amine	CCCNCCC	5.69E+00	1.84E+00	1.87E-01	4.67E-02	1.02E-02	2.57E-02
64	dipropylene glycol monomethyl ether	CC(CO)OCC(C)OC	4.93E+00	2.81E+00	2.59E-01	6.04E-02	1.02E-02	1.95E-02
65	DTPA	C(CN(CC(=O)O)CC(=O)O)N(CCN(CC(=O)O)CC(=O)O)CC(=O)O	4.05E+00	1.54E+00	2.04E-01	6.41E-02	6.69E-03	1.57E-02
66	EDTA	C(CN(CC(=O)O)CC(=O)O)N(CC(=O)O)CC(=O)O	4.17E+00	1.57E+00	2.05E-01	6.52E-02	6.98E-03	1.61E-02
67	epichlorohydrin	C1C(O1)CCl	3.10E+00	1.33E+00	1.79E-01	3.42E-02	5.57E-03	1.12E-02
68	ethyl acetate	CCOC(=O)C	2.69E+00	9.77E-01	1.49E-01	2.60E-02	4.72E-03	1.15E-02
69	ethyl benzene	CCC1=CC=CC=C1	2.44E+00	6.97E-01	6.17E-02	1.83E-02	4.94E-03	9.15E-03
70	ethylamine	CCN	3.02E+00	8.18E-01	1.45E-01	1.96E-02	4.21E-03	1.17E-02
71	ethylene bromide	C(CBr)Br	6.47E+00	1.81E+00	1.99E-01	4.58E-02	8.92E-03	2.22E-02
72	ethylene carbonate	C1COC(=O)O1	1.62E+00	6.26E-01	1.08E-01	1.59E-02	2.47E-03	5.38E-03
73	ethylene dichloride	C(CCl)Cl	1.43E+00	7.59E-01	1.01E-01	1.85E-02	2.95E-03	5.92E-03
74	ethylene glycol diethyl ether	CCOCCOCC	3.56E+00	1.48E+00	2.17E-01	3.78E-02	6.35E-03	1.30E-02
75	ethylene glycol dimethyl ether	COCCOC	2.42E+00	8.81E-01	1.39E-01	2.73E-02	3.79E-03	8.19E-03
76	ethylene glycol monoethyl ether	CCOCCO	2.33E+00	7.05E-01	1.13E-01	1.86E-02	3.45E-03	7.67E-03
77	ethylene oxide	C1CO1	2.18E+00	4.93E-01	5.86E-02	1.46E-02	3.12E-03	6.76E-03
78	ethylenediamine	C(CN)N	5.29E+00	2.24E+00	2.59E-01	5.18E-02	9.66E-03	2.21E-02
79	formic acid	C(=O)O	2.50E+00	1.04E+00	1.05E-01	2.73E-02	3.45E-03	1.06E-02
80	glycerine	C(C(CO)O)O	2.10E+00	6.83E-01	1.09E-01	4.17E-02	7.06E-03	1.83E-02
81	glycine	C(C(=O)O)N	4.96E+00	2.98E+00	3.32E-01	8.00E-02	1.08E-02	2.29E-02

82	glyoxal	<chem>C(=O)C=O</chem>	2.99E+00	9.79E-01	1.07E-01	2.81E-02	5.11E-03	1.04E-02
83	hexafluoroethane	<chem>C(C(F)(F)F)(F)(F)F</chem>	1.06E+01	7.14E+00	7.70E-01	1.68E-01	2.97E-02	6.43E-02
84	hydroquinone	<chem>C1=CC(=CC=C1O)O</chem>	3.84E+00	1.33E+00	1.68E-01	4.24E-02	7.23E-03	1.40E-02
85	imidazole	<chem>C1=CN=CN1</chem>	4.93E+00	1.77E+00	2.26E-01	4.66E-02	8.12E-03	1.96E-02
86	isobutyl acetate	<chem>CC(C)COC(=O)C</chem>	3.83E+00	1.31E+00	1.69E-01	3.49E-02	6.70E-03	1.62E-02
87	isohexane	<chem>CCCC(C)C</chem>	9.79E-01	5.03E-01	1.04E-01	1.19E-02	2.15E-03	6.06E-03
88	isopropanol	<chem>CC(C)O</chem>	2.10E+00	4.14E-01	6.80E-02	1.08E-02	2.63E-03	7.07E-03
89	isopropyl acetate	<chem>CC(C)OC(=O)C</chem>	4.48E+00	1.52E+00	1.95E-01	4.12E-02	7.76E-03	1.85E-02
90	isopropylamine	<chem>CC(C)N</chem>	3.80E+00	9.39E-01	1.53E-01	2.38E-02	5.12E-03	1.40E-02
91	lactic acid	<chem>CC(C(=O)O)O</chem>	4.36E+00	1.53E+00	2.06E-01	4.32E-02	6.86E-03	1.68E-02
92	maleic anhydride	<chem>C1=CC(=O)OC1=O</chem>	2.50E+00	6.31E-01	6.36E-02	1.79E-02	2.80E-03	7.11E-03
93	melamine	<chem>C1(=NC(=NC(=N1)N)N)N</chem>	5.23E+00	1.87E+00	3.35E-01	4.53E-02	1.13E-02	3.36E-02
94	meta-phenylene diamine	<chem>C1=CC(=CC(=C1)N)N</chem>	2.15E+01	3.82E+00	5.16E-01	1.07E-01	2.74E-02	7.50E-02
95	methacrylic acid	<chem>CC(=C)C(=O)O</chem>	6.42E+00	2.14E+00	3.50E-01	6.88E-02	1.09E-02	3.09E-02
96	methane sulfonic acid	<chem>CS(=O)(=O)O</chem>	1.14E+00	1.07E+00	1.87E-01	2.50E-02	4.36E-03	1.38E-02
97	methanol	<chem>CO</chem>	3.15E-01	2.26E+00	4.13E-02	1.05E-02	9.27E-04	2.05E-03
98	methyl acrylate	<chem>COC(=O)C=C</chem>	2.73E+00	1.25E+00	1.17E-01	1.73E-02	2.71E-03	6.22E-03
99	methyl ethyl ketone	<chem>CCC(=O)C</chem>	1.83E+00	3.76E-01	6.05E-02	1.01E-02	2.39E-03	5.87E-03
100	methyl formate	<chem>COC=O</chem>	2.83E+00	1.16E+00	1.30E-01	3.82E-02	5.66E-03	1.24E-02
101	methyl iodide	<chem>CI</chem>	6.79E+00	1.86E+00	1.90E-01	5.43E-02	1.03E-02	2.34E-02
102	methyl tert-butyl ether	<chem>CC(C)(C)OC</chem>	1.13E+00	2.84E-01	6.40E-02	8.48E-03	1.48E-03	3.93E-03
103	methyl-3-methoxypropionate	<chem>COCCC(=O)OC</chem>	2.83E+00	1.32E+00	1.53E-01	3.62E-02	3.40E-03	7.42E-03

104	methylamine	CN	2.63E+00	8.32E-01	1.34E-01	2.59E-02	3.92E-03	1.16E-02
105	methylchloride	CCl	3.10E+00	3.81E-01	4.63E-03	3.57E-03	8.83E-03	1.97E-02
106	methylcyclohexane	CC1CCCCC1	3.65E+00	7.37E-01	7.59E-02	1.83E-02	5.28E-03	1.45E-02
107	N-methyl-2-pyrrolidone	CN1CCCC1=O	7.10E+00	2.66E+00	3.20E-01	7.71E-02	1.37E-02	2.92E-02
108	N, N-dimethylformamide	CN(C)C=O	2.84E+00	1.15E+00	1.68E-01	3.53E-02	5.22E-03	1.26E-02
109	naphthalene sulfonic acid	C1=CC=C2C(=C1)C=CC=C2S(=O)(=O)O	1.52E+00	1.18E+00	1.31E-01	2.89E-02	5.83E-03	1.04E-02
110	nitrobenzene	C1=CC=C(C=C1)[N+](=O)[O-]	3.57E+00	1.18E+00	2.23E-01	2.84E-02	7.20E-03	1.96E-02
111	o-aminophenol	C1=CC=C(C(=C1)N)O	6.31E+00	1.87E+00	3.55E-01	4.85E-02	1.00E-02	2.39E-02
112	o-chlorobenzaldehyde	C1=CC=C(C(=C1)C=O)Cl	8.96E+00	4.10E+00	4.67E-01	1.00E-01	1.68E-02	3.24E-02
113	o-chlorotoluene	CC1=CC=CC=C1Cl	2.91E+00	1.23E+00	1.18E-01	2.64E-02	5.18E-03	1.06E-02
114	o-cresol	CC1=CC=CC=C1O	3.92E+00	1.28E+00	1.58E-01	3.69E-02	7.06E-03	1.37E-02
115	o-nitrophenol	C1=CC=C(C(=C1)[N+](=O)[O-])O	4.07E+00	1.13E+00	2.23E-01	2.95E-02	6.48E-03	1.56E-02
116	ortho-phenylene diamine	C1=CC=C(C(=C1)N)N	1.52E+01	4.15E+00	5.77E-01	1.61E-01	2.27E-02	5.68E-02
117	p-chlorophenol	C1=CC(=CC=C1O)Cl	4.34E+00	1.97E+00	1.94E-01	4.69E-02	8.91E-03	1.66E-02
118	p-nitrophenol	C1=CC(=CC=C1[N+](=O)[O-])O	4.07E+00	1.13E+00	2.23E-01	2.95E-02	6.48E-03	1.56E-02
119	p-nitrotoluene	CC1=CC=C(C(=C1)[N+](=O)[O-])	3.62E+00	5.54E-01	1.57E-01	1.36E-02	3.81E-03	1.24E-02
120	para-phenylene diamine	C1=CC(=CC=C1N)N	1.22E+01	4.31E+00	6.07E-01	1.87E-01	2.04E-02	4.79E-02
121	pentaerythritol	C(C(CO)(CO)CO)O	2.41E+00	9.87E-01	1.43E-01	2.95E-02	4.53E-03	1.00E-02
122	perfluoropentane	C(C(C(F)(F)F)(F)F)(C(C(F)(F)F)(F)F)F	1.64E+01	3.73E+00	4.06E-01	8.05E-02	1.93E-02	4.36E-02
123	phenyl acetic acid	C1=CC=C(C(=C1)CC(=O)O)	5.78E+00	2.14E+00	2.59E-01	5.91E-02	8.98E-03	2.10E-02
124	phenyl isocyanate	C1=CC=C(C(=C1)N=C=O)	7.76E+00	5.15E+00	5.00E-01	9.65E-02	1.66E-02	3.82E-02
125	phosgene	C(=O)(Cl)Cl	1.38E+00	2.72E+00	1.23E-01	2.98E-02	2.62E-03	7.38E-03

126	phthalic anhydride	<chem>C1=CC=C2C(=C1)C(=O)OC2=O</chem>	2.61E+00	4.93E-01	6.06E-02	1.25E-02	4.29E-03	1.12E-02
127	phthalimide	<chem>C1=CC=C2C(=C1)C(=O)NC2=O</chem>	3.73E+00	9.30E-01	1.32E-01	2.33E-02	6.22E-03	1.64E-02
128	piperidine	<chem>C1CCNCC1</chem>	8.88E+00	2.67E+00	3.67E-01	7.40E-02	1.28E-02	3.04E-02
129	polyacrylamide	<chem>C=CC(=O)N</chem>	2.84E+00	6.96E-01	1.16E-01	1.74E-02	4.45E-03	1.49E-02
130	propanal	<chem>CCC=O</chem>	3.74E+00	1.17E+00	9.81E-02	3.00E-02	6.92E-03	1.73E-02
131	propionic acid	<chem>CCC(=O)O</chem>	2.02E+00	6.91E-01	8.38E-02	2.00E-02	3.71E-03	8.10E-03
132	propyl amine	<chem>CCCN</chem>	6.45E+00	2.24E+00	2.51E-01	5.75E-02	1.19E-02	2.90E-02
133	propylene	<chem>CC=C</chem>	1.44E+00	9.46E-03	6.68E-04	9.71E-04	1.25E-03	3.61E-03
134	propylene glycol	<chem>CC(CO)O</chem>	4.54E+00	2.67E+00	2.46E-01	5.58E-02	9.47E-03	1.81E-02
135	propylene oxide	<chem>CC1CO1</chem>	5.00E+00	2.84E+00	2.39E-01	5.97E-02	1.05E-02	2.01E-02
136	pyrazole	<chem>C1=CN=C1</chem>	1.84E+01	2.03E+01	9.27E-01	2.01E-01	3.23E-02	6.60E-02
137	pyridine	<chem>C1=CC=NC=C1</chem>	8.17E+00	2.37E+00	3.17E-01	6.64E-02	1.17E-02	2.80E-02
138	sodium methoxide	<chem>C[O-].[Na+]</chem>	1.70E+00	8.67E-01	1.09E-01	2.51E-02	3.79E-03	7.15E-03
139	styrene	<chem>C=CC1=CC=CC=C1</chem>	3.11E+00	8.70E-01	6.71E-02	2.41E-02	6.30E-03	1.14E-02
140	tert-butyl amine	<chem>CC(C)(C)N</chem>	7.82E+00	2.70E+00	3.62E-01	7.58E-02	1.36E-02	3.40E-02
141	tetrachloroethylene	<chem>C(=C(Cl)Cl)(Cl)Cl</chem>	3.92E+00	7.63E-01	4.47E-03	4.57E-03	6.86E-03	1.47E-02
142	tetraethyl orthosilicate	<chem>CCO[Si](OCC)(OCC)OC</chem>	5.20E+00	2.43E+00	2.20E-01	5.53E-02	9.93E-03	2.03E-02
143	tetrafluoroethane	<chem>C(C(F)(F)F)F</chem>	7.57E+00	4.96E+00	6.16E-01	1.18E-01	2.07E-02	4.41E-02
144	toluene	<chem>CC1=CC=CC=C1</chem>	1.55E+00	2.39E-02	3.78E-03	1.12E-03	1.35E-03	3.81E-03
145	trichloroacetic acid	<chem>C(=O)(C(Cl)(Cl)Cl)O</chem>	4.07E+00	2.75E+00	2.38E-01	5.85E-02	9.76E-03	1.81E-02
146	trichloroethylene	<chem>C(=C(Cl)Cl)Cl</chem>	4.28E+00	2.43E+00	2.35E-01	5.93E-02	1.04E-02	1.85E-02
147	trichloromethane	<chem>C(Cl)(Cl)Cl</chem>	3.53E+00	7.38E+00	1.16E-01	2.58E-02	3.17E-03	6.94E-03

148	trichloropropane	<chem>CCC(Cl)(Cl)Cl</chem>	2.97E+00	2.06E+00	1.94E-01	9.96E-02	9.31E-03	2.93E-02
149	triethyl amine	<chem>CCN(CC)CC</chem>	3.10E+00	8.19E-01	1.49E-01	1.97E-02	4.13E-03	1.08E-02
150	trifluoroacetic acid	<chem>C(=O)(C(F)(F)F)O</chem>	9.03E+00	6.23E+00	6.67E-01	1.38E-01	2.35E-02	4.87E-02
151	trifluoromethane	<chem>C(F)(F)F</chem>	8.24E+00	1.57E+01	5.50E-01	8.81E-02	1.30E-02	3.43E-02
152	trimesoyl chloride	<chem>C1=C(C=C(C=C1C(=O)Cl)C(=O)Cl)C(=O)Cl</chem>	8.78E+00	3.21E+00	3.23E-01	6.02E-02	2.50E-02	6.60E-02
153	trimethyl borate	<chem>B(OC)(OC)OC</chem>	2.52E+00	1.01E+00	1.71E-01	2.99E-02	6.93E-03	1.43E-02
154	vinyl acetate	<chem>CC(=O)OC=C</chem>	2.29E+00	8.83E-01	1.23E-01	2.64E-02	4.24E-03	8.98E-03
155	vinyl chloride	<chem>C=CCl</chem>	1.60E+00	1.71E-01	2.59E-03	3.97E-03	1.36E-03	3.96E-03
156	vinyl fluoride	<chem>C=CF</chem>	9.50E+00	3.24E+00	3.86E-01	8.90E-02	1.71E-02	3.43E-02
157	xylene	<chem>CC1=CC=C(C=C1)C</chem>	1.69E+00	3.03E-02	3.86E-03	1.36E-03	1.55E-03	4.47E-03
158	2,4-di-tert-butylphenol	<chem>CC(C)(C)C1=CC(=C(C=C1)O)C(C)(C)C</chem>	3.43E+00	9.04E-01	1.14E-01	2.57E-02	5.29E-03	1.03E-02
159	2,6-di-tert-butylphenol	<chem>CC(C)(C)C1=C(C(=CC=C1)C(C)(C)C)O</chem>	3.57E+00	9.31E-01	1.17E-01	2.65E-02	5.48E-03	1.06E-02
160	sodium phenolate	<chem>C1=CC=C(C=C1)[O-].[Na+]</chem>	3.93E+00	1.43E+00	1.68E-01	3.92E-02	7.68E-03	1.45E-02
161	dichloropropene	<chem>CC=C(Cl)Cl</chem>	4.08E+00	1.85E+00	2.03E-01	4.58E-02	7.23E-03	1.59E-02
162	dimethyldichlorosilane	<chem>C[Si](C)(Cl)Cl</chem>	6.18E+00	1.55E+00	7.51E-02	3.51E-02	1.43E-02	2.97E-02
163	monochlorobenzene	<chem>C1=CC=C(C=C1)Cl</chem>	3.05E+00	1.48E+00	1.33E-01	1.02E-01	7.47E-03	1.34E-02
164	monochloropentafluoroethane	<chem>C(C(F)(F)Cl)(F)(F)F</chem>	9.46E+00	7.41E+00	8.30E-01	1.56E-01	2.77E-02	6.21E-02
165	o-dichlorobenzene	<chem>C1=CC=C(C(=C1)Cl)Cl</chem>	2.84E+00	1.45E+00	1.30E-01	1.18E-01	7.02E-03	1.25E-02
166	p-dichlorobenzene	<chem>C1=CC(=CC=C1Cl)Cl</chem>	2.84E+00	1.45E+00	1.30E-01	1.18E-01	7.02E-03	1.25E-02
167	sodium chloroacetate	<chem>C(C(=O)[O-])Cl.[Na+]</chem>	3.46E+00	2.08E+00	2.64E-01	5.20E-02	7.21E-03	1.64E-02
168	benzene	<chem>C1=CC=CC=C1</chem>	2.03E+00	5.14E-01	9.68E-03	1.36E-02	4.75E-03	8.22E-03
169	ethanol	<chem>CCO</chem>	1.25E+00	2.67E-01	5.39E-02	6.20E-03	1.57E-03	4.14E-03



170	ethylene glycol	<chem>C(CO)O</chem>	1.98E+00	6.72E-01	9.72E-02	1.85E-02	3.43E-03	6.96E-03
171	glucose	<chem>C(C1C(C(C(C(O1)O)O)O)O)O</chem>	1.39E+00	7.00E-01	1.27E-01	2.40E-02	3.35E-03	1.05E-02
172	1-pentanol	<chem>CCCCCO</chem>	5.05E+00	1.27E+00	7.56E-02	3.07E-02	8.32E-03	2.22E-02
173	2-methyl-1-butanol	<chem>CCC(C)CO</chem>	5.05E+00	1.27E+00	7.56E-02	3.07E-02	8.32E-03	2.22E-02
174	acetonitrile	<chem>CC#N</chem>	4.02E+00	6.61E-01	1.11E-01	1.63E-02	5.65E-03	2.21E-02
175	acrylonitrile	<chem>C=CC#N</chem>	2.98E+00	4.92E-01	8.25E-02	1.21E-02	4.21E-03	1.64E-02
176	benzoic acid	<chem>C1=CC=C(C=C1)C(=O)O</chem>	2.22E+00	4.81E-01	6.42E-02	1.38E-02	3.25E-03	7.00E-03
177	butyrolactone	<chem>C1CC(=O)OC1</chem>	6.28E+00	2.28E+00	2.43E-01	6.59E-02	1.26E-02	2.61E-02
178	decabromodiphenyl ether	<chem>C1(=C(C(=C(C(=C1Br)Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br</chem>	1.35E+01	3.73E+00	4.27E-01	1.23E-01	2.83E-02	7.63E-02
179	dimethyl carbonate	<chem>COC(=O)OC</chem>	2.22E+00	9.40E-01	1.59E-01	2.58E-02	3.59E-03	7.59E-03
180	ethane	<chem>CC</chem>	8.15E-01	2.23E-01	2.74E-02	1.19E-02	1.52E-03	3.76E-03
181	hexamethyldisilazane	<chem>C[Si](C)(C)N[Si](C)(C)C</chem>	5.84E+00	1.96E+00	3.73E-01	5.95E-02	1.14E-02	2.49E-02
182	methyl acetate	<chem>CC(=O)OC</chem>	1.15E+00	4.30E-01	6.48E-02	1.07E-02	2.42E-03	6.72E-03
183	monoethanolamine	<chem>C(CO)N</chem>	2.87E+00	8.64E-01	1.21E-01	2.28E-02	4.44E-03	1.08E-02
184	morpholine	<chem>C1COCCN1</chem>	9.53E+00	2.73E+00	2.35E-01	8.33E-02	1.99E-02	5.86E-02
185	polydimethylsiloxane	<chem>C[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C</chem>	1.55E+01	4.77E+00	3.64E-01	1.18E-01	3.55E-02	7.23E-02
186	propane	<chem>CCC</chem>	8.28E-01	1.39E-01	1.73E-02	4.46E-03	1.78E-03	5.62E-03
187	salicylic acid	<chem>C1=CC=C(C(=C1)C(=O)O)O</chem>	4.90E+00	2.32E+00	3.27E-01	5.96E-02	1.10E-02	2.59E-02