Supplementary Information for :

Polarization charge densities provide a predictive quantification of hydrogen bond energies

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Algorithm for the generation of vdW-HB-clusters:

Input: geometries of the educts A and B and the optimized HB-cluster AB

1) Identify all hydrogen bonds

2) For each HB: Define a translation vector $\underline{t} = (\underline{x}_{don}-\underline{x}_{acc})*(d_{vdW}-d_{HB})/d_{HB}$, where $\underline{x}_{don}$ and $\underline{x}_{acc}$ are the positions of the donor hydrogen atom and the acceptor atom, respectively, d_{HB} is their distance in the HB cluster, and d_{vdW} is their vdW distance, which was set to the sum of COSMO radii divided by 1.17 in the present study. Move the atoms of the educt with the donor by 0.5 $\underline{t}$ and the atoms of the acceptor educt by -0.5 $\underline{t}$ and store the resulting atom positions as one set of shifted atom positions. Assign a weight to each of the atoms positions i as $\exp\{-3d_{i,HB}\}$ where $d_{i,HB}$ is the distance of the atom i to the donor hydrogen in the donor educt and the distance of i to the acceptor atom in the acceptor educt, respectively.

3) For each educt A and B, respectively: Move and rotate the stiff educt geometry in order to achieve a least weighted squared deviation of the atom positions from the atom positions in all sets of shifted atom positions generated in step 2 using the weigh of each atom shifted atom position as described in step 2.

At the end two stiff educts are arranged in a way that the intermolecular hydrogen bonds of the HB cluster are roughly stretched to vdW distance.

Table SI1: COSMO radii (in Å) used in the DFT/COSMO calculations.

H	1.30	P	2.11
C	2.00	S	2.16
N	1.83	Cl	2.05
O	1.72	Br	2.16
F	1.72	I	2.32

Table SI2: Listing of the 2465 HB complexes studied in this paper:

acceptor molecule	donor molecule	acc. type	donor type	σ_acc [e/nm²]	σ_don [e/nm²]	DFT/COSMO HBE [kcal/mol]	HBE(eq. 1) [kcal/mol]	ref-name of HB-complex
1-decene	h2o	C	OH	0.97	-1.74	0.12	-0.12	1-decene_acc_01_h2o
cyclopentene	h2o	C	OH	1.06	-1.74	-0.22	-0.15	cyclopentene_acc_01_h2o
pentene2	h2o	C	OH	1.03	-1.74	-0.10	-0.12	pentene2_acc_01_h2o
pentene4	h2o	C	OH	0.99	-1.74	0.05	-0.15	pentene4_acc_01_h2o
2,4-dimethylpyridine	h2o	N	OH	2.24	-1.74	-4.42	-4.01	2,4-dimethylpyridine_acc_01_h2o
2,6-dimethylpyridine	h2o	N	OH	2.22	-1.74	-4.35	-3.30	2,6-dimethylpyridine_acc_01_h2o
2-propenenitrile	h2o	N	OH	1.44	-1.74	-1.53	-1.43	2-propenenitrile_acc_01_h2o
4-cyanophenol	h2o	N	OH	1.49	-1.74	-1.71	-1.72	4-cyanophenol_acc_01_h2o
acetonitrile	h2o	N	OH	1.51	-1.74	-1.79	-1.79	acetonitrile_acc_01_h2o
aziridine	h2o	N	OH	2.22	-1.74	-4.35	-4.79	aziridine_acc_01_h2o
butyronitrile	h2o	N	OH	1.51	-1.74	-1.79	-1.71	butyronitrile_acc_01_h2o
dibutylamine	h2o	N	OH	2.5	-1.74	-5.35	-4.56	dibutylamine_acc_01_h2o
diethylamine0	h2o	N	OH	2.53	-1.74	-5.46	-4.61	diethylamine0_acc_01_h2o
diethylamine1	h2o	N	OH	2.51	-1.74	-5.39	-4.93	diethylamine1_acc_01_h2o

dipropylamine	h2o	N	OH	2.5	-1.74	-5.35	-4.56	dipropylamine_acc_01_h2o
morpholine	h2o	N	OH	2.43	-1.74	-5.10	-4.42	morpholine_acc_01_h2o
piperidine	h2o	N	OH	2.53	-1.74	-5.46	-4.93	piperidine_acc_01_h2o
propionitrile	h2o	N	OH	1.51	-1.74	-1.79	-1.82	propionitrile_acc_01_h2o
pyridine	h2o	N	OH	2.17	-1.74	-4.16	-4.15	pyridine_acc_01_h2o
pyrrolidin	h2o	N	OH	2.49	-1.74	-5.32	-5.32	pyrrolidin_acc_01_h2o
triethylamine1	h2o	N	OH	2.29	-1.74	-4.60	-4.34	triethylamine1_acc_01_h2o
triethylamine2	h2o	N	OH	2.19	-1.74	-4.24	-4.12	triethylamine2_acc_01_h2o
triethylamine3	h2o	N	OH	2.17	-1.74	-4.16	-4.63	triethylamine3_acc_01_h2o
1,2-epoxypropane	h2o	O	OH	1.63	-1.74	-1.71	-2.10	1,2-epoxypropane_acc_01_h2o
3-cyanophenol	h2o	O	OH	1.21	-1.74	-0.41	-0.35	3-cyanophenol_acc_01_h2o
acetaldehyde	h2o	O	OH	1.65	-1.74	-1.77	-1.69	acetaldehyde_acc_01_h2o
acetamide	h2o	O	OH	1.94	-1.74	-2.67	-2.67	acetamide_acc_01_h2o
butanal	h2o	O	OH	1.65	-1.74	-1.77	-2.14	butanal_acc_01_h2o
butoxide	h2o	O	OH	1.63	-1.74	-1.71	-2.12	butoxide_acc_01_h2o
diethylcarbonate0	h2o	O	OH	1.48	-1.74	-1.25	-0.91	diethylcarbonate0_acc_01_h2o
diethylcarbonate2	h2o	O	OH	1.42	-1.74	-1.06	-0.75	diethylcarbonate2_acc_01_h2o
diethylcarbonate3	h2o	O	OH	1.65	-1.74	-1.77	-1.74	diethylcarbonate3_acc_01_h2o
diethylcarbonate4	h2o	O	OH	1.64	-1.74	-1.74	-1.73	diethylcarbonate4_acc_01_h2o
dimethylcarbonate0	h2o	O	OH	1.45	-1.74	-1.16	-0.75	dimethylcarbonate0_acc_01_h2o
dimethylcarbonate1	h2o	O	OH	1.61	-1.74	-1.65	-1.76	dimethylcarbonate1_acc_01_h2o
dimethylether	h2o	O	OH	1.68	-1.74	-1.86	-2.17	dimethylether_acc_01_h2o
dimethylformamide	h2o	O	OH	1.89	-1.74	-2.51	-3.12	dimethylformamide_acc_01_h2o
di-n-butylether0	h2o	O	OH	1.76	-1.74	-2.11	-1.40	di-n-butylether0_acc_01_h2o
di-n-butylether1	h2o	O	OH	1.74	-1.74	-2.05	-2.33	di-n-butylether1_acc_01_h2o
dioxolane	h2o	O	OH	1.54	-1.74	-1.43	-1.63	dioxolane_acc_01_h2o
ethanol1	h2o	O	OH	1.82	-1.74	-2.30	-2.20	ethanol1_acc_01_h2o
ethyleneoxide	h2o	O	OH	1.57	-1.74	-1.53	-1.92	ethyleneoxide_acc_01_h2o
formaldehyde	h2o	O	OH	1.49	-1.74	-1.28	-1.56	formaldehyde_acc_01_h2o
formamide	h2o	O	OH	1.85	-1.74	-2.39	-2.97	formamide_acc_01_h2o

formicacid	h2o	O	OH	1.06	-1.74	0.05	-0.01	formicacid_acc_01_h2o
furane	h2o	O	OH	1.07	-1.74	0.02	0.03	furane_acc_01_h2o
hexanal	h2o	O	OH	1.65	-1.74	-1.77	-2.15	hexanal_acc_01_h2o
isobutanal	h2o	O	OH	1.62	-1.74	-1.68	-1.22	isobutanal_acc_01_h2o
methylformamide	h2o	O	OH	1.9	-1.74	-2.54	-3.09	methylformamide_acc_01_h2o
n,n-dimethylacetamide	h2o	O	OH	1.99	-1.74	-2.82	-3.04	n,n-dimethylacetamide_acc_01_h2o
n-methylacetamide	h2o	O	OH	1.96	-1.74	-2.73	-3.10	n-methylacetamide_acc_01_h2o
octanal	h2o	O	OH	1.65	-1.74	-1.77	-2.16	octanal_acc_01_h2o
propanal	h2o	O	OH	1.64	-1.74	-1.74	-1.34	propanal_acc_01_h2o
propanol0	h2o	O	OH	1.83	-1.74	-2.33	-2.18	propanol0_acc_01_h2o
propanone	h2o	O	OH	1.75	-1.74	-2.08	-2.15	propanone_acc_01_h2o
thf	h2o	O	OH	1.79	-1.74	-2.20	-2.59	thf_acc_01_h2o
thp	h2o	O	OH	1.8	-1.74	-2.23	-2.13	thp_acc_01_h2o
2,2'-dichlorodiethylsulfide0	h2o	S	OH	1.07	-1.74	-0.23	-0.42	2,2'-dichlorodiethylsulfide0_acc_01_h2o
2,2'-dichlorodiethylsulfide1	h2o	S	OH	1.15	-1.74	-0.53	-0.56	2,2'-dichlorodiethylsulfide1_acc_01_h2o
2,2'-dichlorodiethylsulfide2	h2o	S	OH	1.14	-1.74	-0.49	-0.29	2,2'-dichlorodiethylsulfide2_acc_01_h2o
2,2'-dichlorodiethylsulfide3	h2o	S	OH	1.2	-1.74	-0.71	-0.59	2,2'-dichlorodiethylsulfide3_acc_01_h2o
butanethiol0	h2o	S	OH	1.31	-1.74	-1.12	-1.04	butanethiol0_acc_01_h2o
butanethiol1	h2o	S	OH	1.32	-1.74	-1.15	-1.20	butanethiol1_acc_01_h2o
diethylsulfide	h2o	S	OH	1.49	-1.74	-1.78	-1.43	diethylsulfide_acc_01_h2o
h2s	h2o	S	OH	1.15	-1.74	-0.53	-0.81	h2s_acc_01_h2o
methanethiol	h2o	S	OH	1.3	-1.74	-1.08	-1.26	methanethiol_acc_01_h2o
2-methyl-2-butene	h2o	C	OH	1.01	-1.74	-0.03	0.02	2-methyl-2-butene_acc_02_h2o
cyclohexene	h2o	C	OH	0.97	-1.74	0.12	-0.05	cyclohexene_acc_02_h2o
pentene0	h2o	C	OH	0.98	-1.74	0.08	0.09	pentene0_acc_02_h2o
propyne	h2o	C	OH	1	-1.74	0.01	-0.08	propyne_acc_02_h2o
pyridazine	h2o	N	OH	2.01	-1.74	-3.59	-3.66	pyridazine_acc_02_h2o
1,2-dimethoxyethane5	h2o	O	OH	1.67	-1.74	-1.83	-1.70	1,2-dimethoxyethane5_acc_02_h2o
3-pentanone	h2o	O	OH	1.65	-1.74	-1.77	-1.65	3-pentanone_acc_02_h2o
aceticacid0	h2o	O	OH	1.6	-1.74	-1.62	-1.57	aceticacid0_acc_02_h2o

aceticacid1	h2o	O	OH	1.66	-1.74	-1.80	-1.82	aceticacid1_acc_02_h2o
benzophenone	h2o	O	OH	1.66	-1.74	-1.80	-1.68	benzophenone_acc_02_h2o
butyricacid0	h2o	O	OH	1.52	-1.74	-1.37	-1.17	butyricacid0_acc_02_h2o
butyricacid1	h2o	O	OH	1.66	-1.74	-1.80	-1.85	butyricacid1_acc_02_h2o
diethylsulfate0	h2o	O	OH	1.05	-1.74	0.08	-0.32	diethylsulfate0_acc_02_h2o
diethylsulfate1	h2o	O	OH	1.06	-1.74	0.05	-0.20	diethylsulfate1_acc_02_h2o
dimethoxymethane0	h2o	O	OH	1.57	-1.74	-1.53	-1.28	dimethoxymethane0_acc_02_h2o
dimethoxymethane1	h2o	O	OH	1.57	-1.74	-1.53	-1.46	dimethoxymethane1_acc_02_h2o
dimethoxymethane2	h2o	O	OH	1.65	-1.74	-1.77	-1.67	dimethoxymethane2_acc_02_h2o
dimethoxymethane3	h2o	O	OH	1.58	-1.74	-1.56	-1.27	dimethoxymethane3_acc_02_h2o
dimethylsulfate1	h2o	O	OH	0.86	-1.74	0.66	1.10	dimethylsulfate1_acc_02_h2o
di-n-propylether0	h2o	O	OH	1.76	-1.74	-2.11	-1.41	di-n-propylether0_acc_02_h2o
di-n-propylether1	h2o	O	OH	1.76	-1.74	-2.11	-2.23	di-n-propylether1_acc_02_h2o
ethylacetate0	h2o	O	OH	1.64	-1.74	-1.74	-1.82	ethylacetate0_acc_02_h2o
ethylacetate1	h2o	O	OH	1.63	-1.74	-1.71	-1.85	ethylacetate1_acc_02_h2o
ethylformate0	h2o	O	OH	1.56	-1.74	-1.49	-1.76	ethylformate0_acc_02_h2o
ethylformate1	h2o	O	OH	1.55	-1.74	-1.46	-1.73	ethylformate1_acc_02_h2o
ethylpropionate0	h2o	O	OH	1.57	-1.74	-1.53	-1.39	ethylpropionate0_acc_02_h2o
ethylpropionate1	h2o	O	OH	1.55	-1.74	-1.46	-1.36	ethylpropionate1_acc_02_h2o
ethylpropionate2	h2o	O	OH	1.57	-1.74	-1.53	-1.25	ethylpropionate2_acc_02_h2o
h2o2	h2o	O	OH	1.42	-1.74	-1.06	-1.39	h2o2_acc_02_h2o
methanol	h2o	O	OH	1.79	-1.74	-2.20	-2.45	methanol_acc_02_h2o
methylacetate	h2o	O	OH	1.62	-1.74	-1.68	-1.79	methylacetate_acc_02_h2o
methylformate	h2o	O	OH	1.54	-1.74	-1.43	-1.67	methylformate_acc_02_h2o
n-propylacetate0	h2o	O	OH	1.64	-1.74	-1.74	-1.87	n-propylacetate0_acc_02_h2o
n-propylacetate1	h2o	O	OH	1.62	-1.74	-1.68	-1.80	n-propylacetate1_acc_02_h2o
propionicacid0	h2o	O	OH	1.57	-1.74	-1.53	-1.14	propionicacid0_acc_02_h2o
propionicacid1	h2o	O	OH	1.66	-1.74	-1.80	-1.87	propionicacid1_acc_02_h2o
trifluoroaceticacid0	h2o	O	OH	1.16	-1.74	-0.26	-0.31	trifluoroaceticacid0_acc_02_h2o
trifluoroaceticacid1	h2o	O	OH	1.27	-1.74	-0.60	-0.72	trifluoroaceticacid1_acc_02_h2o

(methylthio)-ethane	h2o	S	OH	1.46	-1.74	-1.67	-1.58	(methylthio)-ethane_acc_02_h2o
1-methylcyclohexene	h2o	C	OH	1	-1.74	0.01	0.11	1-methylcyclohexene_acc_03_h2o
cis-2-butene	h2o	C	OH	1.05	-1.74	-0.18	-0.22	cis-2-butene_acc_03_h2o
cyclohexene	h2o	C	OH	0.97	-1.74	0.12	-0.10	cyclohexene_acc_03_h2o
isobutene	h2o	C	OH	1	-1.74	0.01	-0.26	isobutene_acc_03_h2o
propene	h2o	C	OH	1	-1.74	0.01	-0.17	propene_acc_03_h2o
pyrrole	h2o	C	OH	1.08	-1.74	-0.29	-0.28	pyrrole_acc_03_h2o
1-butylamine	h2o	N	OH	2.5	-1.74	-5.35	-5.27	1-butylamine_acc_03_h2o
2-methylpyrazine	h2o	N	OH	1.99	-1.74	-3.52	-3.39	2-methylpyrazine_acc_03_h2o
3-picoline	h2o	N	OH	2.19	-1.74	-4.24	-4.20	3-picoline_acc_03_h2o
ethylamine0	h2o	N	OH	2.52	-1.74	-5.43	-5.08	ethylamine0_acc_03_h2o
ethylamine1	h2o	N	OH	2.49	-1.74	-5.32	-5.30	ethylamine1_acc_03_h2o
hexylamine	h2o	N	OH	2.5	-1.74	-5.35	-5.31	hexylamine_acc_03_h2o
imidazole	h2o	N	OH	2.25	-1.74	-4.45	-4.36	imidazole_acc_03_h2o
methylimidazol	h2o	N	OH	2.3	-1.74	-4.63	-4.26	methylimidazol_acc_03_h2o
n-pentylamine	h2o	N	OH	2.5	-1.74	-5.35	-5.33	n-pentylamine_acc_03_h2o
n-propylamine	h2o	N	OH	2.49	-1.74	-5.32	-5.31	n-propylamine_acc_03_h2o
pyrimidine	h2o	N	OH	1.99	-1.74	-3.52	-3.35	pyrimidine_acc_03_h2o
2-propen-1-ol0	h2o	O	OH	1.75	-1.74	-2.08	-2.04	2-propen-1-ol0_acc_03_h2o
2-propen-1-ol2	h2o	O	OH	1.79	-1.74	-2.20	-1.97	2-propen-1-ol2_acc_03_h2o
aceticacid0	h2o	O	OH	1.1	-1.74	-0.08	0.12	aceticacid0_acc_03_h2o
aceticacid1	h2o	O	OH	1.17	-1.74	-0.29	-0.18	aceticacid1_acc_03_h2o
butyricacid0	h2o	O	OH	1.13	-1.74	-0.17	0.04	butyricacid0_acc_03_h2o
butyricacid1	h2o	O	OH	1.19	-1.74	-0.35	-0.16	butyricacid1_acc_03_h2o
diethylcarbonate0	h2o	O	OH	1.15	-1.74	-0.23	0.64	diethylcarbonate0_acc_03_h2o
diethylcarbonate1	h2o	O	OH	1.17	-1.74	-0.29	0.22	diethylcarbonate1_acc_03_h2o
diethylcarbonate2	h2o	O	OH	1.18	-1.74	-0.32	0.07	diethylcarbonate2_acc_03_h2o
diethylether0	h2o	O	OH	1.73	-1.74	-2.02	-1.44	diethylether0_acc_03_h2o
diethylether1	h2o	O	OH	1.78	-1.74	-2.17	-1.87	diethylether1_acc_03_h2o
diethylsulfate0	h2o	O	OH	1.05	-1.74	0.08	-0.21	diethylsulfate0_acc_03_h2o

diethylsulfate1	h2o	O	OH	1.04	-1.74	0.11	-0.28	diethylsulfate1_acc_03_h2o
dimethoxymethane0	h2o	O	OH	1.58	-1.74	-1.56	-1.63	dimethoxymethane0_acc_03_h2o
dimethoxymethane1	h2o	O	OH	1.57	-1.74	-1.53	-1.28	dimethoxymethane1_acc_03_h2o
dimethoxymethane2	h2o	O	OH	1.54	-1.74	-1.43	-1.30	dimethoxymethane2_acc_03_h2o
dimethoxymethane3	h2o	O	OH	1.58	-1.74	-1.56	-1.21	dimethoxymethane3_acc_03_h2o
dimethylcarbonate1	h2o	O	OH	1.12	-1.74	-0.14	0.10	dimethylcarbonate1_acc_03_h2o
ethoxyethanol0	h2o	O	OH	1.63	-1.74	-1.71	-1.12	ethoxyethanol0_acc_03_h2o
ethoxyethanol1	h2o	O	OH	1.63	-1.74	-1.71	-1.06	ethoxyethanol1_acc_03_h2o
ethoxyethanol2	h2o	O	OH	1.66	-1.74	-1.80	-1.53	ethoxyethanol2_acc_03_h2o
ethoxyethanol4	h2o	O	OH	1.64	-1.74	-1.74	-1.13	ethoxyethanol4_acc_03_h2o
ethoxyethanol5	h2o	O	OH	1.64	-1.74	-1.74	-1.18	ethoxyethanol5_acc_03_h2o
ethoxyethanol7	h2o	O	OH	1.73	-1.74	-2.02	-1.68	ethoxyethanol7_acc_03_h2o
ethoxyethanol8	h2o	O	OH	1.75	-1.74	-2.08	-1.59	ethoxyethanol8_acc_03_h2o
ethylacetate0	h2o	O	OH	1.17	-1.74	-0.29	0.64	ethylacetate0_acc_03_h2o
ethylacetate1	h2o	O	OH	1.17	-1.74	-0.29	0.70	ethylacetate1_acc_03_h2o
ethylformate0	h2o	O	OH	1.11	-1.74	-0.11	0.45	ethylformate0_acc_03_h2o
ethylpropionate0	h2o	O	OH	1.19	-1.74	-0.35	0.67	ethylpropionate0_acc_03_h2o
ethylpropionate1	h2o	O	OH	1.21	-1.74	-0.41	0.15	ethylpropionate1_acc_03_h2o
ethylpropionate2	h2o	O	OH	1.19	-1.74	-0.35	0.61	ethylpropionate2_acc_03_h2o
formicacid	h2o	O	OH	1.49	-1.74	-1.28	-1.48	formicacid_acc_03_h2o
methylacetate	h2o	O	OH	1.13	-1.74	-0.17	0.35	methylacetate_acc_03_h2o
methylformate	h2o	O	OH	1.1	-1.74	-0.08	0.07	methylformate_acc_03_h2o
n-propylacetate0	h2o	O	OH	1.18	-1.74	-0.32	0.64	n-propylacetate0_acc_03_h2o
n-propylacetate1	h2o	O	OH	1.19	-1.74	-0.35	0.31	n-propylacetate1_acc_03_h2o
propionicacid0	h2o	O	OH	1.16	-1.74	-0.26	-0.03	propionicacid0_acc_03_h2o
propionicacid1	h2o	O	OH	1.19	-1.74	-0.35	-0.19	propionicacid1_acc_03_h2o
ethanethiol0	h2o	S	OH	1.31	-1.74	-1.12	-1.02	ethanethiol0_acc_03_h2o
ethanethiol1	h2o	S	OH	1.32	-1.74	-1.15	-1.16	ethanethiol1_acc_03_h2o
2-propen-1-ol1	h2o	C	OH	0.98	-1.74	0.08	0.05	2-propen-1-ol1_acc_04_h2o
4-methylpyridine	h2o	N	OH	2.21	-1.74	-4.31	-4.29	4-methylpyridine_acc_04_h2o

dicyanomethane	h2o	N	OH	1.32	-1.74	-1.10	-1.21	dicyanomethane_acc_04_h2o
pyrazine	h2o	N	OH	1.95	-1.74	-3.37	-3.28	pyrazine_acc_04_h2o
2-propanol0	h2o	O	OH	1.81	-1.74	-2.27	-2.14	2-propanol0_acc_04_h2o
2-propanol1	h2o	O	OH	1.83	-1.74	-2.33	-2.26	2-propanol1_acc_04_h2o
acrolein0	h2o	O	OH	1.64	-1.74	-1.74	-2.13	acrolein0_acc_04_h2o
acrolein1	h2o	O	OH	1.63	-1.74	-1.71	-2.12	acrolein1_acc_04_h2o
diethylcarbonate1	h2o	O	OH	1.16	-1.74	-0.26	0.45	diethylcarbonate1_acc_04_h2o
diethylcarbonate3	h2o	O	OH	1.2	-1.74	-0.38	0.52	diethylcarbonate3_acc_04_h2o
diethylcarbonate4	h2o	O	OH	1.2	-1.74	-0.38	0.52	diethylcarbonate4_acc_04_h2o
diethylsulfate0	h2o	O	OH	0.88	-1.74	0.60	1.31	diethylsulfate0_acc_04_h2o
diethylsulfate1	h2o	O	OH	0.88	-1.74	0.60	0.80	diethylsulfate1_acc_04_h2o
dimethylcarbonate0	h2o	O	OH	1.11	-1.74	-0.11	0.07	dimethylcarbonate0_acc_04_h2o
dimethylsulfate0	h2o	O	OH	1.02	-1.74	0.17	-0.14	dimethylsulfate0_acc_04_h2o
dimethylsulfate1	h2o	O	OH	1.04	-1.74	0.11	-0.34	dimethylsulfate1_acc_04_h2o
dioxolane	h2o	O	OH	1.54	-1.74	-1.43	-1.55	dioxolane_acc_04_h2o
methylbutyrate	h2o	O	OH	1.58	-1.74	-1.56	-1.31	methylbutyrate_acc_04_h2o
morpholine	h2o	O	OH	1.77	-1.74	-2.14	-1.89	morpholine_acc_04_h2o
n-propylformate0	h2o	O	OH	1.15	-1.74	-0.23	0.43	n-propylformate0_acc_04_h2o
1-propanethiol0	h2o	S	OH	1.32	-1.74	-1.15	-1.03	1-propanethiol0_acc_04_h2o
1-propanethiol1	h2o	S	OH	1.32	-1.74	-1.15	-1.11	1-propanethiol1_acc_04_h2o
1,4-pentadiene1	h2o	C	OH	0.98	-1.74	0.08	0.27	1,4-pentadiene1_acc_05_h2o
pyrrole	h2o	C	OH	1.08	-1.74	-0.29	-0.36	pyrrole_acc_05_h2o
2-amino-2-methylpropane0	h2o	N	OH	2.53	-1.74	-5.46	-4.74	2-amino-2-methylpropane0_acc_05_h2o
2-amino-2-methylpropane1	h2o	N	OH	2.53	-1.74	-5.46	-4.72	2-amino-2-methylpropane1_acc_05_h2o
isopropylamine	h2o	N	OH	2.45	-1.74	-5.17	-4.72	isopropylamine_acc_05_h2o
1,2-dimethoxyethane1	h2o	O	OH	1.64	-1.74	-1.74	-1.58	1,2-dimethoxyethane1_acc_05_h2o
1,2-dimethoxyethane2	h2o	O	OH	1.67	-1.74	-1.83	-1.58	1,2-dimethoxyethane2_acc_05_h2o
1,2-dimethoxyethane4	h2o	O	OH	1.67	-1.74	-1.83	-1.96	1,2-dimethoxyethane4_acc_05_h2o
1,2-dimethoxyethane5	h2o	O	OH	1.67	-1.74	-1.83	-2.07	1,2-dimethoxyethane5_acc_05_h2o
1-butanol1	h2o	O	OH	1.81	-1.74	-2.27	-2.24	1-butanol1_acc_05_h2o

2-butanol0	h2o	O	OH	1.85	-1.74	-2.39	-2.39	2-butanol0_acc_05_h2o
2-butanol1	h2o	O	OH	1.8	-1.74	-2.23	-2.09	2-butanol1_acc_05_h2o
2-butanol2	h2o	O	OH	1.81	-1.74	-2.27	-2.09	2-butanol2_acc_05_h2o
2-butanol3	h2o	O	OH	1.83	-1.74	-2.33	-2.24	2-butanol3_acc_05_h2o
butadione	h2o	O	OH	1.48	-1.74	-1.25	-0.34	butadione_acc_05_h2o
butanone	h2o	O	OH	1.73	-1.74	-2.02	-1.66	butanone_acc_05_h2o
dimethylsulfate1	h2o	O	OH	1.05	-1.74	0.08	-0.33	dimethylsulfate1_acc_05_h2o
glycol1	h2o	O	OH	1.77	-1.74	-2.14	-2.18	glycol1_acc_05_h2o
glycol2	h2o	O	OH	1.77	-1.74	-2.14	-2.33	glycol2_acc_05_h2o
isobutanol0	h2o	O	OH	1.8	-1.74	-2.23	-1.99	isobutanol0_acc_05_h2o
isobutanol1	h2o	O	OH	1.78	-1.74	-2.17	-2.09	isobutanol1_acc_05_h2o
isobutanol2	h2o	O	OH	1.83	-1.74	-2.33	-2.26	isobutanol2_acc_05_h2o
methylbutyrate	h2o	O	OH	1.18	-1.74	-0.32	0.10	methylbutyrate_acc_05_h2o
methyl-t-butylether	h2o	O	OH	1.8	-1.74	-2.23	-1.94	methyl-t-butylether_acc_05_h2o
dimethylsulfide	h2o	S	OH	1.42	-1.74	-1.52	-1.71	dimethylsulfide_acc_05_h2o
1-heptene0	h2o	C	OH	1.02	-1.74	-0.07	0.10	1-heptene0_acc_06_h2o
1-heptene1	h2o	C	OH	1.02	-1.74	-0.07	-0.12	1-heptene1_acc_06_h2o
1-heptene2	h2o	C	OH	1.03	-1.74	-0.10	0.15	1-heptene2_acc_06_h2o
1-heptene3	h2o	C	OH	1.02	-1.74	-0.07	0.33	1-heptene3_acc_06_h2o
1-heptene4	h2o	C	OH	1.06	-1.74	-0.22	0.05	1-heptene4_acc_06_h2o
1-heptene5	h2o	C	OH	1.02	-1.74	-0.07	0.45	1-heptene5_acc_06_h2o
1-hexene0	h2o	C	OH	1.02	-1.74	-0.07	0.05	1-hexene0_acc_06_h2o
1-hexene2	h2o	C	OH	1	-1.74	0.01	-0.14	1-hexene2_acc_06_h2o
1-hexene3	h2o	C	OH	1	-1.74	0.01	0.20	1-hexene3_acc_06_h2o
1-hexene4	h2o	C	OH	1.02	-1.74	-0.07	0.38	1-hexene4_acc_06_h2o
2-butyne	h2o	C	OH	1.03	-1.74	-0.10	-0.23	2-butyne_acc_06_h2o
butene	h2o	C	OH	1	-1.74	0.01	-0.16	butene_acc_06_h2o
hexyne	h2o	C	OH	1.01	-1.74	-0.03	0.00	hexyne_acc_06_h2o
octene	h2o	C	OH	1	-1.74	0.01	-0.15	octene_acc_06_h2o
octyne	h2o	C	OH	1.01	-1.74	-0.03	-0.01	octyne_acc_06_h2o

pentyne	h2o	C	OH	1	-1.74	0.01	0.04	pentyne_acc_06_h2o
2-methylpyrazine	h2o	N	OH	1.98	-1.74	-3.48	-2.97	2-methylpyrazine_acc_06_h2o
2-methylpyridine	h2o	N	OH	2.18	-1.74	-4.20	-3.96	2-methylpyridine_acc_06_h2o
1-nitropropane0	h2o	O	OH	1.34	-1.74	-0.82	-0.86	1-nitropropane0_acc_06_h2o
1-nitropropane1	h2o	O	OH	1.35	-1.74	-0.85	-0.67	1-nitropropane1_acc_06_h2o
2-nitropropane	h2o	O	OH	1.33	-1.74	-0.78	-0.72	2-nitropropane_acc_06_h2o
2-pentanone	h2o	O	OH	1.73	-1.74	-2.02	-2.24	2-pentanone_acc_06_h2o
3-methyl-2-butanone	h2o	O	OH	1.77	-1.74	-2.14	-2.13	3-methyl-2-butanone_acc_06_h2o
butadione	h2o	O	OH	1.48	-1.74	-1.25	-1.24	butadione_acc_06_h2o
dimethylsulfate0	h2o	O	OH	0.83	-1.74	0.76	0.92	dimethylsulfate0_acc_06_h2o
dimethylsulfone	h2o	O	OH	1.44	-1.74	-1.12	-0.78	dimethylsulfone_acc_06_h2o
dimethylsulfoxide	h2o	O	OH	1.89	-1.74	-2.51	-2.88	dimethylsulfoxide_acc_06_h2o
di-n-pentylether0	h2o	O	OH	1.75	-1.74	-2.08	-1.43	di-n-pentylether0_acc_06_h2o
di-n-pentylether1	h2o	O	OH	1.78	-1.74	-2.17	-2.30	di-n-pentylether1_acc_06_h2o
ethoxyethanol0	h2o	O	OH	1.79	-1.74	-2.20	-2.07	ethoxyethanol0_acc_06_h2o
ethoxyethanol1	h2o	O	OH	1.79	-1.74	-2.20	-2.04	ethoxyethanol1_acc_06_h2o
ethoxyethanol2	h2o	O	OH	1.77	-1.74	-2.14	-2.05	ethoxyethanol2_acc_06_h2o
ethoxyethanol3	h2o	O	OH	1.75	-1.74	-2.08	-2.02	ethoxyethanol3_acc_06_h2o
ethoxyethanol4	h2o	O	OH	1.71	-1.74	-1.96	-1.94	ethoxyethanol4_acc_06_h2o
ethoxyethanol5	h2o	O	OH	1.72	-1.74	-1.99	-1.96	ethoxyethanol5_acc_06_h2o
ethoxyethanol7	h2o	O	OH	1.74	-1.74	-2.05	-2.38	ethoxyethanol7_acc_06_h2o
ethoxyethanol8	h2o	O	OH	1.77	-1.74	-2.14	-2.08	ethoxyethanol8_acc_06_h2o
ethoxyethanol9	h2o	O	OH	1.75	-1.74	-2.08	-2.04	ethoxyethanol9_acc_06_h2o
nitroethane0	h2o	O	OH	1.34	-1.74	-0.82	-0.73	nitroethane0_acc_06_h2o
nitroethane1	h2o	O	OH	1.34	-1.74	-0.82	-0.72	nitroethane1_acc_06_h2o
nitromethane	h2o	O	OH	1.33	-1.74	-0.78	-0.64	nitromethane_acc_06_h2o
n-propylformate0	h2o	O	OH	1.56	-1.74	-1.49	-1.74	n-propylformate0_acc_06_h2o
n-propylformate1	h2o	O	OH	1.55	-1.74	-1.46	-1.70	n-propylformate1_acc_06_h2o
dimethyldisulfide	h2o	S	OH	1.09	-1.74	-0.31	-0.67	dimethyldisulfide_acc_06_h2o
1-nitropropane0	h2o	O	OH	1.34	-1.74	-0.82	-0.60	1-nitropropane0_acc_07_h2o

1-nitropropane1	h2o	O	OH	1.34	-1.74	-0.82	-0.73	1-nitropropane1_acc_07_h2o
1-nitropropane2	h2o	O	OH	1.35	-1.74	-0.85	-0.76	1-nitropropane2_acc_07_h2o
2-nitropropane	h2o	O	OH	1.34	-1.74	-0.82	-0.64	2-nitropropane_acc_07_h2o
4-bromophenol0	h2o	O	OH	1.27	-1.74	-0.60	-0.48	4-bromophenol0_acc_07_h2o
4-bromophenol1	h2o	O	OH	1.27	-1.74	-0.60	-0.60	4-bromophenol1_acc_07_h2o
cyclohexanone	h2o	O	OH	1.78	-1.74	-2.17	-2.14	cyclohexanone_acc_07_h2o
dimethylsulfone	h2o	O	OH	1.44	-1.74	-1.12	-0.71	dimethylsulfone_acc_07_h2o
furfural0	h2o	O	OH	1.68	-1.74	-1.86	-2.35	furfural0_acc_07_h2o
furfural1	h2o	O	OH	1.67	-1.74	-1.83	-2.32	furfural1_acc_07_h2o
nitroethane0	h2o	O	OH	1.34	-1.74	-0.82	-0.60	nitroethane0_acc_07_h2o
propynol0	h2o	O	OH	1.64	-1.74	-1.74	-1.72	propynol0_acc_07_h2o
propynol1	h2o	O	OH	1.64	-1.74	-1.74	-1.66	propynol1_acc_07_h2o
propynol2	h2o	O	OH	1.64	-1.74	-1.74	-1.78	propynol2_acc_07_h2o
3-cyanophenol	h2o	N	OH	1.44	-1.74	-1.53	-1.56	3-cyanophenol_acc_08_h2o
chinoline	h2o	N	OH	2.18	-1.74	-4.20	-3.59	chinoline_acc_08_h2o
1-heptanol0	h2o	O	OH	1.8	-1.74	-2.23	-2.23	1-heptanol0_acc_08_h2o
1-heptanol1	h2o	O	OH	1.81	-1.74	-2.27	-2.16	1-heptanol1_acc_08_h2o
2-heptanone	h2o	O	OH	1.74	-1.74	-2.05	-2.25	2-heptanone_acc_08_h2o
2-octanone	h2o	O	OH	1.74	-1.74	-2.05	-2.25	2-octanone_acc_08_h2o
3-hydroxybenzaldehyde0	h2o	O	OH	1.26	-1.74	-0.57	-0.48	3-hydroxybenzaldehyde0_acc_08_h2o
3-hydroxybenzaldehyde2	h2o	O	OH	1.25	-1.74	-0.54	-0.34	3-hydroxybenzaldehyde2_acc_08_h2o
dioxane	h2o	O	OH	1.68	-1.74	-1.86	-1.68	dioxane_acc_08_h2o
ethanol0	h2o	O	OH	1.81	-1.74	-2.27	-2.20	ethanol0_acc_08_h2o
methylbenzoate	h2o	O	OH	1.49	-1.74	-1.28	-0.98	methylbenzoate_acc_08_h2o
1-nonene0	h2o	C	OH	1.01	-1.74	-0.03	-0.14	1-nonene0_acc_09_h2o
1-nonene1	h2o	C	OH	0.99	-1.74	0.05	-0.15	1-nonene1_acc_09_h2o
1,2-diaminoethane0	h2o	N	OH	2.43	-1.74	-5.10	-5.11	1,2-diaminoethane0_acc_09_h2o
1,2-diaminoethane1	h2o	N	OH	2.49	-1.74	-5.32	-5.33	1,2-diaminoethane1_acc_09_h2o
1,2-diaminoethane2	h2o	N	OH	2.55	-1.74	-5.53	-5.20	1,2-diaminoethane2_acc_09_h2o
1,2-diaminoethane3	h2o	N	OH	2.49	-1.74	-5.32	-4.76	1,2-diaminoethane3_acc_09_h2o

1,2-dimethoxyethane3	h2o	O	OH	1.67	-1.74	-1.83	-2.17	1,2-dimethoxyethane3_acc_09_h2o
4-(1,1-dimethylethyl)-phenol	h2o	O	OH	1.35	-1.74	-0.85	-1.37	4-(1,1-dimethylethyl)-phenol_acc_09_h2o
4-cyanophenol	h2o	O	OH	1.17	-1.74	-0.29	-0.18	4-cyanophenol_acc_09_h2o
anisole	h2o	O	OH	1.31	-1.74	-0.72	-0.44	anisole_acc_09_h2o
glycol0	h2o	O	OH	1.76	-1.74	-2.11	-2.03	glycol0_acc_09_h2o
glycol2	h2o	O	OH	1.77	-1.74	-2.14	-2.08	glycol2_acc_09_h2o
glycol3	h2o	O	OH	1.71	-1.74	-1.96	-2.00	glycol3_acc_09_h2o
propanol1	h2o	O	OH	1.81	-1.74	-2.27	-2.26	propanol1_acc_09_h2o
1,4-pentadiene1	h2o	C	OH	0.96	-1.74	0.16	0.33	1,4-pentadiene1_acc_10_h2o
aniline	h2o	N	OH	1.69	-1.74	-2.43	-2.75	aniline_acc_10_h2o
2-methylphenol0	h2o	O	OH	1.28	-1.74	-0.63	-0.46	2-methylphenol0_acc_10_h2o
2-methylphenol1	h2o	O	OH	1.33	-1.74	-0.78	-0.65	2-methylphenol1_acc_10_h2o
4-methylphenol	h2o	O	OH	1.36	-1.74	-0.88	-0.71	4-methylphenol_acc_10_h2o
chinone	h2o	O	OH	1.51	-1.74	-1.34	-1.17	chinone_acc_10_h2o
phenol	h2o	O	OH	1.32	-1.74	-0.75	-0.76	phenol_acc_10_h2o
cyclohexanol0	h2o	O	OH	1.85	-1.74	-2.39	-2.18	cyclohexanol0_acc_11_h2o
cyclohexanol1	h2o	O	OH	1.85	-1.74	-2.39	-2.36	cyclohexanol1_acc_11_h2o
methyl-n-propylether	h2o	O	OH	1.7	-1.74	-1.93	-1.83	methyl-n-propylether_acc_11_h2o
2-methyl-propanenitrile	h2o	N	OH	1.51	-1.74	-1.79	-1.75	2-methyl-propanenitrile_acc_12_h2o
3-nitrophenol	h2o	O	OH	1.2	-1.74	-0.38	-0.29	3-nitrophenol_acc_12_h2o
methylthiobenzene	h2o	S	OH	1.06	-1.74	-0.20	-0.70	methylthiobenzene_acc_12_h2o
thiophenol	h2o	S	OH	0.98	-1.74	0.10	-0.44	thiophenol_acc_12_h2o
benzonitrile	h2o	N	OH	1.45	-1.74	-1.57	-1.57	benzonitrile_acc_13_h2o
1-bromo-2-nitrobenzene	h2o	O	OH	1.27	-1.74	-0.60	-0.63	1-bromo-2-nitrobenzene_acc_13_h2o
2-nitrotoluene	h2o	O	OH	1.34	-1.74	-0.82	-0.81	2-nitrotoluene_acc_13_h2o
3-cyano-1-nitrobenzene	h2o	O	OH	1.23	-1.74	-0.48	-0.54	3-cyano-1-nitrobenzene_acc_13_h2o
3-hydroxybenzaldehyde0	h2o	O	OH	1.64	-1.74	-1.74	-2.14	3-hydroxybenzaldehyde0_acc_13_h2o
3-hydroxybenzaldehyde1	h2o	O	OH	1.64	-1.74	-1.74	-2.16	3-hydroxybenzaldehyde1_acc_13_h2o
3-hydroxybenzaldehyde2	h2o	O	OH	1.64	-1.74	-1.74	-2.13	3-hydroxybenzaldehyde2_acc_13_h2o
3-nitrophenol	h2o	O	OH	1.33	-1.74	-0.78	-0.78	3-nitrophenol_acc_13_h2o

3-nitrotoluene	h2o	O	OH	1.34	-1.74	-0.82	-0.80	3-nitrotoluene_acc_13_h2o
4-nitrophenol	h2o	O	OH	1.45	-1.74	-1.16	-1.06	4-nitrophenol_acc_13_h2o
acetophenone	h2o	O	OH	1.74	-1.74	-2.05	-2.11	acetophenone_acc_13_h2o
benzaldehyde	h2o	O	OH	1.65	-1.74	-1.77	-2.15	benzaldehyde_acc_13_h2o
dimethylbenzenesulfonamide	h2o	O	OH	1.34	-1.74	-0.82	-0.43	dimethylbenzenesulfonamide_acc_13_h2o
nitrobenzene	h2o	O	OH	1.33	-1.74	-0.78	-0.78	nitrobenzene_acc_13_h2o
dimethylbenzenesulfonamide	h2o	N	OH	1.24	-1.74	-0.81	0.09	dimethylbenzenesulfonamide_acc_14_h2o
1-bromo-2-nitrobenzene	h2o	O	OH	1.3	-1.74	-0.69	-0.62	1-bromo-2-nitrobenzene_acc_14_h2o
2-nitrotoluene	h2o	O	OH	1.39	-1.74	-0.97	-0.82	2-nitrotoluene_acc_14_h2o
3-nitrophenol	h2o	O	OH	1.36	-1.74	-0.88	-0.76	3-nitrophenol_acc_14_h2o
3-nitrotoluene	h2o	O	OH	1.38	-1.74	-0.94	-0.83	3-nitrotoluene_acc_14_h2o
tert-butanol	h2o	O	OH	1.87	-1.74	-2.45	-2.18	tert-butanol_acc_14_h2o
3-cyano-1-nitrobenzene	h2o	N	OH	1.37	-1.74	-1.28	-1.37	3-cyano-1-nitrobenzene_acc_15_h2o
benzylamine0	h2o	N	OH	2.39	-1.74	-4.96	-4.96	benzylamine0_acc_15_h2o
benzylamine1	h2o	N	OH	2.38	-1.74	-4.92	-4.67	benzylamine1_acc_15_h2o
benzylamine2	h2o	N	OH	2.38	-1.74	-4.92	-4.63	benzylamine2_acc_15_h2o
1-pentanol0	h2o	O	OH	1.84	-1.74	-2.36	-2.22	1-pentanol0_acc_17_h2o
1-pentanol1	h2o	O	OH	1.81	-1.74	-2.27	-2.14	1-pentanol1_acc_17_h2o
1-octanol0	h2o	O	OH	1.8	-1.74	-2.23	-2.39	1-octanol0_acc_26_h2o
1-octanol1	h2o	O	OH	1.81	-1.74	-2.27	-2.24	1-octanol1_acc_26_h2o
1-decene	h2s	C	SH	0.97	-1.18	0.77	0.36	1-decene_acc_01_h2s
cyclopentene	h2s	C	SH	1.06	-1.18	0.62	0.38	cyclopentene_acc_01_h2s
pentene2	h2s	C	SH	1.03	-1.18	0.67	0.43	pentene2_acc_01_h2s
pentene4	h2s	C	SH	0.99	-1.18	0.74	0.41	pentene4_acc_01_h2s
2,4-dimethylpyridine	h2s	N	SH	2.24	-1.18	-1.26	-1.52	2,4-dimethylpyridine_acc_01_h2s
2,6-dimethylpyridine	h2s	N	SH	2.22	-1.18	-1.23	-0.62	2,6-dimethylpyridine_acc_01_h2s
2-propenenitrile	h2s	N	SH	1.44	-1.18	0.03	0.28	2-propenenitrile_acc_01_h2s
4-cyanophenol	h2s	N	SH	1.49	-1.18	-0.05	0.21	4-cyanophenol_acc_01_h2s
acetonitrile	h2s	N	SH	1.51	-1.18	-0.08	0.20	acetonitrile_acc_01_h2s
butyronitrile	h2s	N	SH	1.51	-1.18	-0.08	0.22	butyronitrile_acc_01_h2s

hcn	h2s	N	SH	1.34	-1.18	0.19	0.33	hcn_acc_01_h2s
propionitrile	h2s	N	SH	1.51	-1.18	-0.08	0.20	propionitrile_acc_01_h2s
pyrazine	h2s	N	SH	1.95	-1.18	-0.80	-0.89	pyrazine_acc_01_h2s
pyridazine	h2s	N	SH	2.01	-1.18	-0.89	-1.21	pyridazine_acc_01_h2s
pyridine	h2s	N	SH	2.17	-1.18	-1.15	-1.65	pyridine_acc_01_h2s
1,2-epoxypropane	h2s	O	SH	1.63	-1.18	-0.05	-0.39	1,2-epoxypropane_acc_01_h2s
3-cyanophenol	h2s	O	SH	1.21	-1.18	0.53	0.63	3-cyanophenol_acc_01_h2s
acetaldehyde	h2s	O	SH	1.65	-1.18	-0.08	0.06	acetaldehyde_acc_01_h2s
acetamide	h2s	O	SH	1.94	-1.18	-0.48	-0.19	acetamide_acc_01_h2s
butanal	h2s	O	SH	1.65	-1.18	-0.08	-0.33	butanal_acc_01_h2s
butoxide	h2s	O	SH	1.63	-1.18	-0.05	-0.39	butoxide_acc_01_h2s
diethylcarbonate0	h2s	O	SH	1.48	-1.18	0.16	0.54	diethylcarbonate0_acc_01_h2s
diethylcarbonate2	h2s	O	SH	1.42	-1.18	0.24	0.60	diethylcarbonate2_acc_01_h2s
diethylcarbonate3	h2s	O	SH	1.65	-1.18	-0.08	0.33	diethylcarbonate3_acc_01_h2s
diethylcarbonate4	h2s	O	SH	1.64	-1.18	-0.06	0.28	diethylcarbonate4_acc_01_h2s
dimethylcarbonate0	h2s	O	SH	1.45	-1.18	0.20	0.59	dimethylcarbonate0_acc_01_h2s
dimethylcarbonate1	h2s	O	SH	1.61	-1.18	-0.02	0.17	dimethylcarbonate1_acc_01_h2s
dimethylether	h2s	O	SH	1.68	-1.18	-0.12	-0.31	dimethylether_acc_01_h2s
dimethylformamide	h2s	O	SH	1.89	-1.18	-0.41	-0.84	dimethylformamide_acc_01_h2s
di-n-butylether1	h2s	O	SH	1.74	-1.18	-0.20	-0.35	di-n-butylether1_acc_01_h2s
dioxolane	h2s	O	SH	1.54	-1.18	0.08	-0.03	dioxolane_acc_01_h2s
ethanol1	h2s	O	SH	1.82	-1.18	-0.31	-0.24	ethanol1_acc_01_h2s
ethyleneoxide	h2s	O	SH	1.57	-1.18	0.03	-0.29	ethyleneoxide_acc_01_h2s
formaldehyde	h2s	O	SH	1.49	-1.18	0.14	-0.07	formaldehyde_acc_01_h2s
formamide	h2s	O	SH	1.85	-1.18	-0.35	-0.77	formamide_acc_01_h2s
formicacid	h2s	O	SH	1.06	-1.18	0.74	0.72	formicacid_acc_01_h2s
furane	h2s	O	SH	1.07	-1.18	0.73	0.71	furane_acc_01_h2s
h2o	h2s	O	SH	1.82	-1.18	-0.31	-0.22	h2o_acc_01_h2s
hexanal	h2s	O	SH	1.65	-1.18	-0.08	-0.37	hexanal_acc_01_h2s
isobutanal	h2s	O	SH	1.62	-1.18	-0.04	0.32	isobutanal_acc_01_h2s

methylformamide	h2s	O	SH	1.9	-1.18	-0.42	-0.81	methylformamide_acc_01_h2s
methylurethane	h2s	O	SH	1.71	-1.18	-0.16	0.29	methylurethane_acc_01_h2s
n,n-dimethylacetamide	h2s	O	SH	1.99	-1.18	-0.55	-0.58	n,n-dimethylacetamide_acc_01_h2s
n-methylacetamide	h2s	O	SH	1.96	-1.18	-0.51	-0.64	n-methylacetamide_acc_01_h2s
octanal	h2s	O	SH	1.65	-1.18	-0.08	-0.37	octanal_acc_01_h2s
propanal	h2s	O	SH	1.64	-1.18	-0.06	0.27	propanal_acc_01_h2s
propanol0	h2s	O	SH	1.83	-1.18	-0.33	-0.15	propanol0_acc_01_h2s
propanone	h2s	O	SH	1.75	-1.18	-0.22	-0.16	propanone_acc_01_h2s
thf	h2s	O	SH	1.79	-1.18	-0.27	-0.65	thf_acc_01_h2s
thp	h2s	O	SH	1.8	-1.18	-0.28	-0.23	thp_acc_01_h2s
2,2'-dichlorodiethylsulfide0	h2s	S	SH	1.07	-1.18	0.61	0.26	2,2'-dichlorodiethylsulfide0_acc_01_h2s
2,2'-dichlorodiethylsulfide1	h2s	S	SH	1.15	-1.18	0.48	0.19	2,2'-dichlorodiethylsulfide1_acc_01_h2s
2,2'-dichlorodiethylsulfide2	h2s	S	SH	1.14	-1.18	0.50	0.39	2,2'-dichlorodiethylsulfide2_acc_01_h2s
2,2'-dichlorodiethylsulfide3	h2s	S	SH	1.2	-1.18	0.40	0.37	2,2'-dichlorodiethylsulfide3_acc_01_h2s
butanethiol0	h2s	S	SH	1.31	-1.18	0.22	-0.03	butanethiol0_acc_01_h2s
butanethiol1	h2s	S	SH	1.32	-1.18	0.20	-0.21	butanethiol1_acc_01_h2s
diethylsulfide	h2s	S	SH	1.49	-1.18	-0.08	-0.39	diethylsulfide_acc_01_h2s
h2s	h2s	S	SH	1.15	-1.18	0.48	0.05	h2s_acc_01_h2s
methanethiol	h2s	S	SH	1.3	-1.18	0.23	-0.25	methanethiol_acc_01_h2s
2-methyl-2-butene	h2s	C	SH	1.01	-1.18	0.71	0.38	2-methyl-2-butene_acc_02_h2s
pentene0	h2s	C	SH	0.98	-1.18	0.76	0.56	pentene0_acc_02_h2s
propyne	h2s	C	SH	1	-1.18	0.72	0.46	propyne_acc_02_h2s
pyrimidine	h2s	N	SH	1.99	-1.18	-0.86	-0.89	pyrimidine_acc_02_h2s
1,2-dimethoxyethane2	h2s	O	SH	1.68	-1.18	-0.12	0.19	1,2-dimethoxyethane2_acc_02_h2s
1,2-dimethoxyethane5	h2s	O	SH	1.64	-1.18	-0.06	-0.01	1,2-dimethoxyethane5_acc_02_h2s
3-pentanone	h2s	O	SH	1.65	-1.18	-0.08	0.15	3-pentanone_acc_02_h2s
aceticacid0	h2s	O	SH	1.6	-1.18	-0.01	0.17	aceticacid0_acc_02_h2s
aceticacid1	h2s	O	SH	1.66	-1.18	-0.09	0.13	aceticacid1_acc_02_h2s
benzophenone	h2s	O	SH	1.66	-1.18	-0.09	0.07	benzophenone_acc_02_h2s
butyricacid0	h2s	O	SH	1.52	-1.18	0.10	0.43	butyricacid0_acc_02_h2s

butyricacid1	h2s	O	SH	1.66	-1.18	-0.09	0.11	butyricacid1_acc_02_h2s
diethylsulfate0	h2s	O	SH	1.05	-1.18	0.75	0.56	diethylsulfate0_acc_02_h2s
dimethoxymethane0	h2s	O	SH	1.57	-1.18	0.03	0.26	dimethoxymethane0_acc_02_h2s
dimethoxymethane1	h2s	O	SH	1.57	-1.18	0.03	0.19	dimethoxymethane1_acc_02_h2s
dimethoxymethane2	h2s	O	SH	1.65	-1.18	-0.08	0.21	dimethoxymethane2_acc_02_h2s
dimethoxymethane3	h2s	O	SH	1.58	-1.18	0.02	0.41	dimethoxymethane3_acc_02_h2s
di-n-propylether1	h2s	O	SH	1.76	-1.18	-0.23	-0.25	di-n-propylether1_acc_02_h2s
ethylacetate1	h2s	O	SH	1.63	-1.18	-0.05	0.02	ethylacetate1_acc_02_h2s
ethylformate0	h2s	O	SH	1.56	-1.18	0.05	-0.03	ethylformate0_acc_02_h2s
ethylformate1	h2s	O	SH	1.55	-1.18	0.06	0.03	ethylformate1_acc_02_h2s
ethylpropionate0	h2s	O	SH	1.57	-1.18	0.03	0.34	ethylpropionate0_acc_02_h2s
ethylpropionate1	h2s	O	SH	1.55	-1.18	0.06	0.37	ethylpropionate1_acc_02_h2s
h2o2	h2s	O	SH	1.42	-1.18	0.24	0.11	h2o2_acc_02_h2s
methanol	h2s	O	SH	1.79	-1.18	-0.27	-0.44	methanol_acc_02_h2s
methylacetate	h2s	O	SH	1.62	-1.18	-0.04	0.04	methylacetate_acc_02_h2s
methylformate	h2s	O	SH	1.54	-1.18	0.08	0.04	methylformate_acc_02_h2s
propionicacid0	h2s	O	SH	1.57	-1.18	0.03	0.45	propionicacid0_acc_02_h2s
propionicacid1	h2s	O	SH	1.66	-1.18	-0.09	0.12	propionicacid1_acc_02_h2s
trifluoroaceticacid0	h2s	O	SH	1.16	-1.18	0.60	0.63	trifluoroaceticacid0_acc_02_h2s
trifluoroaceticacid1	h2s	O	SH	1.27	-1.18	0.45	0.43	trifluoroaceticacid1_acc_02_h2s
(methylthio)-ethane	h2s	S	SH	1.46	-1.18	-0.03	-0.50	(methylthio)-ethane_acc_02_h2s
1-methylcyclohexene	h2s	C	SH	1	-1.18	0.72	0.43	1-methylcyclohexene_acc_03_h2s
cis-2-butene	h2s	C	SH	1.05	-1.18	0.64	0.34	cis-2-butene_acc_03_h2s
cyclohexene	h2s	C	SH	0.97	-1.18	0.77	0.41	cyclohexene_acc_03_h2s
isobutene	h2s	C	SH	1	-1.18	0.72	0.23	isobutene_acc_03_h2s
propene	h2s	C	SH	1	-1.18	0.72	0.39	propene_acc_03_h2s
pyrrole	h2s	C	SH	1.08	-1.18	0.59	0.15	pyrrole_acc_03_h2s
2-methylpyrazine	h2s	N	SH	1.99	-1.18	-0.86	-0.99	2-methylpyrazine_acc_03_h2s
3-picoline	h2s	N	SH	2.19	-1.18	-1.18	-1.73	3-picoline_acc_03_h2s
imidazole	h2s	N	SH	2.25	-1.18	-1.28	-1.39	imidazole_acc_03_h2s

methylimidazol	h2s	N	SH	2.3	-1.18	-1.36	-1.28	methylimidazol_acc_03_h2s
2-propen-1-ol0	h2s	O	SH	1.75	-1.18	-0.22	-0.09	2-propen-1-ol0_acc_03_h2s
2-propen-1-ol2	h2s	O	SH	1.79	-1.18	-0.27	-0.07	2-propen-1-ol2_acc_03_h2s
aceticacid0	h2s	O	SH	1.1	-1.18	0.68	0.76	aceticacid0_acc_03_h2s
aceticacid1	h2s	O	SH	1.17	-1.18	0.59	0.78	aceticacid1_acc_03_h2s
butyricacid0	h2s	O	SH	1.13	-1.18	0.64	0.78	butyricacid0_acc_03_h2s
butyricacid1	h2s	O	SH	1.19	-1.18	0.56	0.82	butyricacid1_acc_03_h2s
diethylcarbonate1	h2s	O	SH	1.17	-1.18	0.59	1.03	diethylcarbonate1_acc_03_h2s
diethylcarbonate2	h2s	O	SH	1.17	-1.18	0.59	0.97	diethylcarbonate2_acc_03_h2s
diethylether1	h2s	O	SH	1.78	-1.18	-0.26	0.11	diethylether1_acc_03_h2s
diethylsulfate0	h2s	O	SH	1.05	-1.18	0.75	0.64	diethylsulfate0_acc_03_h2s
diethylsulfate1	h2s	O	SH	1.04	-1.18	0.77	0.58	diethylsulfate1_acc_03_h2s
dimethoxymethane0	h2s	O	SH	1.58	-1.18	0.02	0.05	dimethoxymethane0_acc_03_h2s
dimethoxymethane1	h2s	O	SH	1.57	-1.18	0.03	0.27	dimethoxymethane1_acc_03_h2s
dimethoxymethane2	h2s	O	SH	1.54	-1.18	0.08	0.33	dimethoxymethane2_acc_03_h2s
dimethylcarbonate1	h2s	O	SH	1.12	-1.18	0.66	1.00	dimethylcarbonate1_acc_03_h2s
ethoxyethanol2	h2s	O	SH	1.66	-1.18	-0.09	0.27	ethoxyethanol2_acc_03_h2s
ethoxyethanol3	h2s	O	SH	1.65	-1.18	-0.08	0.28	ethoxyethanol3_acc_03_h2s
ethoxyethanol7	h2s	O	SH	1.73	-1.18	-0.19	0.25	ethoxyethanol7_acc_03_h2s
ethoxyethanol8	h2s	O	SH	1.75	-1.18	-0.22	0.22	ethoxyethanol8_acc_03_h2s
ethylformate1	h2s	O	SH	1.14	-1.18	0.63	0.81	ethylformate1_acc_03_h2s
ethylpropionate1	h2s	O	SH	1.21	-1.18	0.53	0.84	ethylpropionate1_acc_03_h2s
formicacid	h2s	O	SH	1.49	-1.18	0.14	0.13	formicacid_acc_03_h2s
methylacetate	h2s	O	SH	1.13	-1.18	0.64	0.87	methylacetate_acc_03_h2s
methylformate	h2s	O	SH	1.1	-1.18	0.68	0.79	methylformate_acc_03_h2s
n-propylacetate1	h2s	O	SH	1.19	-1.18	0.56	0.93	n-propylacetate1_acc_03_h2s
propionicacid0	h2s	O	SH	1.16	-1.18	0.60	0.79	propionicacid0_acc_03_h2s
propionicacid1	h2s	O	SH	1.19	-1.18	0.56	0.83	propionicacid1_acc_03_h2s
ethanethiol0	h2s	S	SH	1.31	-1.18	0.22	-0.01	ethanethiol0_acc_03_h2s
ethanethiol1	h2s	S	SH	1.32	-1.18	0.20	-0.19	ethanethiol1_acc_03_h2s

2-propen-1-ol1	h2s	C	SH	0.98	-1.18	0.76	0.56	2-propen-1-ol1_acc_04_h2s
4-methylpyridine	h2s	N	SH	2.21	-1.18	-1.22	-1.80	4-methylpyridine_acc_04_h2s
dicyanomethane	h2s	N	SH	1.32	-1.18	0.22	0.36	dicyanomethane_acc_04_h2s
2-propanol0	h2s	O	SH	1.81	-1.18	-0.30	-0.23	2-propanol0_acc_04_h2s
2-propanol1	h2s	O	SH	1.83	-1.18	-0.33	-0.26	2-propanol1_acc_04_h2s
acrolein0	h2s	O	SH	1.64	-1.18	-0.06	-0.33	acrolein0_acc_04_h2s
acrolein1	h2s	O	SH	1.63	-1.18	-0.05	-0.31	acrolein1_acc_04_h2s
diethylcarbonate0	h2s	O	SH	1.15	-1.18	0.61	1.32	diethylcarbonate0_acc_04_h2s
diethylcarbonate1	h2s	O	SH	1.16	-1.18	0.60	1.22	diethylcarbonate1_acc_04_h2s
diethylcarbonate4	h2s	O	SH	1.2	-1.18	0.55	1.29	diethylcarbonate4_acc_04_h2s
diethylsulfate1	h2s	O	SH	0.88	-1.18	0.99	1.14	diethylsulfate1_acc_04_h2s
dimethylcarbonate0	h2s	O	SH	1.11	-1.18	0.67	0.87	dimethylcarbonate0_acc_04_h2s
dimethylsulfate1	h2s	O	SH	1.04	-1.18	0.77	0.60	dimethylsulfate1_acc_04_h2s
dioxolane	h2s	O	SH	1.54	-1.18	0.08	0.11	dioxolane_acc_04_h2s
methylbutyrate	h2s	O	SH	1.58	-1.18	0.02	0.38	methylbutyrate_acc_04_h2s
morpholine	h2s	O	SH	1.77	-1.18	-0.24	-0.10	morpholine_acc_04_h2s
n-propylformate0	h2s	O	SH	1.15	-1.18	0.61	0.98	n-propylformate0_acc_04_h2s
n-propylformate1	h2s	O	SH	1.14	-1.18	0.63	0.79	n-propylformate1_acc_04_h2s
1-propanethiol0	h2s	S	SH	1.32	-1.18	0.20	-0.02	1-propanethiol0_acc_04_h2s
1-propanethiol1	h2s	S	SH	1.32	-1.18	0.20	-0.21	1-propanethiol1_acc_04_h2s
1,4-pentadiene1	h2s	C	SH	0.96	-1.18	0.79	0.77	1,4-pentadiene1_acc_05_h2s
cyclopentene	h2s	C	SH	0.99	-1.18	0.74	0.34	cyclopentene_acc_05_h2s
pyrrole	h2s	C	SH	1.08	-1.18	0.59	0.26	pyrrole_acc_05_h2s
1,2-dimethoxyethane1	h2s	O	SH	1.64	-1.18	-0.06	0.06	1,2-dimethoxyethane1_acc_05_h2s
1,2-dimethoxyethane5	h2s	O	SH	1.67	-1.18	-0.10	-0.27	1,2-dimethoxyethane5_acc_05_h2s
1-butanol1	h2s	O	SH	1.81	-1.18	-0.30	-0.24	1-butanol1_acc_05_h2s
2-butanol0	h2s	O	SH	1.85	-1.18	-0.35	-0.27	2-butanol0_acc_05_h2s
2-butanol1	h2s	O	SH	1.8	-1.18	-0.28	-0.05	2-butanol1_acc_05_h2s
2-butanol2	h2s	O	SH	1.81	-1.18	-0.30	-0.04	2-butanol2_acc_05_h2s
2-butanol3	h2s	O	SH	1.83	-1.18	-0.33	-0.26	2-butanol3_acc_05_h2s

butadione	h2s	O	SH	1.48	-1.18	0.16	0.77	butadione_acc_05_h2s
butanone	h2s	O	SH	1.73	-1.18	-0.19	0.13	butanone_acc_05_h2s
dimethylsulfate0	h2s	O	SH	1.02	-1.18	0.79	0.64	dimethylsulfate0_acc_05_h2s
dimethylsulfate1	h2s	O	SH	1.05	-1.18	0.75	0.49	dimethylsulfate1_acc_05_h2s
glycol0	h2s	O	SH	1.69	-1.18	-0.13	-0.20	glycol0_acc_05_h2s
glycol1	h2s	O	SH	1.77	-1.18	-0.24	-0.16	glycol1_acc_05_h2s
glycol3	h2s	O	SH	1.72	-1.18	-0.17	-0.13	glycol3_acc_05_h2s
isobutanol0	h2s	O	SH	1.8	-1.18	-0.28	-0.05	isobutanol0_acc_05_h2s
isobutanol1	h2s	O	SH	1.78	-1.18	-0.26	-0.11	isobutanol1_acc_05_h2s
isobutanol2	h2s	O	SH	1.83	-1.18	-0.33	-0.22	isobutanol2_acc_05_h2s
methylbutyrate	h2s	O	SH	1.18	-1.18	0.57	0.86	methylbutyrate_acc_05_h2s
methyl-t-butylether	h2s	O	SH	1.8	-1.18	-0.28	0.01	methyl-t-butylether_acc_05_h2s
dimethylsulfide	h2s	S	SH	1.42	-1.18	0.04	-0.62	dimethylsulfide_acc_05_h2s
1-heptene0	h2s	C	SH	1.02	-1.18	0.69	0.58	1-heptene0_acc_06_h2s
1-heptene1	h2s	C	SH	1.02	-1.18	0.69	0.43	1-heptene1_acc_06_h2s
1-heptene2	h2s	C	SH	1.03	-1.18	0.67	0.55	1-heptene2_acc_06_h2s
1-heptene3	h2s	C	SH	1.02	-1.18	0.69	0.72	1-heptene3_acc_06_h2s
1-heptene4	h2s	C	SH	1.06	-1.18	0.62	0.57	1-heptene4_acc_06_h2s
1-heptene5	h2s	C	SH	1.02	-1.18	0.69	0.86	1-heptene5_acc_06_h2s
1-hexene0	h2s	C	SH	1.02	-1.18	0.69	0.56	1-hexene0_acc_06_h2s
1-hexene2	h2s	C	SH	1	-1.18	0.72	0.40	1-hexene2_acc_06_h2s
1-hexene3	h2s	C	SH	1	-1.18	0.72	0.66	1-hexene3_acc_06_h2s
1-hexene4	h2s	C	SH	1.02	-1.18	0.69	0.82	1-hexene4_acc_06_h2s
2-butyne	h2s	C	SH	1.03	-1.18	0.67	0.34	2-butyne_acc_06_h2s
butene	h2s	C	SH	1	-1.18	0.72	0.39	butene_acc_06_h2s
hexyne	h2s	C	SH	1.01	-1.18	0.71	0.46	hexyne_acc_06_h2s
octene	h2s	C	SH	1	-1.18	0.72	0.38	octene_acc_06_h2s
octyne	h2s	C	SH	1.01	-1.18	0.71	0.46	octyne_acc_06_h2s
pentyne	h2s	C	SH	1	-1.18	0.72	0.56	pentyne_acc_06_h2s
2-methylpyrazine	h2s	N	SH	1.98	-1.18	-0.84	-0.66	2-methylpyrazine_acc_06_h2s

2-methylpyridine	h2s	N	SH	2.18	-1.18	-1.17	-1.45	2-methylpyridine_acc_06_h2s
1-nitropropane0	h2s	O	SH	1.34	-1.18	0.35	0.44	1-nitropropane0_acc_06_h2s
1-nitropropane1	h2s	O	SH	1.34	-1.18	0.35	0.65	1-nitropropane1_acc_06_h2s
2-nitropropane	h2s	O	SH	1.33	-1.18	0.37	0.54	2-nitropropane_acc_06_h2s
2-pentanone	h2s	O	SH	1.73	-1.18	-0.19	-0.24	2-pentanone_acc_06_h2s
3-methyl-2-butanone	h2s	O	SH	1.77	-1.18	-0.24	-0.17	3-methyl-2-butanone_acc_06_h2s
butadione	h2s	O	SH	1.48	-1.18	0.16	0.25	butadione_acc_06_h2s
dimethylsulfate0	h2s	O	SH	0.83	-1.18	1.06	1.10	dimethylsulfate0_acc_06_h2s
dimethylsulfone	h2s	O	SH	1.44	-1.18	0.21	0.64	dimethylsulfone_acc_06_h2s
dimethylsulfoxide	h2s	O	SH	1.89	-1.18	-0.41	-0.59	dimethylsulfoxide_acc_06_h2s
di-n-pentylether1	h2s	O	SH	1.78	-1.18	-0.26	-0.28	di-n-pentylether1_acc_06_h2s
ethoxyethanol0	h2s	O	SH	1.79	-1.18	-0.27	-0.09	ethoxyethanol0_acc_06_h2s
ethoxyethanol1	h2s	O	SH	1.79	-1.18	-0.27	-0.08	ethoxyethanol1_acc_06_h2s
ethoxyethanol2	h2s	O	SH	1.77	-1.18	-0.24	-0.10	ethoxyethanol2_acc_06_h2s
ethoxyethanol3	h2s	O	SH	1.75	-1.18	-0.22	-0.09	ethoxyethanol3_acc_06_h2s
ethoxyethanol4	h2s	O	SH	1.71	-1.18	-0.16	-0.08	ethoxyethanol4_acc_06_h2s
ethoxyethanol5	h2s	O	SH	1.72	-1.18	-0.17	-0.11	ethoxyethanol5_acc_06_h2s
ethoxyethanol7	h2s	O	SH	1.74	-1.18	-0.20	-0.39	ethoxyethanol7_acc_06_h2s
ethoxyethanol8	h2s	O	SH	1.77	-1.18	-0.24	-0.15	ethoxyethanol8_acc_06_h2s
nitroethane0	h2s	O	SH	1.34	-1.18	0.35	0.50	nitroethane0_acc_06_h2s
n-propylformate0	h2s	O	SH	1.56	-1.18	0.05	-0.01	n-propylformate0_acc_06_h2s
n-propylformate1	h2s	O	SH	1.55	-1.18	0.06	0.04	n-propylformate1_acc_06_h2s
dimethyldisulfide	h2s	S	SH	1.09	-1.18	0.58	0.05	dimethyldisulfide_acc_06_h2s
1-nitropropane0	h2s	O	SH	1.34	-1.18	0.35	0.65	1-nitropropane0_acc_07_h2s
1-nitropropane1	h2s	O	SH	1.34	-1.18	0.35	0.52	1-nitropropane1_acc_07_h2s
1-nitropropane2	h2s	O	SH	1.35	-1.18	0.34	0.48	1-nitropropane2_acc_07_h2s
4-bromophenol0	h2s	O	SH	1.27	-1.18	0.45	0.52	4-bromophenol0_acc_07_h2s
4-nitrophenol	h2s	O	SH	1.11	-1.18	0.67	0.80	4-nitrophenol_acc_07_h2s
cyclohexanone	h2s	O	SH	1.78	-1.18	-0.26	-0.17	cyclohexanone_acc_07_h2s
dimethylsulfone	h2s	O	SH	1.44	-1.18	0.21	0.70	dimethylsulfone_acc_07_h2s

furfural0	h2s	O	SH	1.68	-1.18	-0.12	-0.42	furfural0_acc_07_h2s
furfural1	h2s	O	SH	1.67	-1.18	-0.10	-0.47	furfural1_acc_07_h2s
nitroethane0	h2s	O	SH	1.34	-1.18	0.35	0.56	nitroethane0_acc_07_h2s
nitroethane1	h2s	O	SH	1.34	-1.18	0.35	0.51	nitroethane1_acc_07_h2s
nitromethane	h2s	O	SH	1.33	-1.18	0.37	0.56	nitromethane_acc_07_h2s
propynol0	h2s	O	SH	1.64	-1.18	-0.06	0.10	propynol0_acc_07_h2s
propynol1	h2s	O	SH	1.64	-1.18	-0.06	0.11	propynol1_acc_07_h2s
3-cyanophenol	h2s	N	SH	1.44	-1.18	0.03	0.26	3-cyanophenol_acc_08_h2s
chinoline	h2s	N	SH	2.18	-1.18	-1.17	-1.09	chinoline_acc_08_h2s
1-heptanol0	h2s	O	SH	1.8	-1.18	-0.28	-0.24	1-heptanol0_acc_08_h2s
1-heptanol1	h2s	O	SH	1.81	-1.18	-0.30	-0.22	1-heptanol1_acc_08_h2s
3-hydroxybenzaldehyde0	h2s	O	SH	1.26	-1.18	0.46	0.56	3-hydroxybenzaldehyde0_acc_08_h2s
3-hydroxybenzaldehyde1	h2s	O	SH	1.25	-1.18	0.48	0.53	3-hydroxybenzaldehyde1_acc_08_h2s
3-hydroxybenzaldehyde2	h2s	O	SH	1.25	-1.18	0.48	0.56	3-hydroxybenzaldehyde2_acc_08_h2s
dioxane	h2s	O	SH	1.68	-1.18	-0.12	0.01	dioxane_acc_08_h2s
ethanol0	h2s	O	SH	1.81	-1.18	-0.30	-0.16	ethanol0_acc_08_h2s
methylbenzoate	h2s	O	SH	1.49	-1.18	0.14	0.49	methylbenzoate_acc_08_h2s
1-nonene0	h2s	C	SH	1.01	-1.18	0.71	0.42	1-nonene0_acc_09_h2s
1-nonene1	h2s	C	SH	0.99	-1.18	0.74	0.40	1-nonene1_acc_09_h2s
1,2-dimethoxyethane3	h2s	O	SH	1.67	-1.18	-0.10	-0.31	1,2-dimethoxyethane3_acc_09_h2s
4-(1,1-dimethylethyl)-phenol	h2s	O	SH	1.35	-1.18	0.34	-0.10	4-(1,1-dimethylethyl)-phenol_acc_09_h2s
4-cyanophenol	h2s	O	SH	1.17	-1.18	0.59	0.70	4-cyanophenol_acc_09_h2s
anisole	h2s	O	SH	1.31	-1.18	0.39	0.61	anisole_acc_09_h2s
glycol0	h2s	O	SH	1.76	-1.18	-0.23	-0.09	glycol0_acc_09_h2s
propanol1	h2s	O	SH	1.81	-1.18	-0.30	-0.27	propanol1_acc_09_h2s
aniline	h2s	N	SH	1.69	-1.18	-0.37	-0.94	aniline_acc_10_h2s
2-methylphenol0	h2s	O	SH	1.28	-1.18	0.44	0.61	2-methylphenol0_acc_10_h2s
2-methylphenol1	h2s	O	SH	1.33	-1.18	0.37	0.49	2-methylphenol1_acc_10_h2s
4-methylphenol	h2s	O	SH	1.36	-1.18	0.32	0.45	4-methylphenol_acc_10_h2s
chinone	h2s	O	SH	1.5	-1.18	0.13	0.33	chinone_acc_10_h2s

phenol	h2s	O	SH	1.32	-1.18	0.38	0.44	phenol_acc_10_h2s
cyclohexanol0	h2s	O	SH	1.85	-1.18	-0.35	-0.17	cyclohexanol0_acc_11_h2s
cyclohexanol1	h2s	O	SH	1.85	-1.18	-0.35	-0.27	cyclohexanol1_acc_11_h2s
methyl-n-propylether	h2s	O	SH	1.7	-1.18	-0.15	-0.05	methyl-n-propylether_acc_11_h2s
3-nitrophenol	h2s	O	SH	1.2	-1.18	0.55	0.63	3-nitrophenol_acc_12_h2s
methylthiobenzene	h2s	S	SH	1.06	-1.18	0.63	-0.04	methylthiobenzene_acc_12_h2s
thiophenol	h2s	S	SH	0.98	-1.18	0.76	0.10	thiophenol_acc_12_h2s
benzonitrile	h2s	N	SH	1.45	-1.18	0.01	0.26	benzonitrile_acc_13_h2s
1-bromo-2-nitrobenzene	h2s	O	SH	1.27	-1.18	0.45	0.57	1-bromo-2-nitrobenzene_acc_13_h2s
2-nitrotoluene	h2s	O	SH	1.34	-1.18	0.35	0.55	2-nitrotoluene_acc_13_h2s
3-cyano-1-nitrobenzene	h2s	O	SH	1.23	-1.18	0.50	0.59	3-cyano-1-nitrobenzene_acc_13_h2s
3-hydroxybenzaldehyde0	h2s	O	SH	1.64	-1.18	-0.06	-0.36	3-hydroxybenzaldehyde0_acc_13_h2s
3-hydroxybenzaldehyde1	h2s	O	SH	1.64	-1.18	-0.06	-0.36	3-hydroxybenzaldehyde1_acc_13_h2s
3-hydroxybenzaldehyde2	h2s	O	SH	1.64	-1.18	-0.06	-0.34	3-hydroxybenzaldehyde2_acc_13_h2s
3-nitrophenol	h2s	O	SH	1.33	-1.18	0.37	0.54	3-nitrophenol_acc_13_h2s
3-nitrotoluene	h2s	O	SH	1.34	-1.18	0.35	0.54	3-nitrotoluene_acc_13_h2s
acetophenone	h2s	O	SH	1.74	-1.18	-0.20	-0.12	acetophenone_acc_13_h2s
benzaldehyde	h2s	O	SH	1.65	-1.18	-0.08	-0.33	benzaldehyde_acc_13_h2s
dimethylbenzenesulfonamide	h2s	O	SH	1.34	-1.18	0.35	0.76	dimethylbenzenesulfonamide_acc_13_h2s
nitrobenzene	h2s	O	SH	1.33	-1.18	0.37	0.53	nitrobenzene_acc_13_h2s
1-bromo-2-nitrobenzene	h2s	O	SH	1.3	-1.18	0.41	0.56	1-bromo-2-nitrobenzene_acc_14_h2s
2-nitrotoluene	h2s	O	SH	1.39	-1.18	0.28	0.53	2-nitrotoluene_acc_14_h2s
3-nitrophenol	h2s	O	SH	1.36	-1.18	0.32	0.57	3-nitrophenol_acc_14_h2s
3-nitrotoluene	h2s	O	SH	1.38	-1.18	0.30	0.52	3-nitrotoluene_acc_14_h2s
4-nitrophenol	h2s	O	SH	1.45	-1.18	0.20	0.48	4-nitrophenol_acc_14_h2s
benzoicacid	h2s	O	SH	1.03	-1.18	0.78	1.13	benzoicacid_acc_14_h2s
tert-butanol	h2s	O	SH	1.87	-1.18	-0.38	-0.13	tert-butanol_acc_14_h2s
3-cyano-1-nitrobenzene	h2s	N	SH	1.37	-1.18	0.14	0.32	3-cyano-1-nitrobenzene_acc_15_h2s
1-pentanol0	h2s	O	SH	1.84	-1.18	-0.34	-0.19	1-pentanol0_acc_17_h2s
1-pentanol1	h2s	O	SH	1.81	-1.18	-0.30	-0.17	1-pentanol1_acc_17_h2s

1-octanol0	h2s	O	SH	1.8	-1.18	-0.28	-0.27	1-octanol0_acc_26_h2s
1-octanol1	h2s	O	SH	1.81	-1.18	-0.30	-0.28	1-octanol1_acc_26_h2s
1-decene	HF	C	FH	0.97	-2.29	-2.06	-2.60	1-decene_acc_01
cyclopentene	HF	C	FH	1.06	-2.29	-3.02	-3.02	cyclopentene_acc_01
pentene2	HF	C	FH	1.03	-2.29	-2.70	-2.68	pentene2_acc_01
pentene4	HF	C	FH	0.99	-2.29	-2.27	-2.72	pentene4_acc_01
2,4-dimethylpyridine	HF	N	FH	2.24	-2.29	-14.97	-14.76	2,4-dimethylpyridine_acc_01
2,6-dimethylpyridine	HF	N	FH	2.22	-2.29	-14.77	-14.16	2,6-dimethylpyridine_acc_01
2-propenenitrile	HF	N	FH	1.44	-2.29	-6.77	-6.46	2-propenenitrile_acc_01
4-cyanophenol	HF	N	FH	1.49	-2.29	-7.28	-6.93	4-cyanophenol_acc_01
acetonitrile	HF	N	FH	1.51	-2.29	-7.49	-7.01	acetonitrile_acc_01
aziridine	HF	N	FH	2.22	-2.29	-14.77	-15.88	aziridine_acc_01
butyronitrile	HF	N	FH	1.51	-2.29	-7.49	-6.96	butyronitrile_acc_01
hcn	HF	N	FH	1.34	-2.29	-5.74	-5.47	hcn_acc_01
morpholine	HF	N	FH	2.43	-2.29	-16.92	-16.08	morpholine_acc_01
nh3	HF	N	FH	2.43	-2.29	-16.92	-16.98	nh3_acc_01
propionitrile	HF	N	FH	1.51	-2.29	-7.49	-6.98	propionitrile_acc_01
pyridazine	HF	N	FH	2.01	-2.29	-12.61	-12.75	pyridazine_acc_01
pyridine	HF	N	FH	2.17	-2.29	-14.25	-14.23	pyridine_acc_01
1,2-epoxypropane	HF	O	FH	1.63	-2.29	-7.27	-8.05	1,2-epoxypropane_acc_01
3-cyanophenol	HF	O	FH	1.21	-2.29	-3.59	-3.83	3-cyanophenol_acc_01
acetaldehyde	HF	O	FH	1.65	-2.29	-7.45	-7.36	acetaldehyde_acc_01
acetamide	HF	O	FH	1.94	-2.29	-9.99	-10.30	acetamide_acc_01
butanal	HF	O	FH	1.65	-2.29	-7.45	-8.02	butanal_acc_01
butoxide	HF	O	FH	1.63	-2.29	-7.27	-8.08	butoxide_acc_01
diethylcarbonate0	HF	O	FH	1.48	-2.29	-5.95	-5.67	diethylcarbonate0_acc_01
diethylcarbonate1	HF	O	FH	1.47	-2.29	-5.87	-5.67	diethylcarbonate1_acc_01
diethylcarbonate2	HF	O	FH	1.42	-2.29	-5.43	-5.37	diethylcarbonate2_acc_01
diethylcarbonate3	HF	O	FH	1.65	-2.29	-7.45	-7.56	diethylcarbonate3_acc_01
diethylcarbonate4	HF	O	FH	1.64	-2.29	-7.36	-7.52	diethylcarbonate4_acc_01

dimethylcarbonate0	HF	O	FH	1.45	-2.29	-5.69	-5.43	dimethylcarbonate0_acc_01
dimethylcarbonate1	HF	O	FH	1.61	-2.29	-7.09	-7.30	dimethylcarbonate1_acc_01
dimethylether	HF	O	FH	1.68	-2.29	-7.71	-8.33	dimethylether_acc_01
dimethylformamide	HF	O	FH	1.89	-2.29	-9.55	-10.80	dimethylformamide_acc_01
di-n-butylether0	HF	O	FH	1.76	-2.29	-8.41	-7.85	di-n-butylether0_acc_01
di-n-butylether1	HF	O	FH	1.74	-2.29	-8.24	-8.75	di-n-butylether1_acc_01
dioxolane	HF	O	FH	1.54	-2.29	-6.48	-7.22	dioxolane_acc_01
ethanol1	HF	O	FH	1.82	-2.29	-8.94	-8.67	ethanol1_acc_01
ethyleneoxide	HF	O	FH	1.57	-2.29	-6.74	-7.57	ethyleneoxide_acc_01
formaldehyde	HF	O	FH	1.49	-2.29	-6.04	-6.46	formaldehyde_acc_01
formamide	HF	O	FH	1.85	-2.29	-9.20	-10.28	formamide_acc_01
formicacid	HF	O	FH	1.06	-2.29	-2.27	-2.47	formicacid_acc_01
furane	HF	O	FH	1.07	-2.29	-2.36	-2.59	furane_acc_01
h2o	HF	O	FH	1.82	-2.29	-8.94	-8.43	h2o_acc_01
h2o2	HF	O	FH	1.42	-2.29	-5.43	-5.73	h2o2_acc_01
hexanal	HF	O	FH	1.65	-2.29	-7.45	-8.03	hexanal_acc_01
isobutanal	HF	O	FH	1.62	-2.29	-7.18	-6.29	isobutanal_acc_01
methylformamide	HF	O	FH	1.9	-2.29	-9.64	-10.74	methylformamide_acc_01
methylurethane	HF	O	FH	1.71	-2.29	-7.97	-8.44	methylurethane_acc_01
n,n-dimethylacetamide	HF	O	FH	1.99	-2.29	-10.43	-11.33	n,n-dimethylacetamide_acc_01
n-methylacetamide	HF	O	FH	1.96	-2.29	-10.17	-11.14	n-methylacetamide_acc_01
octanal	HF	O	FH	1.65	-2.29	-7.45	-8.04	octanal_acc_01
propanal	HF	O	FH	1.64	-2.29	-7.36	-6.54	propanal_acc_01
propanol0	HF	O	FH	1.83	-2.29	-9.02	-8.58	propanol0_acc_01
propanone	HF	O	FH	1.75	-2.29	-8.32	-8.46	propanone_acc_01
thf	HF	O	FH	1.79	-2.29	-8.67	-9.38	thf_acc_01
thp	HF	O	FH	1.8	-2.29	-8.76	-8.57	thp_acc_01
2,2'-dichlorodiethylsulfide0	HF	S	FH	1.07	-2.29	-3.07	-3.96	2,2'-dichlorodiethylsulfide0_acc_01
2,2'-dichlorodiethylsulfide1	HF	S	FH	1.15	-2.29	-3.91	-4.42	2,2'-dichlorodiethylsulfide1_acc_01
2,2'-dichlorodiethylsulfide2	HF	S	FH	1.14	-2.29	-3.80	-4.09	2,2'-dichlorodiethylsulfide2_acc_01

2,2'-dichlorodiethylsulfide3	HF	S	FH	1.2	-2.29	-4.43	-4.23	2,2'-dichlorodiethylsulfide3_acc_01
butanethiol0	HF	S	FH	1.31	-2.29	-5.58	-5.22	butanethiol0_acc_01
butanethiol1	HF	S	FH	1.32	-2.29	-5.69	-5.36	butanethiol1_acc_01
diethylsulfide	HF	S	FH	1.49	-2.29	-7.47	-6.56	diethylsulfide_acc_01
h2s	HF	S	FH	1.15	-2.29	-3.91	-4.08	h2s_acc_01
methanethiol	HF	S	FH	1.3	-2.29	-5.48	-5.42	methanethiol_acc_01
2-methyl-2-butene	HF	C	FH	1.01	-2.29	-2.49	-3.18	2-methyl-2-butene_acc_02
cis-2-butene	HF	C	FH	1.05	-2.29	-2.91	-2.98	cis-2-butene_acc_02
cyclohexene	HF	C	FH	0.97	-2.29	-2.06	-2.91	cyclohexene_acc_02
pentene0	HF	C	FH	0.98	-2.29	-2.17	-2.36	pentene0_acc_02
propyne	HF	C	FH	1	-2.29	-2.38	-2.50	propyne_acc_02
methylamine	HF	N	FH	2.49	-2.29	-17.54	-18.40	methylamine_acc_02
1,2-dimethoxyethane2	HF	O	FH	1.68	-2.29	-7.71	-7.77	1,2-dimethoxyethane2_acc_02
1,2-dimethoxyethane4	HF	O	FH	1.67	-2.29	-7.62	-8.35	1,2-dimethoxyethane4_acc_02
1,2-dimethoxyethane5	HF	O	FH	1.64	-2.29	-7.36	-7.62	1,2-dimethoxyethane5_acc_02
3-pentanone	HF	O	FH	1.65	-2.29	-7.45	-7.34	3-pentanone_acc_02
aceticacid0	HF	O	FH	1.6	-2.29	-7.01	-7.21	aceticacid0_acc_02
aceticacid1	HF	O	FH	1.66	-2.29	-7.53	-7.50	aceticacid1_acc_02
benzophenone	HF	O	FH	1.66	-2.29	-7.53	-7.62	benzophenone_acc_02
butyricacid0	HF	O	FH	1.52	-2.29	-6.30	-6.23	butyricacid0_acc_02
butyricacid1	HF	O	FH	1.66	-2.29	-7.53	-7.51	butyricacid1_acc_02
diethylsulfate0	HF	O	FH	1.05	-2.29	-2.18	-3.04	diethylsulfate0_acc_02
diethylsulfate2	HF	O	FH	1.02	-2.29	-1.92	-2.56	diethylsulfate2_acc_02
dimethoxymethane0	HF	O	FH	1.58	-2.29	-6.83	-7.18	dimethoxymethane0_acc_02
dimethoxymethane1	HF	O	FH	1.57	-2.29	-6.74	-6.91	dimethoxymethane1_acc_02
dimethoxymethane2	HF	O	FH	1.65	-2.29	-7.45	-7.59	dimethoxymethane2_acc_02
dimethylsulfate1	HF	O	FH	0.86	-2.29	-0.51	-0.82	dimethylsulfate1_acc_02
di-n-propylether0	HF	O	FH	1.76	-2.29	-8.41	-7.82	di-n-propylether0_acc_02
di-n-propylether1	HF	O	FH	1.76	-2.29	-8.41	-8.69	di-n-propylether1_acc_02
ethylacetate1	HF	O	FH	1.63	-2.29	-7.27	-7.72	ethylacetate1_acc_02

ethylformate0	HF	O	FH	1.56	-2.29	-6.66	-7.13	ethylformate0_acc_02
ethylformate1	HF	O	FH	1.55	-2.29	-6.57	-7.10	ethylformate1_acc_02
ethylpropionate0	HF	O	FH	1.57	-2.29	-6.74	-6.69	ethylpropionate0_acc_02
ethylpropionate1	HF	O	FH	1.55	-2.29	-6.57	-6.69	ethylpropionate1_acc_02
methanol	HF	O	FH	1.79	-2.29	-8.67	-8.78	methanol_acc_02
methylacetate	HF	O	FH	1.62	-2.29	-7.18	-7.56	methylacetate_acc_02
n-propylacetate0	HF	O	FH	1.64	-2.29	-7.36	-7.72	n-propylacetate0_acc_02
n-propylacetate1	HF	O	FH	1.62	-2.29	-7.18	-7.76	n-propylacetate1_acc_02
propionicacid0	HF	O	FH	1.57	-2.29	-6.74	-6.23	propionicacid0_acc_02
propionicacid1	HF	O	FH	1.66	-2.29	-7.53	-7.52	propionicacid1_acc_02
trifluoroaceticacid0	HF	O	FH	1.16	-2.29	-3.15	-3.55	trifluoroaceticacid0_acc_02
trifluoroaceticacid1	HF	O	FH	1.27	-2.29	-4.11	-4.35	trifluoroaceticacid1_acc_02
(methylthio)-ethane	HF	S	FH	1.46	-2.29	-7.15	-6.61	(methylthio)-ethane_acc_02
1-methylcyclohexene	HF	C	FH	1	-2.29	-2.38	-3.07	1-methylcyclohexene_acc_03
isobutene	HF	C	FH	1	-2.29	-2.38	-3.19	isobutene_acc_03
propene	HF	C	FH	1	-2.29	-2.38	-2.63	propene_acc_03
pyrrole	HF	C	FH	1.08	-2.29	-3.23	-3.09	pyrrole_acc_03
1-butylamine	HF	N	FH	2.5	-2.29	-17.64	-17.81	1-butylamine_acc_03
2-methylpyrazine	HF	N	FH	1.99	-2.29	-12.41	-11.96	2-methylpyrazine_acc_03
3-picoline	HF	N	FH	2.19	-2.29	-14.46	-14.47	3-picoline_acc_03
ethylamine1	HF	N	FH	2.49	-2.29	-17.54	-17.93	ethylamine1_acc_03
ethylamine2	HF	N	FH	2.52	-2.29	-17.84	-17.85	ethylamine2_acc_03
hexylamine	HF	N	FH	2.5	-2.29	-17.64	-17.82	hexylamine_acc_03
imidazole	HF	N	FH	2.25	-2.29	-15.07	-14.82	imidazole_acc_03
methylimidazol	HF	N	FH	2.3	-2.29	-15.59	-15.04	methylimidazol_acc_03
n-pentylamine	HF	N	FH	2.5	-2.29	-17.64	-17.83	n-pentylamine_acc_03
n-propylamine	HF	N	FH	2.49	-2.29	-17.54	-17.80	n-propylamine_acc_03
pyrimidine	HF	N	FH	1.99	-2.29	-12.41	-11.81	pyrimidine_acc_03
2-propen-1-ol0	HF	O	FH	1.75	-2.29	-8.32	-8.03	2-propen-1-ol0_acc_03
2-propen-1-ol1	HF	O	FH	1.77	-2.29	-8.50	-7.87	2-propen-1-ol1_acc_03

2-propen-1-ol2	HF	O	FH	1.79	-2.29	-8.67	-8.31	2-propen-1-ol2_acc_03
aceticacid0	HF	O	FH	1.1	-2.29	-2.62	-2.92	aceticacid0_acc_03
aceticacid1	HF	O	FH	1.17	-2.29	-3.23	-3.27	aceticacid1_acc_03
butyricacid0	HF	O	FH	1.13	-2.29	-2.88	-3.06	butyricacid0_acc_03
butyricacid1	HF	O	FH	1.19	-2.29	-3.41	-3.31	butyricacid1_acc_03
diethylcarbonate1	HF	O	FH	1.17	-2.29	-3.23	-3.01	diethylcarbonate1_acc_03
diethylcarbonate2	HF	O	FH	1.17	-2.29	-3.23	-3.17	diethylcarbonate2_acc_03
diethylether0	HF	O	FH	1.73	-2.29	-8.15	-7.89	diethylether0_acc_03
diethylether1	HF	O	FH	1.78	-2.29	-8.59	-8.34	diethylether1_acc_03
diethylsulfate1	HF	O	FH	1.04	-2.29	-2.09	-3.01	diethylsulfate1_acc_03
diethylsulfate2	HF	O	FH	1.07	-2.29	-2.36	-2.96	diethylsulfate2_acc_03
dimethoxymethane2	HF	O	FH	1.54	-2.29	-6.48	-6.65	dimethoxymethane2_acc_03
dimethoxymethane3	HF	O	FH	1.58	-2.29	-6.83	-6.66	dimethoxymethane3_acc_03
dimethylcarbonate0	HF	O	FH	1.11	-2.29	-2.71	-2.84	dimethylcarbonate0_acc_03
dimethylcarbonate1	HF	O	FH	1.12	-2.29	-2.80	-2.92	dimethylcarbonate1_acc_03
ethoxyethanol0	HF	O	FH	1.61	-2.29	-7.09	-7.23	ethoxyethanol0_acc_03
ethoxyethanol1	HF	O	FH	1.61	-2.29	-7.09	-7.22	ethoxyethanol1_acc_03
ethoxyethanol2	HF	O	FH	1.66	-2.29	-7.53	-7.59	ethoxyethanol2_acc_03
ethoxyethanol3	HF	O	FH	1.65	-2.29	-7.45	-7.82	ethoxyethanol3_acc_03
ethoxyethanol4	HF	O	FH	1.64	-2.29	-7.36	-7.22	ethoxyethanol4_acc_03
ethoxyethanol7	HF	O	FH	1.73	-2.29	-8.15	-7.90	ethoxyethanol7_acc_03
ethoxyethanol8	HF	O	FH	1.75	-2.29	-8.32	-8.00	ethoxyethanol8_acc_03
ethylacetate0	HF	O	FH	1.17	-2.29	-3.23	-2.68	ethylacetate0_acc_03
ethylformate0	HF	O	FH	1.11	-2.29	-2.71	-2.44	ethylformate0_acc_03
ethylformate1	HF	O	FH	1.14	-2.29	-2.97	-2.85	ethylformate1_acc_03
ethylpropionate0	HF	O	FH	1.19	-2.29	-3.41	-2.81	ethylpropionate0_acc_03
ethylpropionate1	HF	O	FH	1.21	-2.29	-3.59	-3.44	ethylpropionate1_acc_03
ethylpropionate2	HF	O	FH	1.15	-2.29	-3.06	-2.55	ethylpropionate2_acc_03
formicacid	HF	O	FH	1.49	-2.29	-6.04	-6.53	formicacid_acc_03
methylacetate	HF	O	FH	1.13	-2.29	-2.88	-3.05	methylacetate_acc_03

methylformate	HF	O	FH	1.1	-2.29	-2.62	-2.62	methylformate_acc_03
n-propylacetate0	HF	O	FH	1.18	-2.29	-3.32	-2.66	n-propylacetate0_acc_03
n-propylacetate1	HF	O	FH	1.19	-2.29	-3.41	-3.23	n-propylacetate1_acc_03
propionicacid0	HF	O	FH	1.16	-2.29	-3.15	-3.01	propionicacid0_acc_03
propionicacid1	HF	O	FH	1.19	-2.29	-3.41	-3.32	propionicacid1_acc_03
ethanethiol0	HF	S	FH	1.31	-2.29	-5.58	-5.24	ethanethiol0_acc_03
ethanethiol1	HF	S	FH	1.32	-2.29	-5.69	-5.36	ethanethiol1_acc_03
2-propen-1-ol1	HF	C	FH	0.98	-2.29	-2.17	-2.28	2-propen-1-ol1_acc_04
4-methylpyridine	HF	N	FH	2.21	-2.29	-14.66	-14.71	4-methylpyridine_acc_04
dicyanomethane	HF	N	FH	1.32	-2.29	-5.54	-5.43	dicyanomethane_acc_04
pyrazine	HF	N	FH	1.95	-2.29	-12.00	-11.63	pyrazine_acc_04
2-propanol0	HF	O	FH	1.81	-2.29	-8.85	-8.71	2-propanol0_acc_04
2-propanol1	HF	O	FH	1.83	-2.29	-9.02	-8.76	2-propanol1_acc_04
acrolein0	HF	O	FH	1.64	-2.29	-7.36	-8.06	acrolein0_acc_04
acrolein1	HF	O	FH	1.63	-2.29	-7.27	-8.06	acrolein1_acc_04
diethylcarbonate0	HF	O	FH	1.15	-2.29	-3.06	-2.52	diethylcarbonate0_acc_04
diethylcarbonate1	HF	O	FH	1.16	-2.29	-3.15	-2.65	diethylcarbonate1_acc_04
diethylcarbonate2	HF	O	FH	1.18	-2.29	-3.32	-3.17	diethylcarbonate2_acc_04
diethylcarbonate3	HF	O	FH	1.2	-2.29	-3.50	-2.77	diethylcarbonate3_acc_04
diethylcarbonate4	HF	O	FH	1.2	-2.29	-3.50	-2.78	diethylcarbonate4_acc_04
diethylsulfate1	HF	O	FH	0.88	-2.29	-0.69	-0.99	diethylsulfate1_acc_04
dimethylsulfate0	HF	O	FH	1.02	-2.29	-1.92	-2.85	dimethylsulfate0_acc_04
dimethylsulfate1	HF	O	FH	1.04	-2.29	-2.09	-3.17	dimethylsulfate1_acc_04
dioxolane	HF	O	FH	1.54	-2.29	-6.48	-7.04	dioxolane_acc_04
methylbutyrate	HF	O	FH	1.58	-2.29	-6.83	-6.54	methylbutyrate_acc_04
methylurethane	HF	O	FH	1.11	-2.29	-2.71	-2.93	methylurethane_acc_04
morpholine	HF	O	FH	1.77	-2.29	-8.50	-8.05	morpholine_acc_04
n-propylformate0	HF	O	FH	1.15	-2.29	-3.06	-2.40	n-propylformate0_acc_04
n-propylformate1	HF	O	FH	1.14	-2.29	-2.97	-2.80	n-propylformate1_acc_04
1-propanethiol0	HF	S	FH	1.32	-2.29	-5.69	-5.21	1-propanethiol0_acc_04

1-propanethiol1	HF	S	FH	1.32	-2.29	-5.69	-5.37	1-propanethiol1_acc_04
2-amino-2-methylpropane1	HF	N	FH	2.53	-2.29	-17.95	-16.99	2-amino-2-methylpropane1_acc_05
isopropylamine	HF	N	FH	2.45	-2.29	-17.13	-17.01	isopropylamine_acc_05
1,2-dimethoxyethane0	HF	O	FH	1.67	-2.29	-7.62	-6.78	1,2-dimethoxyethane0_acc_05
1,2-dimethoxyethane1	HF	O	FH	1.64	-2.29	-7.36	-7.32	1,2-dimethoxyethane1_acc_05
1,2-dimethoxyethane4	HF	O	FH	1.67	-2.29	-7.62	-8.13	1,2-dimethoxyethane4_acc_05
1,2-dimethoxyethane5	HF	O	FH	1.67	-2.29	-7.62	-7.99	1,2-dimethoxyethane5_acc_05
1-butanol0	HF	O	FH	1.81	-2.29	-8.85	-8.62	1-butanol0_acc_05
1-butanol1	HF	O	FH	1.81	-2.29	-8.85	-8.64	1-butanol1_acc_05
2-butanol0	HF	O	FH	1.85	-2.29	-9.20	-8.84	2-butanol0_acc_05
2-butanol1	HF	O	FH	1.8	-2.29	-8.76	-8.35	2-butanol1_acc_05
2-butanol2	HF	O	FH	1.81	-2.29	-8.85	-8.59	2-butanol2_acc_05
2-butanol3	HF	O	FH	1.83	-2.29	-9.02	-8.75	2-butanol3_acc_05
butadione	HF	O	FH	1.48	-2.29	-5.95	-6.14	butadione_acc_05
butanone	HF	O	FH	1.73	-2.29	-8.15	-7.21	butanone_acc_05
glycol0	HF	O	FH	1.69	-2.29	-7.80	-8.07	glycol0_acc_05
glycol1	HF	O	FH	1.77	-2.29	-8.50	-8.28	glycol1_acc_05
glycol2	HF	O	FH	1.77	-2.29	-8.50	-8.41	glycol2_acc_05
glycol3	HF	O	FH	1.72	-2.29	-8.06	-8.00	glycol3_acc_05
isobutanol0	HF	O	FH	1.8	-2.29	-8.76	-8.27	isobutanol0_acc_05
isobutanol1	HF	O	FH	1.78	-2.29	-8.59	-8.42	isobutanol1_acc_05
isobutanol2	HF	O	FH	1.83	-2.29	-9.02	-8.76	isobutanol2_acc_05
methylbutyrate	HF	O	FH	1.18	-2.29	-3.32	-3.18	methylbutyrate_acc_05
methyl-t-butylether	HF	O	FH	1.8	-2.29	-8.76	-8.59	methyl-t-butylether_acc_05
dimethyldisulfide	HF	S	FH	1.09	-2.29	-3.28	-4.03	dimethyldisulfide_acc_05
dimethylsulfide	HF	S	FH	1.42	-2.29	-6.73	-6.65	dimethylsulfide_acc_05
1-heptene0	HF	C	FH	1.02	-2.29	-2.59	-2.37	1-heptene0_acc_06
1-heptene1	HF	C	FH	1.02	-2.29	-2.59	-2.69	1-heptene1_acc_06
1-heptene2	HF	C	FH	1.03	-2.29	-2.70	-2.43	1-heptene2_acc_06
1-heptene3	HF	C	FH	1.02	-2.29	-2.59	-2.42	1-heptene3_acc_06

1-heptene4	HF	C	FH	1.06	-2.29	-3.02	-2.59	1-heptene4_acc_06
1-heptene5	HF	C	FH	1.02	-2.29	-2.59	-2.30	1-heptene5_acc_06
1-heptene6	HF	C	FH	1.03	-2.29	-2.70	-2.36	1-heptene6_acc_06
1-hexene0	HF	C	FH	1.02	-2.29	-2.59	-2.41	1-hexene0_acc_06
1-hexene2	HF	C	FH	1	-2.29	-2.38	-2.61	1-hexene2_acc_06
1-hexene3	HF	C	FH	1	-2.29	-2.38	-2.33	1-hexene3_acc_06
1-hexene4	HF	C	FH	1.02	-2.29	-2.59	-2.37	1-hexene4_acc_06
2-butyne	HF	C	FH	1.03	-2.29	-2.70	-3.23	2-butyne_acc_06
butene	HF	C	FH	1	-2.29	-2.38	-2.57	butene_acc_06
hexyne	HF	C	FH	1.01	-2.29	-2.49	-2.46	hexyne_acc_06
octene	HF	C	FH	1	-2.29	-2.38	-2.59	octene_acc_06
octyne	HF	C	FH	1.01	-2.29	-2.49	-2.45	octyne_acc_06
pentyne	HF	C	FH	1	-2.29	-2.38	-2.41	pentyne_acc_06
2-methylpyrazine	HF	N	FH	1.98	-2.29	-12.31	-11.74	2-methylpyrazine_acc_06
2-methylpyridine	HF	N	FH	2.18	-2.29	-14.36	-14.28	2-methylpyridine_acc_06
1-nitropropane0	HF	O	FH	1.34	-2.29	-4.73	-4.67	1-nitropropane0_acc_06
1-nitropropane1	HF	O	FH	1.32	-2.29	-4.55	-4.52	1-nitropropane1_acc_06
1-nitropropane2	HF	O	FH	1.34	-2.29	-4.73	-4.51	1-nitropropane2_acc_06
2-nitropropane	HF	O	FH	1.33	-2.29	-4.64	-4.57	2-nitropropane_acc_06
2-pentanone	HF	O	FH	1.73	-2.29	-8.15	-8.55	2-pentanone_acc_06
3-methyl-2-butanone	HF	O	FH	1.77	-2.29	-8.50	-8.53	3-methyl-2-butanone_acc_06
dimethylsulfone	HF	O	FH	1.44	-2.29	-5.60	-4.97	dimethylsulfone_acc_06
di-n-pentylether0	HF	O	FH	1.75	-2.29	-8.32	-7.87	di-n-pentylether0_acc_06
di-n-pentylether1	HF	O	FH	1.78	-2.29	-8.59	-8.73	di-n-pentylether1_acc_06
ethoxyethanol0	HF	O	FH	1.79	-2.29	-8.67	-8.18	ethoxyethanol0_acc_06
ethoxyethanol1	HF	O	FH	1.79	-2.29	-8.67	-8.18	ethoxyethanol1_acc_06
ethoxyethanol2	HF	O	FH	1.77	-2.29	-8.50	-8.23	ethoxyethanol2_acc_06
ethoxyethanol3	HF	O	FH	1.75	-2.29	-8.32	-8.20	ethoxyethanol3_acc_06
ethoxyethanol4	HF	O	FH	1.71	-2.29	-7.97	-7.78	ethoxyethanol4_acc_06
ethoxyethanol5	HF	O	FH	1.72	-2.29	-8.06	-7.90	ethoxyethanol5_acc_06

ethoxyethanol7	HF	O	FH	1.74	-2.29	-8.24	-8.47	ethoxyethanol7_acc_06
ethoxyethanol8	HF	O	FH	1.77	-2.29	-8.50	-8.41	ethoxyethanol8_acc_06
ethoxyethanol9	HF	O	FH	1.75	-2.29	-8.32	-8.20	ethoxyethanol9_acc_06
nitroethane0	HF	O	FH	1.34	-2.29	-4.73	-4.70	nitroethane0_acc_06
n-propylformate0	HF	O	FH	1.56	-2.29	-6.66	-7.10	n-propylformate0_acc_06
n-propylformate1	HF	O	FH	1.55	-2.29	-6.57	-7.06	n-propylformate1_acc_06
1-nitropropane0	HF	O	FH	1.34	-2.29	-4.73	-4.39	1-nitropropane0_acc_07
1-nitropropane1	HF	O	FH	1.35	-2.29	-4.81	-4.50	1-nitropropane1_acc_07
1-nitropropane2	HF	O	FH	1.32	-2.29	-4.55	-4.50	1-nitropropane2_acc_07
2-nitropropane	HF	O	FH	1.34	-2.29	-4.73	-4.43	2-nitropropane_acc_07
4-bromophenol0	HF	O	FH	1.27	-2.29	-4.11	-4.31	4-bromophenol0_acc_07
4-bromophenol1	HF	O	FH	1.45	-2.29	-5.69	-5.79	4-bromophenol1_acc_07
cyclohexanone	HF	O	FH	1.78	-2.29	-8.59	-8.54	cyclohexanone_acc_07
furfural0	HF	O	FH	1.68	-2.29	-7.71	-8.73	furfural0_acc_07
furfural1	HF	O	FH	1.67	-2.29	-7.62	-8.65	furfural1_acc_07
nitroethane0	HF	O	FH	1.34	-2.29	-4.73	-4.40	nitroethane0_acc_07
nitroethane1	HF	O	FH	1.34	-2.29	-4.73	-4.49	nitroethane1_acc_07
nitromethane	HF	O	FH	1.33	-2.29	-4.64	-4.42	nitromethane_acc_07
propynol0	HF	O	FH	1.64	-2.29	-7.36	-7.15	propynol0_acc_07
propynol1	HF	O	FH	1.64	-2.29	-7.36	-7.22	propynol1_acc_07
propynol2	HF	O	FH	1.64	-2.29	-7.36	-7.15	propynol2_acc_07
3-cyanophenol	HF	N	FH	1.44	-2.29	-6.77	-6.48	3-cyanophenol_acc_08
chinoline	HF	N	FH	2.18	-2.29	-14.36	-13.49	chinoline_acc_08
1-heptanol0	HF	O	FH	1.8	-2.29	-8.76	-8.61	1-heptanol0_acc_08
1-heptanol1	HF	O	FH	1.81	-2.29	-8.85	-8.65	1-heptanol1_acc_08
2-heptanone	HF	O	FH	1.74	-2.29	-8.24	-8.66	2-heptanone_acc_08
2-octanone	HF	O	FH	1.74	-2.29	-8.24	-8.54	2-octanone_acc_08
3-hydroxybenzaldehyde0	HF	O	FH	1.26	-2.29	-4.02	-4.07	3-hydroxybenzaldehyde0_acc_08
3-hydroxybenzaldehyde1	HF	O	FH	1.25	-2.29	-3.94	-4.12	3-hydroxybenzaldehyde1_acc_08
3-hydroxybenzaldehyde2	HF	O	FH	1.25	-2.29	-3.94	-4.10	3-hydroxybenzaldehyde2_acc_08

dioxane	HF	O	FH	1.68	-2.29	-7.71	-7.47	dioxane_acc_08
ethanol0	HF	O	FH	1.81	-2.29	-8.85	-8.67	ethanol0_acc_08
methylbenzoate	HF	O	FH	1.49	-2.29	-6.04	-5.96	methylbenzoate_acc_08
1-nonene0	HF	C	FH	1.01	-2.29	-2.49	-2.61	1-nonene0_acc_09
1-nonene1	HF	C	FH	0.99	-2.29	-2.27	-2.56	1-nonene1_acc_09
1,2-diaminoethane0	HF	N	FH	2.43	-2.29	-16.92	-17.08	1,2-diaminoethane0_acc_09
1,2-diaminoethane3	HF	N	FH	2.49	-2.29	-17.54	-16.89	1,2-diaminoethane3_acc_09
1,2-dimethoxyethane3	HF	O	FH	1.67	-2.29	-7.62	-8.25	1,2-dimethoxyethane3_acc_09
4-(1,1-dimethylethyl)-phenol	HF	O	FH	1.35	-2.29	-4.81	-5.00	4-(1,1-dimethylethyl)-phenol_acc_09
4-cyanophenol	HF	O	FH	1.17	-2.29	-3.23	-3.45	4-cyanophenol_acc_09
anisole	HF	O	FH	1.31	-2.29	-4.46	-4.45	anisole_acc_09
glycol0	HF	O	FH	1.76	-2.29	-8.41	-8.27	glycol0_acc_09
glycol1	HF	O	FH	1.73	-2.29	-8.15	-8.03	glycol1_acc_09
glycol2	HF	O	FH	1.77	-2.29	-8.50	-8.28	glycol2_acc_09
glycol3	HF	O	FH	1.71	-2.29	-7.97	-7.84	glycol3_acc_09
propanol1	HF	O	FH	1.81	-2.29	-8.85	-8.65	propanol1_acc_09
1,4-pentadiene1	HF	C	FH	0.98	-2.29	-2.17	-1.98	1,4-pentadiene1_acc_10
aniline	HF	N	FH	1.69	-2.29	-9.33	-10.70	aniline_acc_10
2-methylphenol0	HF	O	FH	1.28	-2.29	-4.20	-4.44	2-methylphenol0_acc_10
2-methylphenol1	HF	O	FH	1.33	-2.29	-4.64	-4.69	2-methylphenol1_acc_10
4-methylphenol	HF	O	FH	1.36	-2.29	-4.90	-5.00	4-methylphenol_acc_10
chinone	HF	O	FH	1.51	-2.29	-6.22	-6.29	chinone_acc_10
phenol	HF	O	FH	1.32	-2.29	-4.55	-4.76	phenol_acc_10
cyclohexanol0	HF	O	FH	1.85	-2.29	-9.20	-8.67	cyclohexanol0_acc_11
cyclohexanol1	HF	O	FH	1.85	-2.29	-9.20	-9.00	cyclohexanol1_acc_11
diisopropylether	HF	O	FH	1.84	-2.29	-9.11	-8.06	diisopropylether_acc_11
methyl-n-propylether	HF	O	FH	1.7	-2.29	-7.88	-8.14	methyl-n-propylether_acc_11
2-methyl-propanenitrile	HF	N	FH	1.51	-2.29	-7.49	-6.93	2-methyl-propanenitrile_acc_12
3-nitrophenol	HF	O	FH	1.2	-2.29	-3.50	-3.67	3-nitrophenol_acc_12
dimethylbenzenesulfonamide	HF	O	FH	1.34	-2.29	-4.73	-4.34	dimethylbenzenesulfonamide_acc_12

methylthiobenzene	HF	S	FH	1.06	-2.29	-2.96	-4.28	methylthiobenzene_acc_12
thiophenol	HF	S	FH	0.98	-2.29	-2.12	-3.42	thiophenol_acc_12
benzonitrile	HF	N	FH	1.45	-2.29	-6.87	-6.51	benzonitrile_acc_13
1-bromo-2-nitrobenzene	HF	O	FH	1.27	-2.29	-4.11	-4.35	1-bromo-2-nitrobenzene_acc_13
2-nitrotoluene	HF	O	FH	1.34	-2.29	-4.73	-4.85	2-nitrotoluene_acc_13
3-cyano-1-nitrobenzene	HF	O	FH	1.23	-2.29	-3.76	-4.09	3-cyano-1-nitrobenzene_acc_13
3-hydroxybenzaldehyde0	HF	O	FH	1.64	-2.29	-7.36	-8.16	3-hydroxybenzaldehyde0_acc_13
3-hydroxybenzaldehyde1	HF	O	FH	1.64	-2.29	-7.36	-8.16	3-hydroxybenzaldehyde1_acc_13
3-hydroxybenzaldehyde2	HF	O	FH	1.64	-2.29	-7.36	-8.09	3-hydroxybenzaldehyde2_acc_13
3-nitrophenol	HF	O	FH	1.33	-2.29	-4.64	-4.75	3-nitrophenol_acc_13
3-nitrotoluene	HF	O	FH	1.34	-2.29	-4.73	-4.85	3-nitrotoluene_acc_13
4-nitrophenol	HF	O	FH	1.45	-2.29	-5.69	-5.55	4-nitrophenol_acc_13
acetophenone	HF	O	FH	1.74	-2.29	-8.24	-8.50	acetophenone_acc_13
benzaldehyde	HF	O	FH	1.65	-2.29	-7.45	-8.18	benzaldehyde_acc_13
nitrobenzene	HF	O	FH	1.33	-2.29	-4.64	-4.75	nitrobenzene_acc_13
1-bromo-2-nitrobenzene	HF	O	FH	1.3	-2.29	-4.37	-4.35	1-bromo-2-nitrobenzene_acc_14
2-nitrotoluene	HF	O	FH	1.39	-2.29	-5.16	-4.98	2-nitrotoluene_acc_14
3-cyano-1-nitrobenzene	HF	O	FH	1.26	-2.29	-4.02	-4.09	3-cyano-1-nitrobenzene_acc_14
3-nitrophenol	HF	O	FH	1.36	-2.29	-4.90	-4.73	3-nitrophenol_acc_14
3-nitrotoluene	HF	O	FH	1.38	-2.29	-5.08	-4.85	3-nitrotoluene_acc_14
tert-butanol	HF	O	FH	1.87	-2.29	-9.38	-8.63	tert-butanol_acc_14
3-cyano-1-nitrobenzene	HF	N	FH	1.37	-2.29	-6.05	-5.91	3-cyano-1-nitrobenzene_acc_15
benzylamine0	HF	N	FH	2.39	-2.29	-16.51	-16.58	benzylamine0_acc_15
benzylamine2	HF	N	FH	2.38	-2.29	-16.41	-16.37	benzylamine2_acc_15
1-pentanol0	HF	O	FH	1.84	-2.29	-9.11	-8.60	1-pentanol0_acc_17
1-pentanol1	HF	O	FH	1.81	-2.29	-8.85	-8.65	1-pentanol1_acc_17
1-octanol0	HF	O	FH	1.8	-2.29	-8.76	-8.62	1-octanol0_acc_26
1-octanol1	HF	O	FH	1.81	-2.29	-8.85	-8.65	1-octanol1_acc_26
1-decene	HCP	C	CH	0.97	-1.34	0.94	0.68	1-decene_accw_1_HCP
pentene2	HCP	C	CH	1.03	-1.34	0.88	0.76	pentene2_accw_1_HCP

pentene4	HCP	C	CH	0.99	-1.34	0.92	0.73	pentene4_accw_1_HCP
2,4-dimethylpyridine	HCP	N	CH	2.24	-1.34	-0.43	-0.06	2,4-dimethylpyridine_accw_1_HCP
2,6-dimethylpyridine	HCP	N	CH	2.22	-1.34	-0.41	0.28	2,6-dimethylpyridine_accw_1_HCP
2-propenenitrile	HCP	N	CH	1.44	-1.34	0.44	0.39	2-propenenitrile_accw_1_HCP
4-cyanophenol	HCP	N	CH	1.49	-1.34	0.39	0.37	4-cyanophenol_accw_1_HCP
acetonitrile	HCP	N	CH	1.51	-1.34	0.37	0.37	acetonitrile_accw_1_HCP
aziridine	HCP	N	CH	2.22	-1.34	-0.41	-0.33	aziridine_accw_1_HCP
butyronitrile	HCP	N	CH	1.51	-1.34	0.37	0.36	butyronitrile_accw_1_HCP
dibutylamine	HCP	N	CH	2.5	-1.34	-0.72	-0.34	dibutylamine_accw_1_HCP
diethylamine0	HCP	N	CH	2.53	-1.34	-0.75	-0.23	diethylamine0_accw_1_HCP
diethylamine1	HCP	N	CH	2.51	-1.34	-0.73	-0.41	diethylamine1_accw_1_HCP
dimethylamine	HCP	N	CH	2.47	-1.34	-0.68	-0.56	dimethylamine_accw_1_HCP
dipropylamine	HCP	N	CH	2.5	-1.34	-0.72	-0.30	dipropylamine_accw_1_HCP
hcn	HCP	N	CH	1.34	-1.34	0.55	0.44	hcn_accw_1_HCP
morpholine	HCP	N	CH	2.43	-1.34	-0.64	-0.14	morpholine_accw_1_HCP
nh3	HCP	N	CH	2.43	-1.34	-0.64	-0.19	nh3_accw_1_HCP
piperidine	HCP	N	CH	2.53	-1.34	-0.75	-0.25	piperidine_accw_1_HCP
propionitrile	HCP	N	CH	1.51	-1.34	0.37	0.37	propionitrile_accw_1_HCP
pyrazine	HCP	N	CH	1.95	-1.34	-0.12	0.01	pyrazine_accw_1_HCP
pyridine	HCP	N	CH	2.17	-1.34	-0.36	-0.17	pyridine_accw_1_HCP
pyrrolidin	HCP	N	CH	2.49	-1.34	-0.71	-0.44	pyrrolidin_accw_1_HCP
triethylamine1	HCP	N	CH	2.29	-1.34	-0.49	-0.28	triethylamine1_accw_1_HCP
triethylamine2	HCP	N	CH	2.19	-1.34	-0.38	-0.33	triethylamine2_accw_1_HCP
1,2-epoxypropane	HCP	O	CH	1.63	-1.34	0.39	0.02	1,2-epoxypropane_accw_1_HCP
3-cyanophenol	HCP	O	CH	1.21	-1.34	0.78	0.68	3-cyanophenol_accw_1_HCP
acetaldehyde	HCP	O	CH	1.65	-1.34	0.37	0.33	acetaldehyde_accw_1_HCP
acetamide	HCP	O	CH	1.94	-1.34	0.10	0.27	acetamide_accw_1_HCP
butanal	HCP	O	CH	1.65	-1.34	0.37	0.09	butanal_accw_1_HCP
diethylcarbonate0	HCP	O	CH	1.48	-1.34	0.53	0.48	diethylcarbonate0_accw_1_HCP
diethylcarbonate2	HCP	O	CH	1.42	-1.34	0.59	0.53	diethylcarbonate2_accw_1_HCP

diethylcarbonate4	HCP	O	CH	1.64	-1.34	0.38	0.37	diethylcarbonate4_accw_1_HCP
dimethylcarbonate0	HCP	O	CH	1.45	-1.34	0.56	0.52	dimethylcarbonate0_accw_1_HCP
dimethylcarbonate1	HCP	O	CH	1.61	-1.34	0.41	0.39	dimethylcarbonate1_accw_1_HCP
dimethylether	HCP	O	CH	1.68	-1.34	0.34	0.10	dimethylether_accw_1_HCP
dimethylformamide	HCP	O	CH	1.89	-1.34	0.15	-0.12	dimethylformamide_accw_1_HCP
di-n-butylether0	HCP	O	CH	1.76	-1.34	0.27	0.61	di-n-butylether0_accw_1_HCP
dioxolane	HCP	O	CH	1.54	-1.34	0.47	0.26	dioxolane_accw_1_HCP
ethanol1	HCP	O	CH	1.82	-1.34	0.21	0.23	ethanol1_accw_1_HCP
ethyleneoxide	HCP	O	CH	1.57	-1.34	0.45	0.08	ethyleneoxide_accw_1_HCP
formaldehyde	HCP	O	CH	1.49	-1.34	0.52	0.26	formaldehyde_accw_1_HCP
formamide	HCP	O	CH	1.85	-1.34	0.18	-0.07	formamide_accw_1_HCP
formicacid	HCP	O	CH	1.06	-1.34	0.92	0.78	formicacid_accw_1_HCP
furane	HCP	O	CH	1.07	-1.34	0.91	0.74	furane_accw_1_HCP
h2o	HCP	O	CH	1.82	-1.34	0.21	0.22	h2o_accw_1_HCP
hexanal	HCP	O	CH	1.65	-1.34	0.37	0.08	hexanal_accw_1_HCP
isobutanal	HCP	O	CH	1.62	-1.34	0.40	0.37	isobutanal_accw_1_HCP
methylformamide	HCP	O	CH	1.9	-1.34	0.14	-0.10	methylformamide_accw_1_HCP
methylurethane	HCP	O	CH	1.71	-1.34	0.31	0.41	methylurethane_accw_1_HCP
n,n-dimethylacetamide	HCP	O	CH	1.99	-1.34	0.05	-0.03	n,n-dimethylacetamide_accw_1_HCP
n-methylacetamide	HCP	O	CH	1.96	-1.34	0.08	0.00	n-methylacetamide_accw_1_HCP
octanal	HCP	O	CH	1.65	-1.34	0.37	0.07	octanal_accw_1_HCP
propanal	HCP	O	CH	1.64	-1.34	0.38	0.34	propanal_accw_1_HCP
propanol0	HCP	O	CH	1.83	-1.34	0.20	0.17	propanol0_accw_1_HCP
propanone	HCP	O	CH	1.75	-1.34	0.28	0.22	propanone_accw_1_HCP
thf	HCP	O	CH	1.79	-1.34	0.24	-0.10	thf_accw_1_HCP
thp	HCP	O	CH	1.8	-1.34	0.23	0.12	thp_accw_1_HCP
2,2'-dichlorodiethylsulfide0	HCP	S	CH	1.07	-1.34	0.84	0.70	2,2'-dichlorodiethylsulfide0_accw_1_HCP
2,2'-dichlorodiethylsulfide1	HCP	S	CH	1.15	-1.34	0.75	0.67	2,2'-dichlorodiethylsulfide1_accw_1_HCP
2,2'-dichlorodiethylsulfide2	HCP	S	CH	1.14	-1.34	0.76	0.73	2,2'-dichlorodiethylsulfide2_accw_1_HCP
2,2'-dichlorodiethylsulfide3	HCP	S	CH	1.2	-1.34	0.69	0.65	2,2'-dichlorodiethylsulfide3_accw_1_HCP

butanethiol0	HCP	S	CH	1.31	-1.34	0.57	0.56	butanethiol0_accw_1_HCP
butanethiol1	HCP	S	CH	1.32	-1.34	0.56	0.51	butanethiol1_accw_1_HCP
diethylsulfide	HCP	S	CH	1.49	-1.34	0.37	0.44	diethylsulfide_accw_1_HCP
h2s	HCP	S	CH	1.15	-1.34	0.75	0.58	h2s_accw_1_HCP
methanethiol	HCP	S	CH	1.3	-1.34	0.58	0.44	methanethiol_accw_1_HCP
2-methyl-2-butene	HCP	C	CH	1.01	-1.34	0.90	0.65	2-methyl-2-butene_accw_2_HCP
pentene0	HCP	C	CH	0.98	-1.34	0.93	0.84	pentene0_accw_2_HCP
propyne	HCP	C	CH	1	-1.34	0.91	0.74	propyne_accw_2_HCP
methylamine	HCP	N	CH	2.49	-1.34	-0.71	-0.35	methylamine_accw_2_HCP
pyridazine	HCP	N	CH	2.01	-1.34	-0.18	-0.01	pyridazine_accw_2_HCP
1,2-dimethoxyethane0	HCP	O	CH	1.67	-1.34	0.35	0.76	1,2-dimethoxyethane0_accw_2_HCP
1,2-dimethoxyethane2	HCP	O	CH	1.68	-1.34	0.34	0.43	1,2-dimethoxyethane2_accw_2_HCP
1,2-dimethoxyethane5	HCP	O	CH	1.67	-1.34	0.35	0.24	1,2-dimethoxyethane5_accw_2_HCP
3-pentanone	HCP	O	CH	1.65	-1.34	0.37	0.23	3-pentanone_accw_2_HCP
aceticacid0	HCP	O	CH	1.6	-1.34	0.42	0.38	aceticacid0_accw_2_HCP
aceticacid1	HCP	O	CH	1.66	-1.34	0.36	0.40	aceticacid1_accw_2_HCP
benzophenone	HCP	O	CH	1.66	-1.34	0.36	0.25	benzophenone_accw_2_HCP
butyricacid0	HCP	O	CH	1.52	-1.34	0.49	0.40	butyricacid0_accw_2_HCP
butyricacid1	HCP	O	CH	1.66	-1.34	0.36	0.40	butyricacid1_accw_2_HCP
dimethoxymethane2	HCP	O	CH	1.65	-1.34	0.37	0.44	dimethoxymethane2_accw_2_HCP
dimethylsulfate1	HCP	O	CH	0.86	-1.34	1.11	1.09	dimethylsulfate1_accw_2_HCP
di-n-propylether0	HCP	O	CH	1.76	-1.34	0.27	0.62	di-n-propylether0_accw_2_HCP
di-n-propylether1	HCP	O	CH	1.76	-1.34	0.27	0.13	di-n-propylether1_accw_2_HCP
ethylacetate1	HCP	O	CH	1.63	-1.34	0.39	0.26	ethylacetate1_accw_2_HCP
ethylformate0	HCP	O	CH	1.56	-1.34	0.45	0.26	ethylformate0_accw_2_HCP
ethylformate1	HCP	O	CH	1.55	-1.34	0.46	0.25	ethylformate1_accw_2_HCP
ethylpropionate0	HCP	O	CH	1.57	-1.34	0.45	0.35	ethylpropionate0_accw_2_HCP
ethylpropionate1	HCP	O	CH	1.55	-1.34	0.46	0.32	ethylpropionate1_accw_2_HCP
h2o2	HCP	O	CH	1.42	-1.34	0.59	0.37	h2o2_accw_2_HCP
methanol	HCP	O	CH	1.79	-1.34	0.24	0.09	methanol_accw_2_HCP

methylacetate	HCP	O	CH	1.62	-1.34	0.40	0.29	methylacetate_accw_2_HCP
methylformate	HCP	O	CH	1.54	-1.34	0.47	0.29	methylformate_accw_2_HCP
propionicacid0	HCP	O	CH	1.57	-1.34	0.45	0.43	propionicacid0_accw_2_HCP
propionicacid1	HCP	O	CH	1.66	-1.34	0.36	0.41	propionicacid1_accw_2_HCP
trifluoroaceticacid0	HCP	O	CH	1.16	-1.34	0.83	0.61	trifluoroaceticacid0_accw_2_HCP
trifluoroaceticacid1	HCP	O	CH	1.27	-1.34	0.73	0.56	trifluoroaceticacid1_accw_2_HCP
(methylthio)-ethane	HCP	S	CH	1.46	-1.34	0.40	0.36	(methylthio)-ethane_accw_2_HCP
1-methylcyclohexene	HCP	C	CH	1	-1.34	0.91	0.67	1-methylcyclohexene_accw_3_HCP
cis-2-butene	HCP	C	CH	1.05	-1.34	0.85	0.68	cis-2-butene_accw_3_HCP
cyclohexene	HCP	C	CH	1.06	-1.34	0.84	0.68	cyclohexene_accw_3_HCP
isobutene	HCP	C	CH	1	-1.34	0.91	0.61	isobutene_accw_3_HCP
propene	HCP	C	CH	1	-1.34	0.91	0.72	propene_accw_3_HCP
2-methylpyrazine	HCP	N	CH	1.99	-1.34	-0.16	-0.03	2-methylpyrazine_accw_3_HCP
3-picoline	HCP	N	CH	2.19	-1.34	-0.38	-0.17	3-picoline_accw_3_HCP
ethylamine1	HCP	N	CH	2.48	-1.34	-0.69	-0.23	ethylamine1_accw_3_HCP
ethylamine2	HCP	N	CH	2.52	-1.34	-0.74	-0.18	ethylamine2_accw_3_HCP
hexylamine	HCP	N	CH	2.5	-1.34	-0.72	-0.26	hexylamine_accw_3_HCP
methylimidazol	HCP	N	CH	2.3	-1.34	-0.50	0.10	methylimidazol_accw_3_HCP
n-pentylamine	HCP	N	CH	2.5	-1.34	-0.72	-0.28	n-pentylamine_accw_3_HCP
n-propylamine	HCP	N	CH	2.49	-1.34	-0.71	-0.28	n-propylamine_accw_3_HCP
pyrimidine	HCP	N	CH	1.99	-1.34	-0.16	0.02	pyrimidine_accw_3_HCP
2-propen-1-ol0	HCP	O	CH	1.75	-1.34	0.28	0.24	2-propen-1-ol0_accw_3_HCP
2-propen-1-ol2	HCP	O	CH	1.79	-1.34	0.24	0.31	2-propen-1-ol2_accw_3_HCP
aceticacid0	HCP	O	CH	1.1	-1.34	0.88	0.79	aceticacid0_accw_3_HCP
aceticacid1	HCP	O	CH	1.17	-1.34	0.82	0.88	aceticacid1_accw_3_HCP
butyricacid0	HCP	O	CH	1.13	-1.34	0.86	0.78	butyricacid0_accw_3_HCP
butyricacid1	HCP	O	CH	1.19	-1.34	0.80	0.88	butyricacid1_accw_3_HCP
diethylcarbonate1	HCP	O	CH	1.17	-1.34	0.82	1.01	diethylcarbonate1_accw_3_HCP
diethylether0	HCP	O	CH	1.73	-1.34	0.30	0.66	diethylether0_accw_3_HCP
diethylether1	HCP	O	CH	1.78	-1.34	0.25	0.33	diethylether1_accw_3_HCP

diethylsulfate0	HCP	O	CH	1.05	-1.34	0.93	0.60	diethylsulfate0_accw_3_HCP
diethylsulfate1	HCP	O	CH	1.04	-1.34	0.94	0.76	diethylsulfate1_accw_3_HCP
dimethoxymethane0	HCP	O	CH	1.57	-1.34	0.45	0.39	dimethoxymethane0_accw_3_HCP
dimethoxymethane1	HCP	O	CH	1.57	-1.34	0.45	0.31	dimethoxymethane1_accw_3_HCP
dimethoxymethane2	HCP	O	CH	1.54	-1.34	0.47	0.42	dimethoxymethane2_accw_3_HCP
dimethoxymethane3	HCP	O	CH	1.58	-1.34	0.44	0.62	dimethoxymethane3_accw_3_HCP
dimethylcarbonate1	HCP	O	CH	1.12	-1.34	0.87	0.99	dimethylcarbonate1_accw_3_HCP
ethoxyethanol0	HCP	O	CH	1.63	-1.34	0.39	0.66	ethoxyethanol0_accw_3_HCP
ethoxyethanol1	HCP	O	CH	1.63	-1.34	0.39	0.83	ethoxyethanol1_accw_3_HCP
ethoxyethanol2	HCP	O	CH	1.66	-1.34	0.36	0.53	ethoxyethanol2_accw_3_HCP
ethoxyethanol3	HCP	O	CH	1.65	-1.34	0.37	0.53	ethoxyethanol3_accw_3_HCP
ethoxyethanol4	HCP	O	CH	1.64	-1.34	0.38	0.72	ethoxyethanol4_accw_3_HCP
ethoxyethanol5	HCP	O	CH	1.64	-1.34	0.38	0.71	ethoxyethanol5_accw_3_HCP
ethoxyethanol7	HCP	O	CH	1.73	-1.34	0.30	0.36	ethoxyethanol7_accw_3_HCP
ethylacetate0	HCP	O	CH	1.17	-1.34	0.82	1.13	ethylacetate0_accw_3_HCP
ethylformate0	HCP	O	CH	1.11	-1.34	0.88	0.99	ethylformate0_accw_3_HCP
ethylformate1	HCP	O	CH	1.14	-1.34	0.85	0.84	ethylformate1_accw_3_HCP
ethylpropionate0	HCP	O	CH	1.19	-1.34	0.80	1.10	ethylpropionate0_accw_3_HCP
ethylpropionate1	HCP	O	CH	1.21	-1.34	0.78	0.83	ethylpropionate1_accw_3_HCP
formicacid	HCP	O	CH	1.49	-1.34	0.52	0.32	formicacid_accw_3_HCP
methylacetate	HCP	O	CH	1.13	-1.34	0.86	0.89	methylacetate_accw_3_HCP
methylformate	HCP	O	CH	1.1	-1.34	0.88	0.85	methylformate_accw_3_HCP
n-propylacetate1	HCP	O	CH	1.19	-1.34	0.80	0.93	n-propylacetate1_accw_3_HCP
propionicacid0	HCP	O	CH	1.16	-1.34	0.83	0.81	propionicacid0_accw_3_HCP
propionicacid1	HCP	O	CH	1.19	-1.34	0.80	0.87	propionicacid1_accw_3_HCP
ethanethiol0	HCP	S	CH	1.31	-1.34	0.57	0.58	ethanethiol0_accw_3_HCP
ethanethiol1	HCP	S	CH	1.32	-1.34	0.56	0.51	ethanethiol1_accw_3_HCP
2-propen-1-ol1	HCP	C	CH	0.98	-1.34	0.93	0.82	2-propen-1-ol1_accw_4_HCP
4-methylpyridine	HCP	N	CH	2.21	-1.34	-0.40	-0.19	4-methylpyridine_accw_4_HCP
2-propanol0	HCP	O	CH	1.81	-1.34	0.22	0.25	2-propanol0_accw_4_HCP

2-propanol1	HCP	O	CH	1.83	-1.34	0.20	0.16	2-propanol1_accw_4_HCP
acrolein0	HCP	O	CH	1.64	-1.34	0.38	0.11	acrolein0_accw_4_HCP
acrolein1	HCP	O	CH	1.63	-1.34	0.39	0.11	acrolein1_accw_4_HCP
diethylcarbonate2	HCP	O	CH	1.17	-1.34	0.82	0.89	diethylcarbonate2_accw_4_HCP
diethylcarbonate3	HCP	O	CH	1.2	-1.34	0.79	1.17	diethylcarbonate3_accw_4_HCP
diethylsulfate1	HCP	O	CH	0.88	-1.34	1.09	1.06	diethylsulfate1_accw_4_HCP
dimethylcarbonate0	HCP	O	CH	1.11	-1.34	0.88	0.84	dimethylcarbonate0_accw_4_HCP
dimethylsulfate1	HCP	O	CH	1.04	-1.34	0.94	0.58	dimethylsulfate1_accw_4_HCP
dioxolane	HCP	O	CH	1.54	-1.34	0.47	0.33	dioxolane_accw_4_HCP
methylbutyrate	HCP	O	CH	1.58	-1.34	0.44	0.35	methylbutyrate_accw_4_HCP
methylurethane	HCP	O	CH	1.11	-1.34	0.88	1.04	methylurethane_accw_4_HCP
morpholine	HCP	O	CH	1.77	-1.34	0.26	0.17	morpholine_accw_4_HCP
n-propylformate0	HCP	O	CH	1.15	-1.34	0.84	1.01	n-propylformate0_accw_4_HCP
n-propylformate1	HCP	O	CH	1.14	-1.34	0.85	0.83	n-propylformate1_accw_4_HCP
1-propanethiol0	HCP	S	CH	1.32	-1.34	0.56	0.56	1-propanethiol0_accw_4_HCP
1-propanethiol1	HCP	S	CH	1.32	-1.34	0.56	0.50	1-propanethiol1_accw_4_HCP
cyclopentene	HCP	C	CH	1.06	-1.34	0.84	0.66	cyclopentene_accw_5_HCP
pyrrole	HCP	C	CH	1.08	-1.34	0.82	0.35	pyrrole_accw_5_HCP
2-amino-2-methylpropane0	HCP	N	CH	2.53	-1.34	-0.75	0.02	2-amino-2-methylpropane0_accw_5_HCP
2-amino-2-methylpropane1	HCP	N	CH	2.53	-1.34	-0.75	0.02	2-amino-2-methylpropane1_accw_5_HCP
dicyanomethane	HCP	N	CH	1.32	-1.34	0.57	0.45	dicyanomethane_accw_5_HCP
isopropylamine	HCP	N	CH	2.45	-1.34	-0.66	0.06	isopropylamine_accw_5_HCP
1,2-dimethoxyethane1	HCP	O	CH	1.64	-1.34	0.38	0.36	1,2-dimethoxyethane1_accw_5_HCP
1,2-dimethoxyethane5	HCP	O	CH	1.67	-1.34	0.35	0.12	1,2-dimethoxyethane5_accw_5_HCP
1-butanol1	HCP	O	CH	1.81	-1.34	0.22	0.23	1-butanol1_accw_5_HCP
2-butanol0	HCP	O	CH	1.85	-1.34	0.18	0.17	2-butanol0_accw_5_HCP
2-butanol1	HCP	O	CH	1.8	-1.34	0.23	0.33	2-butanol1_accw_5_HCP
2-butanol2	HCP	O	CH	1.81	-1.34	0.22	0.31	2-butanol2_accw_5_HCP
2-butanol3	HCP	O	CH	1.83	-1.34	0.20	0.15	2-butanol3_accw_5_HCP
butanone	HCP	O	CH	1.73	-1.34	0.30	0.27	butanone_accw_5_HCP

glycol0	HCP	O	CH	1.69	-1.34	0.33	0.18	glycol0_accw_5_HCP
glycol1	HCP	O	CH	1.77	-1.34	0.26	0.23	glycol1_accw_5_HCP
glycol3	HCP	O	CH	1.72	-1.34	0.30	0.26	glycol3_accw_5_HCP
isobutanol0	HCP	O	CH	1.8	-1.34	0.23	0.15	isobutanol0_accw_5_HCP
isobutanol1	HCP	O	CH	1.78	-1.34	0.25	0.23	isobutanol1_accw_5_HCP
isobutanol2	HCP	O	CH	1.83	-1.34	0.20	0.23	isobutanol2_accw_5_HCP
methylbutyrate	HCP	O	CH	1.18	-1.34	0.81	0.88	methylbutyrate_accw_5_HCP
methyl-t-butylether	HCP	O	CH	1.8	-1.34	0.23	0.32	methyl-t-butylether_accw_5_HCP
dimethyldisulfide	HCP	S	CH	1.09	-1.34	0.81	0.54	dimethyldisulfide_accw_5_HCP
dimethylsulfide	HCP	S	CH	1.42	-1.34	0.45	0.30	dimethylsulfide_accw_5_HCP
1-heptene0	HCP	C	CH	1.02	-1.34	0.89	0.86	1-heptene0_accw_6_HCP
1-heptene1	HCP	C	CH	1.02	-1.34	0.89	0.71	1-heptene1_accw_6_HCP
1-heptene2	HCP	C	CH	1.03	-1.34	0.88	0.82	1-heptene2_accw_6_HCP
1-heptene3	HCP	C	CH	1.02	-1.34	0.89	0.80	1-heptene3_accw_6_HCP
1-heptene4	HCP	C	CH	1.06	-1.34	0.84	0.76	1-heptene4_accw_6_HCP
1-heptene5	HCP	C	CH	1.02	-1.34	0.89	0.92	1-heptene5_accw_6_HCP
1-hexene0	HCP	C	CH	1.02	-1.34	0.89	0.81	1-hexene0_accw_6_HCP
1-hexene2	HCP	C	CH	1	-1.34	0.91	0.71	1-hexene2_accw_6_HCP
1-hexene3	HCP	C	CH	1	-1.34	0.91	0.85	1-hexene3_accw_6_HCP
1-hexene4	HCP	C	CH	1.02	-1.34	0.89	0.84	1-hexene4_accw_6_HCP
2-butyne	HCP	C	CH	1.03	-1.34	0.88	0.69	2-butyne_accw_6_HCP
butene	HCP	C	CH	1	-1.34	0.91	0.70	butene_accw_6_HCP
hexyne	HCP	C	CH	1.01	-1.34	0.90	0.76	hexyne_accw_6_HCP
octene	HCP	C	CH	1	-1.34	0.91	0.69	octene_accw_6_HCP
octyne	HCP	C	CH	1.01	-1.34	0.90	0.77	octyne_accw_6_HCP
pentyne	HCP	C	CH	1	-1.34	0.91	0.77	pentyne_accw_6_HCP
2-methylpyrazine	HCP	N	CH	1.98	-1.34	-0.15	0.12	2-methylpyrazine_accw_6_HCP
2-methylpyridine	HCP	N	CH	2.18	-1.34	-0.37	-0.03	2-methylpyridine_accw_6_HCP
1-nitropropane0	HCP	O	CH	1.34	-1.34	0.66	0.65	1-nitropropane0_accw_6_HCP
1-nitropropane1	HCP	O	CH	1.32	-1.34	0.68	0.66	1-nitropropane1_accw_6_HCP

2-nitropropane	HCP	O	CH	1.33	-1.34	0.67	0.72	2-nitropropane_accw_6_HCP
2-pentanone	HCP	O	CH	1.73	-1.34	0.30	0.22	2-pentanone_accw_6_HCP
3-methyl-2-butanone	HCP	O	CH	1.77	-1.34	0.26	0.20	3-methyl-2-butanone_accw_6_HCP
butadione	HCP	O	CH	1.48	-1.34	0.53	0.42	butadione_accw_6_HCP
dimethylsulfate0	HCP	O	CH	0.83	-1.34	1.14	1.08	dimethylsulfate0_accw_6_HCP
dimethylsulfoxide	HCP	O	CH	1.89	-1.34	0.15	0.06	dimethylsulfoxide_accw_6_HCP
di-n-pentylether0	HCP	O	CH	1.75	-1.34	0.28	0.60	di-n-pentylether0_accw_6_HCP
di-n-pentylether1	HCP	O	CH	1.78	-1.34	0.25	0.16	di-n-pentylether1_accw_6_HCP
ethoxyethanol0	HCP	O	CH	1.8	-1.34	0.23	0.19	ethoxyethanol0_accw_6_HCP
ethoxyethanol1	HCP	O	CH	1.79	-1.34	0.24	0.17	ethoxyethanol1_accw_6_HCP
ethoxyethanol2	HCP	O	CH	1.77	-1.34	0.26	0.20	ethoxyethanol2_accw_6_HCP
ethoxyethanol3	HCP	O	CH	1.75	-1.34	0.28	0.23	ethoxyethanol3_accw_6_HCP
ethoxyethanol4	HCP	O	CH	1.71	-1.34	0.31	0.24	ethoxyethanol4_accw_6_HCP
ethoxyethanol5	HCP	O	CH	1.72	-1.34	0.30	0.29	ethoxyethanol5_accw_6_HCP
ethoxyethanol7	HCP	O	CH	1.74	-1.34	0.29	0.09	ethoxyethanol7_accw_6_HCP
ethoxyethanol8	HCP	O	CH	1.77	-1.34	0.26	0.26	ethoxyethanol8_accw_6_HCP
nitroethane0	HCP	O	CH	1.34	-1.34	0.66	0.66	nitroethane0_accw_6_HCP
nitromethane	HCP	O	CH	1.33	-1.34	0.67	0.70	nitromethane_accw_6_HCP
n-propylformate1	HCP	O	CH	1.55	-1.34	0.46	0.28	n-propylformate1_accw_6_HCP
1-nitropropane0	HCP	O	CH	1.34	-1.34	0.66	0.71	1-nitropropane0_accw_7_HCP
1-nitropropane1	HCP	O	CH	1.35	-1.34	0.65	0.71	1-nitropropane1_accw_7_HCP
1-nitropropane2	HCP	O	CH	1.32	-1.34	0.68	0.68	1-nitropropane2_accw_7_HCP
4-bromophenol0	HCP	O	CH	1.27	-1.34	0.73	0.62	4-bromophenol0_accw_7_HCP
4-nitrophenol	HCP	O	CH	1.11	-1.34	0.88	0.80	4-nitrophenol_accw_7_HCP
cyclohexanone	HCP	O	CH	1.78	-1.34	0.25	0.22	cyclohexanone_accw_7_HCP
dimethylsulfone	HCP	O	CH	1.44	-1.34	0.57	0.73	dimethylsulfone_accw_7_HCP
furfural0	HCP	O	CH	1.68	-1.34	0.34	0.05	furfural0_accw_7_HCP
furfural1	HCP	O	CH	1.67	-1.34	0.35	0.05	furfural1_accw_7_HCP
nitroethane1	HCP	O	CH	1.31	-1.34	0.69	0.68	nitroethane1_accw_7_HCP
propynol0	HCP	O	CH	1.64	-1.34	0.38	0.37	propynol0_accw_7_HCP

propynol1	HCP	O	CH	1.64	-1.34	0.38	0.42	propynol1_accw_7_HCP
3-cyanophenol	HCP	N	CH	1.44	-1.34	0.44	0.40	3-cyanophenol_accw_8_HCP
chinoline	HCP	N	CH	2.18	-1.34	-0.37	0.06	chinoline_accw_8_HCP
1-heptanol0	HCP	O	CH	1.8	-1.34	0.23	0.16	1-heptanol0_accw_8_HCP
1-heptanol1	HCP	O	CH	1.81	-1.34	0.22	0.21	1-heptanol1_accw_8_HCP
3-hydroxybenzaldehyde0	HCP	O	CH	1.26	-1.34	0.74	0.66	3-hydroxybenzaldehyde0_accw_8_HCP
3-hydroxybenzaldehyde1	HCP	O	CH	1.25	-1.34	0.74	0.62	3-hydroxybenzaldehyde1_accw_8_HCP
3-hydroxybenzaldehyde2	HCP	O	CH	1.25	-1.34	0.74	0.65	3-hydroxybenzaldehyde2_accw_8_HCP
dioxane	HCP	O	CH	1.68	-1.34	0.34	0.25	dioxane_accw_8_HCP
ethanol0	HCP	O	CH	1.81	-1.34	0.22	0.18	ethanol0_accw_8_HCP
methylbenzoate	HCP	O	CH	1.49	-1.34	0.52	0.44	methylbenzoate_accw_8_HCP
1-nonene0	HCP	C	CH	1.01	-1.34	0.90	0.74	1-nonene0_accw_9_HCP
1-nonene1	HCP	C	CH	0.99	-1.34	0.92	0.71	1-nonene1_accw_9_HCP
1,2-dimethoxyethane3	HCP	O	CH	1.67	-1.34	0.35	0.10	1,2-dimethoxyethane3_accw_9_HCP
4-(1,1-dimethylethyl)-phenol	HCP	O	CH	1.35	-1.34	0.65	-0.03	4-(1,1-dimethylethyl)-phenol_accw_9_HCP
4-cyanophenol	HCP	O	CH	1.17	-1.34	0.82	0.74	4-cyanophenol_accw_9_HCP
anisole	HCP	O	CH	1.31	-1.34	0.69	0.67	anisole_accw_9_HCP
glycol0	HCP	O	CH	1.76	-1.34	0.27	0.21	glycol0_accw_9_HCP
glycol1	HCP	O	CH	1.73	-1.34	0.30	0.33	glycol1_accw_9_HCP
glycol3	HCP	O	CH	1.71	-1.34	0.31	0.22	glycol3_accw_9_HCP
propanol1	HCP	O	CH	1.81	-1.34	0.22	0.21	propanol1_accw_9_HCP
1,4-pentadiene1	HCP	C	CH	0.98	-1.34	0.93	0.95	1,4-pentadiene1_accw10_HCP
aniline	HCP	N	CH	1.69	-1.34	0.17	-0.02	aniline_accw10_HCP
2-methylphenol0	HCP	O	CH	1.28	-1.34	0.72	0.76	2-methylphenol0_accw10_HCP
2-methylphenol1	HCP	O	CH	1.33	-1.34	0.67	0.56	2-methylphenol1_accw10_HCP
4-methylphenol	HCP	O	CH	1.36	-1.34	0.64	0.52	4-methylphenol_accw10_HCP
chinone	HCP	O	CH	1.5	-1.34	0.51	0.49	chinone_accw10_HCP
phenol	HCP	O	CH	1.32	-1.34	0.68	0.56	phenol_accw10_HCP
cyclohexanol0	HCP	O	CH	1.85	-1.34	0.18	0.18	cyclohexanol0_accw11_HCP
cyclohexanol1	HCP	O	CH	1.85	-1.34	0.18	0.23	cyclohexanol1_accw11_HCP

methyl-n-propylether	HCP	O	CH	1.7	-1.34	0.32	0.27	methyl-n-propylether_accw11_HCP
3-nitrophenol	HCP	O	CH	1.2	-1.34	0.79	0.74	3-nitrophenol_accw12_HCP
methylthiobenzene	HCP	S	CH	1.06	-1.34	0.85	0.51	methylthiobenzene_accw12_HCP
thiophenol	HCP	S	CH	0.98	-1.34	0.94	0.59	thiophenol_accw12_HCP
benzonitrile	HCP	N	CH	1.45	-1.34	0.43	0.39	benzonitrile_accw13_HCP
1-bromo-2-nitrobenzene	HCP	O	CH	1.27	-1.34	0.73	0.68	1-bromo-2-nitrobenzene_accw13_HCP
2-nitrotoluene	HCP	O	CH	1.34	-1.34	0.66	0.69	2-nitrotoluene_accw13_HCP
3-cyano-1-nitrobenzene	HCP	O	CH	1.23	-1.34	0.76	0.69	3-cyano-1-nitrobenzene_accw13_HCP
3-hydroxybenzaldehyde0	HCP	O	CH	1.64	-1.34	0.38	0.10	3-hydroxybenzaldehyde0_accw13_HCP
3-hydroxybenzaldehyde1	HCP	O	CH	1.64	-1.34	0.38	0.10	3-hydroxybenzaldehyde1_accw13_HCP
3-hydroxybenzaldehyde2	HCP	O	CH	1.64	-1.34	0.38	0.11	3-hydroxybenzaldehyde2_accw13_HCP
3-nitrophenol	HCP	O	CH	1.33	-1.34	0.67	0.67	3-nitrophenol_accw13_HCP
3-nitrotoluene	HCP	O	CH	1.34	-1.34	0.66	0.67	3-nitrotoluene_accw13_HCP
4-nitrophenol	HCP	O	CH	1.45	-1.34	0.56	0.63	4-nitrophenol_accw13_HCP
acetophenone	HCP	O	CH	1.74	-1.34	0.29	0.24	acetophenone_accw13_HCP
benzaldehyde	HCP	O	CH	1.65	-1.34	0.37	0.10	benzaldehyde_accw13_HCP
dimethylbenzenesulfonamide	HCP	O	CH	1.34	-1.34	0.66	0.73	dimethylbenzenesulfonamide_accw13_HCP
1-bromo-2-nitrobenzene	HCP	O	CH	1.3	-1.34	0.70	0.68	1-bromo-2-nitrobenzene_accw14_HCP
2-nitrotoluene	HCP	O	CH	1.39	-1.34	0.61	0.68	2-nitrotoluene_accw14_HCP
3-nitrophenol	HCP	O	CH	1.36	-1.34	0.64	0.69	3-nitrophenol_accw14_HCP
3-nitrotoluene	HCP	O	CH	1.38	-1.34	0.62	0.69	3-nitrotoluene_accw14_HCP
benzoicacid	HCP	O	CH	1.03	-1.34	0.95	1.00	benzoicacid_accw14_HCP
nitrobenzene	HCP	O	CH	1.37	-1.34	0.63	0.67	nitrobenzene_accw14_HCP
tert-butanol	HCP	O	CH	1.87	-1.34	0.16	0.25	tert-butanol_accw14_HCP
3-cyano-1-nitrobenzene	HCP	N	CH	1.37	-1.34	0.52	0.43	3-cyano-1-nitrobenzene_accw15_HCP
benzylamine0	HCP	N	CH	2.39	-1.34	-0.60	-0.23	benzylamine0_accw15_HCP
benzylamine1	HCP	N	CH	2.38	-1.34	-0.59	-0.12	benzylamine1_accw15_HCP
1-pentanol0	HCP	O	CH	1.84	-1.34	0.19	0.16	1-pentanol0_accw17_HCP
1-pentanol1	HCP	O	CH	1.81	-1.34	0.22	0.21	1-pentanol1_accw17_HCP
1-octanol0	HCP	O	CH	1.8	-1.34	0.23	0.16	1-octanol0_accw26_HCP

1-octanol1	HCP	O	CH	1.81	-1.34	0.22	0.19	1-octanol1_accw26_HCP
1-decene	HCN	C	CH	0.97	-1.81	0.52	1.03	1-decene_accw_10
pentene2	HCN	C	CH	1.03	-1.81	0.37	1.08	pentene2_accw_10
pentene4	HCN	C	CH	0.99	-1.81	0.47	1.02	pentene4_accw_10
2,4-dimethylpyridine	HCN	N	CH	2.24	-1.81	-2.48	-2.67	2,4-dimethylpyridine_accw_10
2,6-dimethylpyridine	HCN	N	CH	2.22	-1.81	-2.44	-2.08	2,6-dimethylpyridine_accw_10
2-propenenitrile	HCN	N	CH	1.44	-1.81	-0.57	-0.41	2-propenenitrile_accw_10
4-cyanophenol	HCN	N	CH	1.49	-1.81	-0.69	-0.54	4-cyanophenol_accw_10
acetonitrile	HCN	N	CH	1.51	-1.81	-0.74	-0.56	acetonitrile_accw_10
aziridine	HCN	N	CH	2.22	-1.81	-2.44	-3.44	aziridine_accw_10
butyronitrile	HCN	N	CH	1.51	-1.81	-0.74	-0.55	butyronitrile_accw_10
dibutylamine	HCN	N	CH	2.5	-1.81	-3.10	-3.71	dibutylamine_accw_10
diethylamine0	HCN	N	CH	2.53	-1.81	-3.18	-3.56	diethylamine0_accw_10
diethylamine1	HCN	N	CH	2.51	-1.81	-3.13	-4.07	diethylamine1_accw_10
dimethylamine	HCN	N	CH	2.47	-1.81	-3.03	-4.40	dimethylamine_accw_10
dipropylamine	HCN	N	CH	2.5	-1.81	-3.10	-3.67	dipropylamine_accw_10
morpholine	HCN	N	CH	2.43	-1.81	-2.94	-2.99	morpholine_accw_10
nh3	HCN	N	CH	2.43	-1.81	-2.94	-3.35	nh3_accw_10
piperidine	HCN	N	CH	2.53	-1.81	-3.18	-3.66	piperidine_accw_10
propionitrile	HCN	N	CH	1.51	-1.81	-0.74	-0.56	propionitrile_accw_10
pyridazine	HCN	N	CH	2.01	-1.81	-1.93	-2.24	pyridazine_accw_10
pyridine	HCN	N	CH	2.17	-1.81	-2.32	-2.67	pyridine_accw_10
pyrrolidin	HCN	N	CH	2.49	-1.81	-3.08	-4.16	pyrrolidin_accw_10
triethylamine1	HCN	N	CH	2.29	-1.81	-2.60	-3.50	triethylamine1_accw_10
triethylamine2	HCN	N	CH	2.19	-1.81	-2.36	-3.46	triethylamine2_accw_10
1,2-epoxypropane	HCN	O	CH	1.63	-1.81	-0.69	-1.27	1,2-epoxypropane_accw_10
3-cyanophenol	HCN	O	CH	1.21	-1.81	0.17	0.55	3-cyanophenol_accw_10
acetaldehyde	HCN	O	CH	1.65	-1.81	-0.73	-0.67	acetaldehyde_accw_10
acetamide	HCN	O	CH	1.94	-1.81	-1.32	-1.50	acetamide_accw_10
butanal	HCN	O	CH	1.65	-1.81	-0.73	-1.19	butanal_accw_10

butoxide	HCN	O	CH	1.63	-1.81	-0.69	-1.27	butoxide_accw_10
diethylcarbonate0	HCN	O	CH	1.48	-1.81	-0.39	-0.28	diethylcarbonate0_accw_10
diethylcarbonate1	HCN	O	CH	1.47	-1.81	-0.36	-0.28	diethylcarbonate1_accw_10
diethylcarbonate3	HCN	O	CH	1.65	-1.81	-0.73	-0.75	diethylcarbonate3_accw_10
diethylcarbonate4	HCN	O	CH	1.64	-1.81	-0.71	-0.74	diethylcarbonate4_accw_10
dimethylcarbonate0	HCN	O	CH	1.45	-1.81	-0.32	-0.18	dimethylcarbonate0_accw_10
dimethylether	HCN	O	CH	1.68	-1.81	-0.79	-1.23	dimethylether_accw_10
dimethylformamide	HCN	O	CH	1.89	-1.81	-1.22	-2.20	dimethylformamide_accw_10
di-n-butylether0	HCN	O	CH	1.76	-1.81	-0.96	-0.40	di-n-butylether0_accw_10
di-n-butylether1	HCN	O	CH	1.74	-1.81	-0.92	-1.36	di-n-butylether1_accw_10
dioxane	HCN	O	CH	1.68	-1.81	-0.79	-0.86	dioxane_accw_10
dioxolane	HCN	O	CH	1.54	-1.81	-0.51	-0.69	dioxolane_accw_10
ethanol1	HCN	O	CH	1.82	-1.81	-1.08	-1.15	ethanol1_accw_10
ethyleneoxide	HCN	O	CH	1.57	-1.81	-0.57	-1.10	ethyleneoxide_accw_10
formaldehyde	HCN	O	CH	1.49	-1.81	-0.41	-0.63	formaldehyde_accw_10
formamide	HCN	O	CH	1.85	-1.81	-1.14	-1.97	formamide_accw_10
formicacid	HCN	O	CH	1.06	-1.81	0.47	0.85	formicacid_accw_10
furane	HCN	O	CH	1.07	-1.81	0.45	0.88	furane_accw_10
h2o	HCN	O	CH	1.82	-1.81	-1.08	-1.21	h2o_accw_10
hexanal	HCN	O	CH	1.65	-1.81	-0.73	-1.20	hexanal_accw_10
isobutanal	HCN	O	CH	1.62	-1.81	-0.67	-0.56	isobutanal_accw_10
methylformamide	HCN	O	CH	1.9	-1.81	-1.24	-2.16	methylformamide_accw_10
methylurethane	HCN	O	CH	1.71	-1.81	-0.85	-0.92	methylurethane_accw_10
n,n-dimethylacetamide	HCN	O	CH	1.99	-1.81	-1.43	-2.14	n,n-dimethylacetamide_accw_10
n-methylacetamide	HCN	O	CH	1.96	-1.81	-1.37	-2.14	n-methylacetamide_accw_10
octanal	HCN	O	CH	1.65	-1.81	-0.73	-1.21	octanal_accw_10
propanal	HCN	O	CH	1.64	-1.81	-0.71	-0.67	propanal_accw_10
propanol0	HCN	O	CH	1.83	-1.81	-1.10	-1.26	propanol0_accw_10
propanone	HCN	O	CH	1.75	-1.81	-0.94	-1.05	propanone_accw_10
thf	HCN	O	CH	1.79	-1.81	-1.02	-1.74	thf_accw_10

thp	HCN	O	CH	1.8	-1.81	-1.04	-1.28	thp_accw_10
2,2'-dichlorodiethylsulfide0	HCN	S	CH	1.07	-1.81	0.29	0.84	2,2'-dichlorodiethylsulfide0_accw_10
2,2'-dichlorodiethylsulfide1	HCN	S	CH	1.15	-1.81	0.09	0.70	2,2'-dichlorodiethylsulfide1_accw_10
2,2'-dichlorodiethylsulfide2	HCN	S	CH	1.14	-1.81	0.12	0.73	2,2'-dichlorodiethylsulfide2_accw_10
2,2'-dichlorodiethylsulfide3	HCN	S	CH	1.2	-1.81	-0.03	0.32	2,2'-dichlorodiethylsulfide3_accw_10
butanethiol0	HCN	S	CH	1.31	-1.81	-0.30	0.35	butanethiol0_accw_10
butanethiol1	HCN	S	CH	1.32	-1.81	-0.32	0.21	butanethiol1_accw_10
diethylsulfide	HCN	S	CH	1.49	-1.81	-0.74	-0.06	diethylsulfide_accw_10
h2s	HCN	S	CH	1.15	-1.81	0.09	0.50	h2s_accw_10
methanethiol	HCN	S	CH	1.3	-1.81	-0.27	0.09	methanethiol_accw_10
2-methyl-2-butene	HCN	C	CH	1.01	-1.81	0.42	0.82	2-methyl-2-butene_accw_20
pentene0	HCN	C	CH	0.98	-1.81	0.50	1.28	pentene0_accw_20
propyne	HCN	C	CH	1	-1.81	0.45	0.99	propyne_accw_20
methylamine	HCN	N	CH	2.49	-1.81	-3.08	-4.06	methylamine_accw_20
pyrimidine	HCN	N	CH	1.99	-1.81	-1.89	-1.83	pyrimidine_accw_20
1,2-dimethoxyethane0	HCN	O	CH	1.67	-1.81	-0.77	-0.90	1,2-dimethoxyethane0_accw_20
1,2-dimethoxyethane2	HCN	O	CH	1.68	-1.81	-0.79	-0.64	1,2-dimethoxyethane2_accw_20
1,2-dimethoxyethane4	HCN	O	CH	1.67	-1.81	-0.77	-1.30	1,2-dimethoxyethane4_accw_20
1,2-dimethoxyethane5	HCN	O	CH	1.64	-1.81	-0.71	-0.90	1,2-dimethoxyethane5_accw_20
3-pentanone	HCN	O	CH	1.65	-1.81	-0.73	-1.04	3-pentanone_accw_20
aceticacid0	HCN	O	CH	1.6	-1.81	-0.63	-0.64	aceticacid0_accw_20
aceticacid1	HCN	O	CH	1.66	-1.81	-0.75	-0.79	aceticacid1_accw_20
benzophenone	HCN	O	CH	1.66	-1.81	-0.75	-0.92	benzophenone_accw_20
butyricacid1	HCN	O	CH	1.66	-1.81	-0.75	-0.79	butyricacid1_accw_20
diethylsulfate1	HCN	O	CH	1.06	-1.81	0.47	0.46	diethylsulfate1_accw_20
dimethoxymethane0	HCN	O	CH	1.57	-1.81	-0.57	-0.60	dimethoxymethane0_accw_20
dimethoxymethane1	HCN	O	CH	1.57	-1.81	-0.57	-0.68	dimethoxymethane1_accw_20
dimethoxymethane2	HCN	O	CH	1.65	-1.81	-0.73	-0.73	dimethoxymethane2_accw_20
dimethoxymethane3	HCN	O	CH	1.58	-1.81	-0.59	-0.32	dimethoxymethane3_accw_20
dimethylsulfate1	HCN	O	CH	0.86	-1.81	0.88	1.84	dimethylsulfate1_accw_20

di-n-propylether0	HCN	O	CH	1.76	-1.81	-0.96	-0.39	di-n-propylether0_accw_20
di-n-propylether1	HCN	O	CH	1.76	-1.81	-0.96	-1.29	di-n-propylether1_accw_20
ethylacetate0	HCN	O	CH	1.64	-1.81	-0.71	-0.91	ethylacetate0_accw_20
ethylacetate1	HCN	O	CH	1.63	-1.81	-0.69	-0.92	ethylacetate1_accw_20
ethylformate0	HCN	O	CH	1.56	-1.81	-0.55	-0.79	ethylformate0_accw_20
ethylformate1	HCN	O	CH	1.55	-1.81	-0.53	-0.79	ethylformate1_accw_20
ethylpropionate0	HCN	O	CH	1.57	-1.81	-0.57	-0.73	ethylpropionate0_accw_20
ethylpropionate1	HCN	O	CH	1.55	-1.81	-0.53	-0.74	ethylpropionate1_accw_20
h2o2	HCN	O	CH	1.42	-1.81	-0.26	-0.43	h2o2_accw_20
methanol	HCN	O	CH	1.79	-1.81	-1.02	-1.40	methanol_accw_20
methylacetate	HCN	O	CH	1.62	-1.81	-0.67	-0.79	methylacetate_accw_20
methylformate	HCN	O	CH	1.54	-1.81	-0.51	-0.73	methylformate_accw_20
n-propylacetate0	HCN	O	CH	1.64	-1.81	-0.71	-0.82	n-propylacetate0_accw_20
n-propylacetate1	HCN	O	CH	1.62	-1.81	-0.67	-0.90	n-propylacetate1_accw_20
propionicacid0	HCN	O	CH	1.57	-1.81	-0.57	-0.52	propionicacid0_accw_20
trifluoroaceticacid0	HCN	O	CH	1.16	-1.81	0.27	0.33	trifluoroaceticacid0_accw_20
trifluoroaceticacid1	HCN	O	CH	1.27	-1.81	0.04	0.17	trifluoroaceticacid1_accw_20
(methylthio)-ethane	HCN	S	CH	1.46	-1.81	-0.66	-0.19	(methylthio)-ethane_accw_20
1-methylcyclohexene	HCN	C	CH	1	-1.81	0.45	0.89	1-methylcyclohexene_accw_30
cis-2-butene	HCN	C	CH	1.05	-1.81	0.32	0.89	cis-2-butene_accw_30
cyclohexene	HCN	C	CH	1.06	-1.81	0.30	0.99	cyclohexene_accw_30
isobutene	HCN	C	CH	1	-1.81	0.45	0.82	isobutene_accw_30
propene	HCN	C	CH	1	-1.81	0.45	1.02	propene_accw_30
1-butylamine	HCN	N	CH	2.5	-1.81	-3.10	-3.80	1-butylamine_accw_30
2-methylpyrazine	HCN	N	CH	1.99	-1.81	-1.89	-1.93	2-methylpyrazine_accw_30
3-picoline	HCN	N	CH	2.19	-1.81	-2.36	-2.76	3-picoline_accw_30
ethylamine0	HCN	N	CH	2.48	-1.81	-3.06	-3.79	ethylamine0_accw_30
ethylamine1	HCN	N	CH	2.48	-1.81	-3.06	-3.79	ethylamine1_accw_30
ethylamine2	HCN	N	CH	2.52	-1.81	-3.15	-3.62	ethylamine2_accw_30
hexylamine	HCN	N	CH	2.5	-1.81	-3.10	-3.80	hexylamine_accw_30

imidazole	HCN	N	CH	2.25	-1.81	-2.51	-2.70	imidazole_accw_30
methylimidazol	HCN	N	CH	2.3	-1.81	-2.63	-2.66	methylimidazol_accw_30
n-pentylamine	HCN	N	CH	2.5	-1.81	-3.10	-3.82	n-pentylamine_accw_30
n-propylamine	HCN	N	CH	2.49	-1.81	-3.08	-3.82	n-propylamine_accw_30
2-propen-1-ol0	HCN	O	CH	1.75	-1.81	-0.94	-1.04	2-propen-1-ol0_accw_30
2-propen-1-ol2	HCN	O	CH	1.79	-1.81	-1.02	-1.05	2-propen-1-ol2_accw_30
aceticacid0	HCN	O	CH	1.1	-1.81	0.39	0.82	aceticacid0_accw_30
aceticacid1	HCN	O	CH	1.17	-1.81	0.25	0.74	aceticacid1_accw_30
butyricacid0	HCN	O	CH	1.13	-1.81	0.33	0.82	butyricacid0_accw_30
butyricacid1	HCN	O	CH	1.19	-1.81	0.21	0.74	butyricacid1_accw_30
diethylcarbonate1	HCN	O	CH	1.17	-1.81	0.25	0.88	diethylcarbonate1_accw_30
diethylether0	HCN	O	CH	1.73	-1.81	-0.90	-0.38	diethylether0_accw_30
diethylether1	HCN	O	CH	1.78	-1.81	-1.00	-0.90	diethylether1_accw_30
diethylsulfate0	HCN	O	CH	1.05	-1.81	0.49	0.52	diethylsulfate0_accw_30
diethylsulfate1	HCN	O	CH	1.04	-1.81	0.51	0.69	diethylsulfate1_accw_30
dimethoxymethane2	HCN	O	CH	1.54	-1.81	-0.51	-0.45	dimethoxymethane2_accw_30
dimethylcarbonate1	HCN	O	CH	1.12	-1.81	0.35	0.92	dimethylcarbonate1_accw_30
ethoxyethanol0	HCN	O	CH	1.63	-1.81	-0.69	0.03	ethoxyethanol0_accw_30
ethoxyethanol1	HCN	O	CH	1.63	-1.81	-0.69	0.04	ethoxyethanol1_accw_30
ethoxyethanol2	HCN	O	CH	1.66	-1.81	-0.75	-0.43	ethoxyethanol2_accw_30
ethoxyethanol3	HCN	O	CH	1.65	-1.81	-0.73	-0.63	ethoxyethanol3_accw_30
ethoxyethanol4	HCN	O	CH	1.64	-1.81	-0.71	-0.06	ethoxyethanol4_accw_30
ethoxyethanol5	HCN	O	CH	1.64	-1.81	-0.71	-0.05	ethoxyethanol5_accw_30
ethoxyethanol6	HCN	O	CH	1.91	-1.81	-1.26	-0.91	ethoxyethanol6_accw_30
ethoxyethanol7	HCN	O	CH	1.73	-1.81	-0.90	-0.71	ethoxyethanol7_accw_30
ethoxyethanol8	HCN	O	CH	1.75	-1.81	-0.94	-0.83	ethoxyethanol8_accw_30
ethylacetate0	HCN	O	CH	1.17	-1.81	0.25	1.42	ethylacetate0_accw_30
ethylacetate1	HCN	O	CH	1.18	-1.81	0.23	1.00	ethylacetate1_accw_30
ethylformate0	HCN	O	CH	1.11	-1.81	0.37	1.29	ethylformate0_accw_30
ethylformate1	HCN	O	CH	1.14	-1.81	0.31	1.01	ethylformate1_accw_30

ethylpropionate0	HCN	O	CH	1.19	-1.81	0.21	1.37	ethylpropionate0_accw_30
ethylpropionate1	HCN	O	CH	1.21	-1.81	0.17	0.93	ethylpropionate1_accw_30
ethylpropionate2	HCN	O	CH	1.19	-1.81	0.21	1.38	ethylpropionate2_accw_30
formicacid	HCN	O	CH	1.49	-1.81	-0.41	-0.57	formicacid_accw_30
methylacetate	HCN	O	CH	1.13	-1.81	0.33	1.01	methylacetate_accw_30
methylformate	HCN	O	CH	1.1	-1.81	0.39	1.01	methylformate_accw_30
n-propylacetate0	HCN	O	CH	1.18	-1.81	0.23	1.42	n-propylacetate0_accw_30
n-propylacetate1	HCN	O	CH	1.19	-1.81	0.21	1.04	n-propylacetate1_accw_30
propionicacid0	HCN	O	CH	1.16	-1.81	0.27	0.83	propionicacid0_accw_30
propionicacid1	HCN	O	CH	1.19	-1.81	0.21	0.76	propionicacid1_accw_30
ethanethiol0	HCN	S	CH	1.31	-1.81	-0.30	0.34	ethanethiol0_accw_30
ethanethiol1	HCN	S	CH	1.32	-1.81	-0.32	0.20	ethanethiol1_accw_30
2-propen-1-ol1	HCN	C	CH	0.98	-1.81	0.50	1.22	2-propen-1-ol1_accw_40
4-methylpyridine	HCN	N	CH	2.21	-1.81	-2.41	-2.82	4-methylpyridine_accw_40
dicyanomethane	HCN	N	CH	1.32	-1.81	-0.29	-0.12	dicyanomethane_accw_40
pyrazine	HCN	N	CH	1.95	-1.81	-1.79	-1.80	pyrazine_accw_40
2-propanol0	HCN	O	CH	1.81	-1.81	-1.06	-1.15	2-propanol0_accw_40
2-propanol1	HCN	O	CH	1.83	-1.81	-1.10	-1.32	2-propanol1_accw_40
acrolein0	HCN	O	CH	1.64	-1.81	-0.71	-1.16	acrolein0_accw_40
acrolein1	HCN	O	CH	1.63	-1.81	-0.69	-1.17	acrolein1_accw_40
diethylcarbonate0	HCN	O	CH	1.15	-1.81	0.29	1.13	diethylcarbonate0_accw_40
diethylcarbonate1	HCN	O	CH	1.16	-1.81	0.27	1.05	diethylcarbonate1_accw_40
diethylcarbonate2	HCN	O	CH	1.17	-1.81	0.25	0.76	diethylcarbonate2_accw_40
diethylcarbonate3	HCN	O	CH	1.2	-1.81	0.19	1.06	diethylcarbonate3_accw_40
diethylcarbonate4	HCN	O	CH	1.2	-1.81	0.19	1.04	diethylcarbonate4_accw_40
diethylsulfate0	HCN	O	CH	0.88	-1.81	0.84	1.71	diethylsulfate0_accw_40
diethylsulfate1	HCN	O	CH	0.88	-1.81	0.84	1.58	diethylsulfate1_accw_40
dimethylcarbonate0	HCN	O	CH	1.11	-1.81	0.37	0.78	dimethylcarbonate0_accw_40
dimethylsulfate0	HCN	O	CH	1.02	-1.81	0.55	0.60	dimethylsulfate0_accw_40
dimethylsulfate1	HCN	O	CH	1.04	-1.81	0.51	0.47	dimethylsulfate1_accw_40

dioxolane	HCN	O	CH	1.54	-1.81	-0.51	-0.55	dioxolane_accw_40
methylbutyrate	HCN	O	CH	1.58	-1.81	-0.59	-0.68	methylbutyrate_accw_40
methylurethane	HCN	O	CH	1.11	-1.81	0.37	1.26	methylurethane_accw_40
morpholine	HCN	O	CH	1.77	-1.81	-0.98	-1.05	morpholine_accw_40
n-propylformate0	HCN	O	CH	1.15	-1.81	0.29	1.29	n-propylformate0_accw_40
n-propylformate1	HCN	O	CH	1.14	-1.81	0.31	1.01	n-propylformate1_accw_40
1-propanethiol0	HCN	S	CH	1.32	-1.81	-0.32	0.34	1-propanethiol0_accw_40
1-propanethiol1	HCN	S	CH	1.32	-1.81	-0.32	0.21	1-propanethiol1_accw_40
1,4-pentadiene1	HCN	C	CH	0.98	-1.81	0.50	1.30	1,4-pentadiene1_accw_50
2-butyne	HCN	C	CH	1.03	-1.81	0.37	0.80	2-butyne_accw_50
cyclopentene	HCN	C	CH	0.99	-1.81	0.47	0.97	cyclopentene_accw_50
pyrrole	HCN	C	CH	1.08	-1.81	0.25	-0.05	pyrrole_accw_50
1,2-diaminoethane1	HCN	N	CH	2.24	-1.81	-2.48	-3.06	1,2-diaminoethane1_accw_50
1,2-diaminoethane2	HCN	N	CH	2.2	-1.81	-2.39	-2.79	1,2-diaminoethane2_accw_50
1,2-diaminoethane3	HCN	N	CH	2.49	-1.81	-3.08	-3.17	1,2-diaminoethane3_accw_50
2-amino-2-methylpropane0	HCN	N	CH	2.53	-1.81	-3.18	-3.22	2-amino-2-methylpropane0_accw_50
2-amino-2-methylpropane1	HCN	N	CH	2.53	-1.81	-3.18	-3.21	2-amino-2-methylpropane1_accw_50
isopropylamine	HCN	N	CH	2.45	-1.81	-2.98	-3.12	isopropylamine_accw_50
1,2-dimethoxyethane1	HCN	O	CH	1.64	-1.81	-0.71	-0.53	1,2-dimethoxyethane1_accw_50
1,2-dimethoxyethane2	HCN	O	CH	1.68	-1.81	-0.79	-1.34	1,2-dimethoxyethane2_accw_50
1,2-dimethoxyethane5	HCN	O	CH	1.67	-1.81	-0.77	-1.15	1,2-dimethoxyethane5_accw_50
1-butanol0	HCN	O	CH	1.81	-1.81	-1.06	-1.28	1-butanol0_accw_50
1-butanol1	HCN	O	CH	1.81	-1.81	-1.06	-1.14	1-butanol1_accw_50
2-butanol0	HCN	O	CH	1.85	-1.81	-1.14	-1.35	2-butanol0_accw_50
2-butanol1	HCN	O	CH	1.8	-1.81	-1.04	-0.98	2-butanol1_accw_50
2-butanol2	HCN	O	CH	1.81	-1.81	-1.06	-1.07	2-butanol2_accw_50
2-butanol3	HCN	O	CH	1.83	-1.81	-1.10	-1.33	2-butanol3_accw_50
butadione	HCN	O	CH	1.48	-1.81	-0.39	-0.29	butadione_accw_50
butanone	HCN	O	CH	1.73	-1.81	-0.90	-0.96	butanone_accw_50
diethylsulfate1	HCN	O	CH	0.86	-1.81	0.88	1.81	diethylsulfate1_accw_50

dimethylsulfate1	HCN	O	CH	1.05	-1.81	0.49	0.50	dimethylsulfate1_accw_50
glycol0	HCN	O	CH	1.69	-1.81	-0.81	-1.12	glycol0_accw_50
glycol1	HCN	O	CH	1.77	-1.81	-0.98	-1.14	glycol1_accw_50
glycol2	HCN	O	CH	1.71	-1.81	-0.85	-1.17	glycol2_accw_50
glycol3	HCN	O	CH	1.72	-1.81	-0.88	-0.94	glycol3_accw_50
isobutanol0	HCN	O	CH	1.8	-1.81	-1.04	-1.27	isobutanol0_accw_50
isobutanol1	HCN	O	CH	1.78	-1.81	-1.00	-1.18	isobutanol1_accw_50
isobutanol2	HCN	O	CH	1.83	-1.81	-1.10	-1.20	isobutanol2_accw_50
methylbutyrate	HCN	O	CH	1.18	-1.81	0.23	0.98	methylbutyrate_accw_50
methyl-t-butylether	HCN	O	CH	1.8	-1.81	-1.04	-1.09	methyl-t-butylether_accw_50
dimethyldisulfide	HCN	S	CH	1.09	-1.81	0.24	0.60	dimethyldisulfide_accw_50
dimethylsulfide	HCN	S	CH	1.42	-1.81	-0.57	-0.30	dimethylsulfide_accw_50
1-heptene0	HCN	C	CH	1.02	-1.81	0.40	1.30	1-heptene0_accw_60
1-heptene1	HCN	C	CH	1.02	-1.81	0.40	1.05	1-heptene1_accw_60
1-heptene2	HCN	C	CH	1.03	-1.81	0.37	1.25	1-heptene2_accw_60
1-heptene3	HCN	C	CH	1.02	-1.81	0.40	1.23	1-heptene3_accw_60
1-heptene4	HCN	C	CH	1.06	-1.81	0.30	1.13	1-heptene4_accw_60
1-heptene5	HCN	C	CH	1.02	-1.81	0.40	1.36	1-heptene5_accw_60
1-heptene6	HCN	C	CH	1.03	-1.81	0.37	1.31	1-heptene6_accw_60
1-hexene0	HCN	C	CH	1.02	-1.81	0.40	1.26	1-hexene0_accw_60
1-hexene2	HCN	C	CH	1	-1.81	0.45	1.03	1-hexene2_accw_60
1-hexene3	HCN	C	CH	1	-1.81	0.45	1.32	1-hexene3_accw_60
1-hexene4	HCN	C	CH	1.02	-1.81	0.40	1.29	1-hexene4_accw_60
butene	HCN	C	CH	1	-1.81	0.45	1.04	butene_accw_60
hexyne	HCN	C	CH	1.01	-1.81	0.42	1.02	hexyne_accw_60
octene	HCN	C	CH	1	-1.81	0.45	1.03	octene_accw_60
octyne	HCN	C	CH	1.01	-1.81	0.42	1.02	octyne_accw_60
pentyne	HCN	C	CH	1	-1.81	0.45	1.02	pentyne_accw_60
2-methylpyrazine	HCN	N	CH	1.98	-1.81	-1.86	-1.66	2-methylpyrazine_accw_60
2-methylpyridine	HCN	N	CH	2.18	-1.81	-2.34	-2.51	2-methylpyridine_accw_60

1-nitropropane0	HCN	O	CH	1.34	-1.81	-0.10	0.23	1-nitropropane0_accw_60
1-nitropropane1	HCN	O	CH	1.32	-1.81	-0.06	0.27	1-nitropropane1_accw_60
1-nitropropane2	HCN	O	CH	1.34	-1.81	-0.10	0.26	1-nitropropane2_accw_60
2-nitropropane	HCN	O	CH	1.33	-1.81	-0.08	0.31	2-nitropropane_accw_60
2-pentanone	HCN	O	CH	1.73	-1.81	-0.90	-1.09	2-pentanone_accw_60
3-methyl-2-butanone	HCN	O	CH	1.77	-1.81	-0.98	-1.10	3-methyl-2-butanone_accw_60
dimethylsulfate0	HCN	O	CH	0.83	-1.81	0.94	1.60	dimethylsulfate0_accw_60
dimethylsulfoxide	HCN	O	CH	1.89	-1.81	-1.22	-1.88	dimethylsulfoxide_accw_60
di-n-pentylether0	HCN	O	CH	1.75	-1.81	-0.94	-0.41	di-n-pentylether0_accw_60
di-n-pentylether1	HCN	O	CH	1.78	-1.81	-1.00	-1.30	di-n-pentylether1_accw_60
ethoxyethanol0	HCN	O	CH	1.79	-1.81	-1.02	-1.16	ethoxyethanol0_accw_60
ethoxyethanol1	HCN	O	CH	1.79	-1.81	-1.02	-1.16	ethoxyethanol1_accw_60
ethoxyethanol2	HCN	O	CH	1.77	-1.81	-0.98	-1.15	ethoxyethanol2_accw_60
ethoxyethanol3	HCN	O	CH	1.75	-1.81	-0.94	-1.14	ethoxyethanol3_accw_60
ethoxyethanol4	HCN	O	CH	1.71	-1.81	-0.85	-0.98	ethoxyethanol4_accw_60
ethoxyethanol5	HCN	O	CH	1.72	-1.81	-0.88	-0.85	ethoxyethanol5_accw_60
ethoxyethanol6	HCN	O	CH	1.81	-1.81	-1.06	-0.97	ethoxyethanol6_accw_60
ethoxyethanol7	HCN	O	CH	1.74	-1.81	-0.92	-1.31	ethoxyethanol7_accw_60
ethoxyethanol8	HCN	O	CH	1.77	-1.81	-0.98	-1.06	ethoxyethanol8_accw_60
ethoxyethanol9	HCN	O	CH	1.75	-1.81	-0.94	-1.14	ethoxyethanol9_accw_60
nitroethane0	HCN	O	CH	1.34	-1.81	-0.10	0.21	nitroethane0_accw_60
nitroethane1	HCN	O	CH	1.34	-1.81	-0.10	0.28	nitroethane1_accw_60
nitromethane	HCN	O	CH	1.33	-1.81	-0.08	0.31	nitromethane_accw_60
n-propylformate0	HCN	O	CH	1.56	-1.81	-0.55	-0.78	n-propylformate0_accw_60
n-propylformate1	HCN	O	CH	1.55	-1.81	-0.53	-0.77	n-propylformate1_accw_60
1-nitropropane0	HCN	O	CH	1.34	-1.81	-0.10	0.34	1-nitropropane0_accw_70
1-nitropropane1	HCN	O	CH	1.35	-1.81	-0.12	0.30	1-nitropropane1_accw_70
1-nitropropane2	HCN	O	CH	1.32	-1.81	-0.06	0.28	1-nitropropane2_accw_70
2-nitropropane	HCN	O	CH	1.34	-1.81	-0.10	0.34	2-nitropropane_accw_70
4-bromophenol0	HCN	O	CH	1.27	-1.81	0.04	0.34	4-bromophenol0_accw_70

4-bromophenol1	HCN	O	CH	1.27	-1.81	0.04	0.34	4-bromophenol1_accw_70
4-nitrophenol	HCN	O	CH	1.11	-1.81	0.37	0.88	4-nitrophenol_accw_70
chinone	HCN	O	CH	1.5	-1.81	-0.43	-0.23	chinone_accw_70
cyclohexanone	HCN	O	CH	1.78	-1.81	-1.00	-1.08	cyclohexanone_accw_70
dimethylsulfone	HCN	O	CH	1.44	-1.81	-0.30	0.20	dimethylsulfone_accw_70
furfural0	HCN	O	CH	1.68	-1.81	-0.79	-1.41	furfural0_accw_70
furfural1	HCN	O	CH	1.67	-1.81	-0.77	-1.37	furfural1_accw_70
nitroethane0	HCN	O	CH	1.34	-1.81	-0.10	0.32	nitroethane0_accw_70
nitroethane1	HCN	O	CH	1.31	-1.81	-0.04	0.28	nitroethane1_accw_70
propynol0	HCN	O	CH	1.64	-1.81	-0.71	-0.68	propynol0_accw_70
propynol1	HCN	O	CH	1.64	-1.81	-0.71	-0.63	propynol1_accw_70
propynol2	HCN	O	CH	1.64	-1.81	-0.71	-0.68	propynol2_accw_70
3-cyanophenol	HCN	N	CH	1.44	-1.81	-0.57	-0.40	3-cyanophenol_accw_80
chinoline	HCN	N	CH	2.18	-1.81	-2.34	-2.09	chinoline_accw_80
1-heptanol0	HCN	O	CH	1.8	-1.81	-1.04	-1.28	1-heptanol0_accw_80
1-heptanol1	HCN	O	CH	1.81	-1.81	-1.06	-1.16	1-heptanol1_accw_80
2-heptanone	HCN	O	CH	1.74	-1.81	-0.92	-1.18	2-heptanone_accw_80
2-octanone	HCN	O	CH	1.74	-1.81	-0.92	-1.14	2-octanone_accw_80
3-hydroxybenzaldehyde0	HCN	O	CH	1.26	-1.81	0.06	0.45	3-hydroxybenzaldehyde0_accw_80
3-hydroxybenzaldehyde1	HCN	O	CH	1.25	-1.81	0.08	0.42	3-hydroxybenzaldehyde1_accw_80
3-hydroxybenzaldehyde2	HCN	O	CH	1.25	-1.81	0.08	0.43	3-hydroxybenzaldehyde2_accw_80
ethanol0	HCN	O	CH	1.81	-1.81	-1.06	-1.29	ethanol0_accw_80
methylbenzoate	HCN	O	CH	1.49	-1.81	-0.41	-0.40	methylbenzoate_accw_80
1-nonene0	HCN	C	CH	1.01	-1.81	0.42	1.06	1-nonene0_accw_90
1-nonene1	HCN	C	CH	0.99	-1.81	0.47	1.03	1-nonene1_accw_90
1,2-diaminoethane0	HCN	N	CH	2.43	-1.81	-2.94	-3.61	1,2-diaminoethane0_accw_90
1,2-diaminoethane1	HCN	N	CH	2.49	-1.81	-3.08	-3.81	1,2-diaminoethane1_accw_90
1,2-diaminoethane2	HCN	N	CH	2.55	-1.81	-3.22	-3.69	1,2-diaminoethane2_accw_90
1,2-dimethoxyethane3	HCN	O	CH	1.67	-1.81	-0.77	-1.19	1,2-dimethoxyethane3_accw_90
4-(1,1-dimethylethyl)-phenol	HCN	O	CH	1.35	-1.81	-0.12	0.03	4-(1,1-dimethylethyl)-phenol_accw_90

4-cyanophenol	HCN	O	CH	1.17	-1.81	0.25	0.67	4-cyanophenol_accw_90
anisole	HCN	O	CH	1.31	-1.81	-0.04	0.49	anisole_accw_90
glycol0	HCN	O	CH	1.76	-1.81	-0.96	-1.16	glycol0_accw_90
glycol1	HCN	O	CH	1.73	-1.81	-0.90	-0.93	glycol1_accw_90
glycol2	HCN	O	CH	1.77	-1.81	-0.98	-1.14	glycol2_accw_90
glycol3	HCN	O	CH	1.71	-1.81	-0.85	-1.01	glycol3_accw_90
propanol1	HCN	O	CH	1.81	-1.81	-1.06	-1.17	propanol1_accw_90
aniline	HCN	N	CH	1.69	-1.81	-1.17	-1.54	aniline_accw100
2-methylphenol0	HCN	O	CH	1.28	-1.81	0.02	0.55	2-methylphenol0_accw100
2-methylphenol1	HCN	O	CH	1.33	-1.81	-0.08	0.21	2-methylphenol1_accw100
4-methylphenol	HCN	O	CH	1.36	-1.81	-0.14	0.07	4-methylphenol_accw100
phenol	HCN	O	CH	1.32	-1.81	-0.06	0.18	phenol_accw100
cyclohexanol0	HCN	O	CH	1.85	-1.81	-1.14	-1.27	cyclohexanol0_accw110
cyclohexanol1	HCN	O	CH	1.85	-1.81	-1.14	-1.28	cyclohexanol1_accw110
diisopropylether	HCN	O	CH	1.84	-1.81	-1.12	-0.57	diisopropylether_accw110
methyl-n-propylether	HCN	O	CH	1.7	-1.81	-0.83	-0.90	methyl-n-propylether_accw110
2-methyl-propanenitrile	HCN	N	CH	1.51	-1.81	-0.74	-0.52	2-methyl-propanenitrile_accw120
3-nitrophenol	HCN	O	CH	1.2	-1.81	0.19	0.62	3-nitrophenol_accw120
methylthiobenzene	HCN	S	CH	1.06	-1.81	0.31	0.51	methylthiobenzene_accw120
thiophenol	HCN	S	CH	0.98	-1.81	0.51	0.73	thiophenol_accw120
benzonitrile	HCN	N	CH	1.45	-1.81	-0.60	-0.41	benzonitrile_accw130
1-bromo-2-nitrobenzene	HCN	O	CH	1.27	-1.81	0.04	0.32	1-bromo-2-nitrobenzene_accw130
2-nitrotoluene	HCN	O	CH	1.34	-1.81	-0.10	0.20	2-nitrotoluene_accw130
3-cyano-1-nitrobenzene	HCN	O	CH	1.23	-1.81	0.13	0.40	3-cyano-1-nitrobenzene_accw130
3-hydroxybenzaldehyde0	HCN	O	CH	1.64	-1.81	-0.71	-1.19	3-hydroxybenzaldehyde0_accw130
3-hydroxybenzaldehyde1	HCN	O	CH	1.64	-1.81	-0.71	-1.20	3-hydroxybenzaldehyde1_accw130
3-hydroxybenzaldehyde2	HCN	O	CH	1.64	-1.81	-0.71	-1.16	3-hydroxybenzaldehyde2_accw130
3-nitrophenol	HCN	O	CH	1.33	-1.81	-0.08	0.21	3-nitrophenol_accw130
3-nitrotoluene	HCN	O	CH	1.34	-1.81	-0.10	0.17	3-nitrotoluene_accw130
4-nitrophenol	HCN	O	CH	1.45	-1.81	-0.32	-0.02	4-nitrophenol_accw130

acetophenone	HCN	O	CH	1.74	-1.81	-0.92	-1.03	acetophenone_accw130
benzaldehyde	HCN	O	CH	1.65	-1.81	-0.73	-1.20	benzaldehyde_accw130
benzoicacid	HCN	O	CH	1.5	-1.81	-0.43	-0.11	benzoicacid_accw130
dimethylbenzenesulfonamide	HCN	O	CH	1.34	-1.81	-0.10	0.37	dimethylbenzenesulfonamide_accw130
nitrobenzene	HCN	O	CH	1.33	-1.81	-0.08	0.21	nitrobenzene_accw130
1-bromo-2-nitrobenzene	HCN	O	CH	1.3	-1.81	-0.02	0.32	1-bromo-2-nitrobenzene_accw140
2-nitrotoluene	HCN	O	CH	1.39	-1.81	-0.20	0.17	2-nitrotoluene_accw140
3-cyano-1-nitrobenzene	HCN	O	CH	1.26	-1.81	0.06	0.42	3-cyano-1-nitrobenzene_accw140
3-nitrophenol	HCN	O	CH	1.36	-1.81	-0.14	0.24	3-nitrophenol_accw140
3-nitrotoluene	HCN	O	CH	1.38	-1.81	-0.18	0.19	3-nitrotoluene_accw140
benzoicacid	HCN	O	CH	1.03	-1.81	0.53	1.36	benzoicacid_accw140
tert-butanol	HCN	O	CH	1.87	-1.81	-1.18	-1.12	tert-butanol_accw140
3-cyano-1-nitrobenzene	HCN	N	CH	1.37	-1.81	-0.41	-0.24	3-cyano-1-nitrobenzene_accw150
benzylamine0	HCN	N	CH	2.39	-1.81	-2.84	-3.39	benzylamine0_accw150
benzylamine1	HCN	N	CH	2.38	-1.81	-2.82	-3.22	benzylamine1_accw150
benzylamine2	HCN	N	CH	2.38	-1.81	-2.82	-3.23	benzylamine2_accw150
1-pentanol0	HCN	O	CH	1.84	-1.81	-1.12	-1.26	1-pentanol0_accw170
1-pentanol1	HCN	O	CH	1.81	-1.81	-1.06	-1.16	1-pentanol1_accw170
1-octanol0	HCN	O	CH	1.8	-1.81	-1.04	-1.28	1-octanol0_accw260
1-octanol1	HCN	O	CH	1.81	-1.81	-1.06	-1.16	1-octanol1_accw260
h2o	propyne	O	CH	1.82	-1.35	0.18	0.41	propyne_don_01_h2o
h2o	propynol0	O	CH	1.82	-1.41	0.02	0.31	propynol0_don_01_h2o
h2o	propynol1	O	CH	1.82	-1.42	-0.01	0.13	propynol1_don_01_h2o
h2o	propynol2	O	CH	1.82	-1.41	0.02	0.13	propynol2_don_01_h2o
h2o	1,2,4,5-tetrafluorobenzene	O	CH	1.82	-1.19	0.62	0.86	1,2,4,5-tetrafluorobenzene_don_02_h2o
h2o	1,3,5-tribromobenzene	O	CH	1.82	-1.08	0.93	1.22	1,3,5-tribromobenzene_don_02_h2o
h2o	1-bromo-2-nitrobenzene	O	CH	1.82	-1.06	0.98	1.52	1-bromo-2-nitrobenzene_don_02_h2o
h2o	1-nitropropane0	O	CH	1.82	-1.14	0.76	1.16	1-nitropropane0_don_02_h2o
h2o	butanethiol0	O	SH	1.82	-1.04	0.64	0.44	butanethiol0_don_02_h2o
h2o	butanethiol1	O	SH	1.82	-1.04	0.64	0.24	butanethiol1_don_02_h2o

h2o	chcl3	O	CH	1.82	-1.38	0.10	0.35	chcl3_don_02_h2o
h2o	h2s	O	SH	1.82	-1.18	-0.31	-0.23	h2s_don_02_h2o
h2o	methanethiol	O	SH	1.82	-1.04	0.64	0.26	methanethiol_don_02_h2o
h2o	nitromethane	O	CH	1.82	-1.3	0.32	0.90	nitromethane_don_02_h2o
h2o	1,1-dichloroethane	O	CH	1.82	-1.13	0.79	1.10	1,1-dichloroethane_don_03_h2o
h2o	1,1-dichloroethylene	O	CH	1.82	-1.01	1.12	0.96	1,1-dichloroethylene_don_03_h2o
h2o	butenyne	O	CH	1.82	-1.41	0.02	0.11	butenyne_don_03_h2o
h2o	ch2cl2	O	CH	1.82	-1.14	0.76	0.74	ch2cl2_don_03_h2o
h2o	diiodomethane	O	CH	1.82	-1.11	0.84	0.68	diiodomethane_don_03_h2o
h2o	dimethylsulfone	O	CH	1.82	-1.06	0.98	1.51	dimethylsulfone_don_03_h2o
h2o	h2o	O	OH	1.82	-1.74	-2.30	-2.38	h2o_don_03_h2o
h2o	hcn	O	CH	1.82	-1.81	-1.08	-1.21	hcn_don_03_h2o
h2o	trichloroethene	O	CH	1.82	-1.24	0.49	0.70	trichloroethene_don_03_h2o
h2o	1,3-dibromobenzene	O	CH	1.82	-1.03	1.06	1.29	1,3-dibromobenzene_don_04_h2o
h2o	1-nitropropane1	O	CH	1.82	-1.14	0.76	1.22	1-nitropropane1_don_04_h2o
h2o	aceticacid0	O	OH	1.82	-1.99	-3.42	-3.71	aceticacid0_don_04_h2o
h2o	aceticacid1	O	OH	1.82	-2.12	-4.01	-4.24	aceticacid1_don_04_h2o
h2o	aziridine	O	NH	1.82	-1.25	0.32	0.04	aziridine_don_04_h2o
h2o	butyricacid0	O	OH	1.82	-1.97	-3.33	-3.61	butyricacid0_don_04_h2o
h2o	ch2br2	O	CH	1.82	-1.17	0.68	0.61	ch2br2_don_04_h2o
h2o	chcl2br	O	CH	1.82	-1.4	0.05	0.23	chcl2br_don_04_h2o
h2o	dimethylamine	O	NH	1.82	-1.17	0.57	0.26	dimethylamine_don_04_h2o
h2o	ethine	O	CH	1.82	-1.45	-0.09	0.08	ethine_don_04_h2o
h2o	h2o2	O	OH	1.82	-1.89	-2.97	-3.52	h2o2_don_04_h2o
h2o	methylformate	O	CH	1.82	-1.02	1.09	0.95	methylformate_don_04_h2o
h2o	nh3	O	NH	1.82	-1.18	0.54	0.10	nh3_don_04_h2o
h2o	nitroethane0	O	CH	1.82	-1.1	0.87	0.98	nitroethane0_don_04_h2o
h2o	propionicacid0	O	OH	1.82	-1.97	-3.33	-3.57	propionicacid0_don_04_h2o
h2o	2-propanol0	O	OH	1.82	-1.7	-2.12	-1.87	2-propanol0_don_05_h2o
h2o	2-propanol1	O	OH	1.82	-1.7	-2.12	-1.59	2-propanol1_don_05_h2o

h2o	2-propenenitrile	O	CH	1.82	-1.09	0.90	0.79	2-propenenitrile_don_05_h2o
h2o	acetamide	O	NH	1.82	-1.69	-1.09	-1.01	acetamide_don_05_h2o
h2o	ch2clbr	O	CH	1.82	-1.16	0.71	0.65	ch2clbr_don_05_h2o
h2o	ch2fcl	O	CH	1.82	-1.09	0.90	0.82	ch2fcl_don_05_h2o
h2o	chbr3	O	CH	1.82	-1.39	0.07	0.09	chbr3_don_05_h2o
h2o	chf2cl	O	CH	1.82	-1.34	0.21	0.62	chf2cl_don_05_h2o
h2o	chfcl2	O	CH	1.82	-1.36	0.16	0.75	chfcl2_don_05_h2o
h2o	formamide	O	NH	1.82	-1.69	-1.09	-1.14	formamide_don_05_h2o
h2o	formicacid	O	CH	1.82	-1.06	0.98	0.78	formicacid_don_05_h2o
h2o	methylurethane	O	NH	1.82	-1.69	-1.09	-0.80	methylurethane_don_05_h2o
h2o	1,1-difluoroethene	O	CH	1.82	-1.01	1.12	0.87	1,1-difluoroethene_don_06_h2o
h2o	1,2-diaminoethane1	O	NH	1.82	-1.17	0.57	0.27	1,2-diaminoethane1_don_06_h2o
h2o	1,2-diaminoethane2	O	NH	1.82	-1.17	0.57	0.27	1,2-diaminoethane2_don_06_h2o
h2o	1,2-dibromoethane1	O	CH	1.82	-1	1.14	0.94	1,2-dibromoethane1_don_06_h2o
h2o	2-butanol0	O	OH	1.82	-1.69	-2.07	-1.50	2-butanol0_don_06_h2o
h2o	2-butanol1	O	OH	1.82	-1.69	-2.07	-1.65	2-butanol1_don_06_h2o
h2o	2-butanol2	O	OH	1.82	-1.7	-2.12	-1.85	2-butanol2_don_06_h2o
h2o	2-butanol3	O	OH	1.82	-1.7	-2.12	-1.61	2-butanol3_don_06_h2o
h2o	acetamide	O	NH	1.82	-1.62	-0.87	-0.59	acetamide_don_06_h2o
h2o	cis-1,2-dichloroethene	O	CH	1.82	-1.15	0.73	0.74	cis-1,2-dichloroethene_don_06_h2o
h2o	dibutylamine	O	NH	1.82	-1.13	0.70	0.78	dibutylamine_don_06_h2o
h2o	diethylamine0	O	NH	1.82	-1.13	0.70	0.88	diethylamine0_don_06_h2o
h2o	diethylamine1	O	NH	1.82	-1.13	0.70	0.77	diethylamine1_don_06_h2o
h2o	dipropylamine	O	NH	1.82	-1.13	0.70	0.82	dipropylamine_don_06_h2o
h2o	formamide	O	NH	1.82	-1.66	-1.00	-0.83	formamide_don_06_h2o
h2o	glycol0	O	OH	1.82	-1.76	-2.39	-2.28	glycol0_don_06_h2o
h2o	glycol2	O	OH	1.82	-1.77	-2.43	-2.51	glycol2_don_06_h2o
h2o	glycol3	O	OH	1.82	-1.76	-2.39	-2.50	glycol3_don_06_h2o
h2o	imidazole	O	CH	1.82	-1.04	1.04	0.90	imidazole_don_06_h2o
h2o	isobutanol0	O	OH	1.82	-1.71	-2.16	-1.99	isobutanol0_don_06_h2o

h2o	isobutanol1	O	OH	1.82	-1.71	-2.16	-1.77	isobutanol1_don_06_h2o
h2o	isobutanol2	O	OH	1.82	-1.71	-2.16	-2.21	isobutanol2_don_06_h2o
h2o	methanol	O	OH	1.82	-1.73	-2.25	-2.31	methanol_don_06_h2o
h2o	methylformamide	O	NH	1.82	-1.66	-1.00	-1.03	methylformamide_don_06_h2o
h2o	methylimidazol	O	CH	1.82	-1.01	1.12	0.94	methylimidazol_don_06_h2o
h2o	methylurethane	O	NH	1.82	-1.69	-1.09	-0.96	methylurethane_don_06_h2o
h2o	n-methylacetamide	O	NH	1.82	-1.66	-1.00	-0.84	n-methylacetamide_don_06_h2o
h2o	thiophene	O	CH	1.82	-0.99	1.17	0.87	thiophene_don_06_h2o
h2o	trans-1,2-dichloroethene	O	CH	1.82	-1.18	0.65	0.83	trans-1,2-dichloroethene_don_06_h2o
h2o	3-cyano-1-nitrobenzene	O	CH	1.82	-1.09	0.90	1.07	3-cyano-1-nitrobenzene_don_07_h2o
h2o	aceticacid1	O	CH	1.82	-1.04	1.04	1.26	aceticacid1_don_07_h2o
h2o	butyricacid1	O	CH	1.82	-0.99	1.17	1.49	butyricacid1_don_07_h2o
h2o	dicyanomethane	O	CH	1.82	-1.46	-0.12	0.16	dicyanomethane_don_07_h2o
h2o	ethanol1	O	OH	1.82	-1.71	-2.16	-2.23	ethanol1_don_07_h2o
h2o	methylamine	O	NH	1.82	-1.15	0.64	0.23	methylamine_don_07_h2o
h2o	methylindole	O	NH	1.82	-1.73	-1.22	-1.14	methylindole_don_07_h2o
h2o	pentyne	O	CH	1.82	-1.35	0.18	0.24	pentyne_don_07_h2o
h2o	piperidine	O	NH	1.82	-1.16	0.60	0.28	piperidine_don_07_h2o
h2o	1,2,3,5-tetrafluorobenzene	O	CH	1.82	-1.16	0.71	0.88	1,2,3,5-tetrafluorobenzene_don_08_h2o
h2o	2-propen-1-ol0	O	OH	1.82	-1.75	-2.34	-2.01	2-propen-1-ol0_don_08_h2o
h2o	2-propen-1-ol1	O	OH	1.82	-1.76	-2.39	-2.46	2-propen-1-ol1_don_08_h2o
h2o	2-propen-1-ol2	O	OH	1.82	-1.74	-2.30	-2.42	2-propen-1-ol2_don_08_h2o
h2o	aceticacid1	O	CH	1.82	-1.04	1.04	1.17	aceticacid1_don_08_h2o
h2o	butyricacid1	O	OH	1.82	-2.12	-4.01	-4.07	butyricacid1_don_08_h2o
h2o	dimethylsulfoxide	O	CH	1.82	-0.97	1.23	1.34	dimethylsulfoxide_don_08_h2o
h2o	furfural0	O	CH	1.82	-1	1.14	0.84	furfural0_don_08_h2o
h2o	furfural1	O	CH	1.82	-1	1.14	0.84	furfural1_don_08_h2o
h2o	hexyne	O	CH	1.82	-1.35	0.18	0.22	hexyne_don_08_h2o
h2o	imidazole	O	CH	1.82	-1.01	1.12	0.88	imidazole_don_08_h2o
h2o	octyne	O	CH	1.82	-1.35	0.18	0.22	octyne_don_08_h2o

h2o	propanol0	O	OH	1.82	-1.73	-2.25	-2.04	propanol0_don_08_h2o
h2o	propionicacid1	O	OH	1.82	-2.12	-4.01	-4.02	propionicacid1_don_08_h2o
h2o	propynol1	O	OH	1.82	-1.8	-2.57	-2.71	propynol1_don_08_h2o
h2o	propynol2	O	OH	1.82	-1.83	-2.70	-2.48	propynol2_don_08_h2o
h2o	1-bromo-2-nitrobenzene	O	CH	1.82	-1.02	1.09	1.09	1-bromo-2-nitrobenzene_don_09_h2o
h2o	1-butylamine	O	NH	1.82	-1.14	0.67	0.42	1-butylamine_don_09_h2o
h2o	3-cyano-1-nitrobenzene	O	CH	1.82	-1.19	0.62	1.41	3-cyano-1-nitrobenzene_don_09_h2o
h2o	dimethylsulfone	O	CH	1.82	-1.05	1.01	1.21	dimethylsulfone_don_09_h2o
h2o	ethanethiol0	O	SH	1.82	-1.04	0.64	0.46	ethanethiol0_don_09_h2o
h2o	ethanethiol1	O	SH	1.82	-1.04	0.64	0.25	ethanethiol1_don_09_h2o
h2o	ethanol0	O	OH	1.82	-1.72	-2.21	-1.99	ethanol0_don_09_h2o
h2o	ethylamine0	O	NH	1.82	-1.14	0.67	0.47	ethylamine0_don_09_h2o
h2o	ethylamine1	O	NH	1.82	-1.14	0.67	0.46	ethylamine1_don_09_h2o
h2o	ethylamine2	O	NH	1.82	-1.15	0.64	0.24	ethylamine2_don_09_h2o
h2o	furane	O	CH	1.82	-1.04	1.04	0.79	furane_don_09_h2o
h2o	furfural0	O	CH	1.82	-1.18	0.65	0.67	furfural0_don_09_h2o
h2o	furfural1	O	CH	1.82	-1.17	0.68	0.76	furfural1_don_09_h2o
h2o	hexylamine	O	NH	1.82	-1.14	0.67	0.42	hexylamine_don_09_h2o
h2o	imidazole	O	NH	1.82	-1.81	-1.48	-1.58	imidazole_don_09_h2o
h2o	1,2-diaminoethane0	O	NH	1.82	-1.18	0.54	0.49	1,2-diaminoethane0_don_10_h2o
h2o	1,2-diaminoethane1	O	NH	1.82	-1.14	0.67	0.47	1,2-diaminoethane1_don_10_h2o
h2o	1,2-diaminoethane3	O	NH	1.82	-1.17	0.57	0.18	1,2-diaminoethane3_don_10_h2o
h2o	butyne	O	CH	1.82	-1.35	0.18	0.25	butyne_don_10_h2o
h2o	ethylamine2	O	NH	1.82	-1.13	0.70	0.44	ethylamine2_don_10_h2o
h2o	furfural0	O	CH	1.82	-1.06	0.98	0.97	furfural0_don_10_h2o
h2o	furfural1	O	CH	1.82	-1.07	0.95	1.27	furfural1_don_10_h2o
h2o	glycol1	O	OH	1.82	-1.77	-2.43	-2.49	glycol1_don_10_h2o
h2o	glycol3	O	OH	1.82	-1.77	-2.43	-2.37	glycol3_don_10_h2o
h2o	methylimidazol	O	NH	1.82	-1.79	-1.42	-1.48	methylimidazol_don_10_h2o
h2o	n-pentylamine	O	NH	1.82	-1.14	0.67	0.45	n-pentylamine_don_10_h2o

h2o	n-propylamine	O	NH	1.82	-1.14	0.67	0.45	n-propylamine_don_10_h2o
h2o	pyrrole	O	NH	1.82	-1.71	-1.16	-1.20	pyrrole_don_10_h2o
h2o	1,2-diaminoethane2	O	NH	1.82	-1.17	0.57	0.40	1,2-diaminoethane2_don_11_h2o
h2o	1,2-dibromopropane1	O	CH	1.82	-1	1.14	1.12	1,2-dibromopropane1_don_11_h2o
h2o	2-amino-2-methylpropane0	O	NH	1.82	-1.13	0.70	0.62	2-amino-2-methylpropane0_don_11_h2o
h2o	3-cyano-1-nitrobenzene	O	CH	1.82	-1.02	1.09	1.24	3-cyano-1-nitrobenzene_don_11_h2o
h2o	dimethylsulfone	O	CH	1.82	-1.06	0.98	1.42	dimethylsulfone_don_11_h2o
h2o	morpholine	O	NH	1.82	-1.21	0.44	0.19	morpholine_don_11_h2o
h2o	1,2-diaminoethane2	O	NH	1.82	-1.15	0.64	0.23	1,2-diaminoethane2_don_12_h2o
h2o	1-propanethiol0	O	SH	1.82	-1.04	0.64	0.44	1-propanethiol0_don_12_h2o
h2o	1-propanethiol1	O	SH	1.82	-1.04	0.64	0.26	1-propanethiol1_don_12_h2o
h2o	chinone	O	CH	1.82	-1.01	1.12	1.21	chinone_don_12_h2o
h2o	isopropylamine	O	NH	1.82	-1.13	0.70	0.41	isopropylamine_don_12_h2o
h2o	propanol1	O	OH	1.82	-1.71	-2.16	-2.24	propanol1_don_12_h2o
h2o	2-methylphenol0	O	OH	1.82	-1.95	-3.24	-3.12	2-methylphenol0_don_13_h2o
h2o	4-bromophenol0	O	OH	1.82	-2.01	-3.51	-3.48	4-bromophenol0_don_13_h2o
h2o	4-bromophenol1	O	OH	1.82	-2.01	-3.51	-3.48	4-bromophenol1_don_13_h2o
h2o	4-methylphenol	O	OH	1.82	-1.96	-3.29	-3.15	4-methylphenol_don_13_h2o
h2o	aniline	O	NH	1.82	-1.46	-0.36	-0.32	aniline_don_13_h2o
h2o	phenol	O	OH	1.82	-1.98	-3.38	-3.24	phenol_don_13_h2o
h2o	thiophenol	O	SH	1.82	-1.24	-0.72	0.04	thiophenol_don_13_h2o
h2o	3-cyanophenol	O	OH	1.82	-2.05	-3.69	-3.70	3-cyanophenol_don_14_h2o
h2o	3-hydroxybenzaldehyde0	O	OH	1.82	-2.02	-3.56	-3.56	3-hydroxybenzaldehyde0_don_14_h2o
h2o	3-hydroxybenzaldehyde1	O	OH	1.82	-2.03	-3.60	-3.55	3-hydroxybenzaldehyde1_don_14_h2o
h2o	3-hydroxybenzaldehyde2	O	OH	1.82	-2.02	-3.56	-3.70	3-hydroxybenzaldehyde2_don_14_h2o
h2o	4-cyanophenol	O	OH	1.82	-2.06	-3.74	-4.06	4-cyanophenol_don_14_h2o
h2o	pyrrolidin	O	NH	1.82	-1.18	0.54	0.40	pyrrolidin_don_14_h2o
h2o	1-butanol0	O	OH	1.82	-1.72	-2.21	-2.02	1-butanol0_don_15_h2o
h2o	1-butanol1	O	OH	1.82	-1.71	-2.16	-2.23	1-butanol1_don_15_h2o
h2o	3-nitrophenol	O	OH	1.82	-2.07	-3.78	-3.90	3-nitrophenol_don_15_h2o

h2o	4-nitrophenol	O	OH	1.82	-2.1	-3.92	-4.40	4-nitrophenol_don_15_h2o
h2o	benzoicacid	O	OH	1.82	-2	-3.47	-3.84	benzoicacid_don_15_h2o
h2o	tert-butanol	O	OH	1.82	-1.69	-2.07	-1.51	tert-butanol_don_15_h2o
h2o	2-amino-2-methylpropane1	O	NH	1.82	-1.13	0.70	0.65	2-amino-2-methylpropane1_don_16_h2o
h2o	benzylamine1	O	NH	1.82	-1.18	0.54	0.29	benzylamine1_don_16_h2o
h2o	benzylamine2	O	NH	1.82	-1.18	0.54	0.22	benzylamine2_don_16_h2o
h2o	ethoxyethanol4	O	OH	1.82	-1.77	-2.43	-2.36	ethoxyethanol4_don_16_h2o
h2o	ethoxyethanol5	O	OH	1.82	-1.76	-2.39	-2.51	ethoxyethanol5_don_16_h2o
h2o	ethoxyethanol6	O	OH	1.82	-1.75	-2.34	-2.04	ethoxyethanol6_don_16_h2o
h2o	ethoxyethanol7	O	OH	1.82	-1.75	-2.34	-2.01	ethoxyethanol7_don_16_h2o
h2o	ethoxyethanol8	O	OH	1.82	-1.73	-2.25	-2.36	ethoxyethanol8_don_16_h2o
h2o	benzylamine0	O	NH	1.82	-1.21	0.44	0.59	benzylamine0_don_17_h2o
h2o	benzylamine1	O	NH	1.82	-1.18	0.54	0.48	benzylamine1_don_17_h2o
h2o	benzylamine2	O	NH	1.82	-1.18	0.54	0.50	benzylamine2_don_17_h2o
h2o	1-pentanol0	O	OH	1.82	-1.73	-2.25	-2.02	1-pentanol0_don_18_h2o
h2o	1-pentanol1	O	OH	1.82	-1.71	-2.16	-2.23	1-pentanol1_don_18_h2o
h2o	cyclohexanol0	O	OH	1.82	-1.71	-2.16	-1.65	cyclohexanol0_don_19_h2o
h2o	cyclohexanol1	O	OH	1.82	-1.68	-2.03	-1.70	cyclohexanol1_don_19_h2o
h2o	1-heptanol0	O	OH	1.82	-1.72	-2.21	-2.02	1-heptanol0_don_24_h2o
h2o	1-heptanol1	O	OH	1.82	-1.71	-2.16	-2.24	1-heptanol1_don_24_h2o
h2o	4-(1,1-dimethylethyl)-phenol	O	OH	1.82	-1.96	-3.29	-3.70	4-(1,1-dimethylethyl)-phenol_don_25_h2o
h2o	1-octanol0	O	OH	1.82	-1.72	-2.21	-2.02	1-octanol0_don_27_h2o
h2o	1-octanol1	O	OH	1.82	-1.71	-2.16	-2.23	1-octanol1_don_27_h2o
h2s	propyne	S	CH	1.15	-1.35	0.73	0.60	propyne_don_01_h2s
h2s	propynol0	S	CH	1.15	-1.41	0.65	0.60	propynol0_don_01_h2s
h2s	propynol1	S	CH	1.15	-1.42	0.64	0.61	propynol1_don_01_h2s
h2s	1,2,4,5-tetrafluorobenzene	S	CH	1.15	-1.19	0.96	0.79	1,2,4,5-tetrafluorobenzene_don_02_h2s
h2s	1-bromo-2-nitrobenzene	S	CH	1.15	-1.06	1.14	1.16	1-bromo-2-nitrobenzene_don_02_h2s
h2s	1-nitropropane0	S	CH	1.15	-1.14	1.03	0.90	1-nitropropane0_don_02_h2s
h2s	butanethiol0	S	SH	1.15	-1.04	0.97	0.36	butanethiol0_don_02_h2s

h2s	butanethiol1	S	SH	1.15	-1.04	0.97	0.23	butanethiol1_don_02_h2s
h2s	ch2cl2	S	CH	1.15	-1.14	1.03	0.69	ch2cl2_don_02_h2s
h2s	chcl3	S	CH	1.15	-1.38	0.69	0.60	chcl3_don_02_h2s
h2s	diiodomethane	S	CH	1.15	-1.11	1.07	0.60	diiodomethane_don_02_h2s
h2s	dimethylsulfone	S	CH	1.15	-1.05	1.15	1.02	dimethylsulfone_don_02_h2s
h2s	h2o	S	OH	1.15	-1.74	-0.53	-0.81	h2o_don_02_h2s
h2s	methanethiol	S	SH	1.15	-1.04	0.97	0.24	methanethiol_don_02_h2s
h2s	nh3	S	NH	1.15	-1.18	0.92	0.26	nh3_don_02_h2s
h2s	1,1-dichloroethane	S	CH	1.15	-1.13	1.04	0.79	1,1-dichloroethane_don_03_h2s
h2s	1,1-dichloroethylene	S	CH	1.15	-1.01	1.21	0.74	1,1-dichloroethylene_don_03_h2s
h2s	butenyne	S	CH	1.15	-1.41	0.65	0.58	butenyne_don_03_h2s
h2s	h2o2	S	OH	1.15	-1.89	-0.87	-1.45	h2o2_don_03_h2s
h2s	hcn	S	CH	1.15	-1.81	0.09	0.50	hcn_don_03_h2s
h2s	nitromethane	S	CH	1.15	-1.3	0.80	0.87	nitromethane_don_03_h2s
h2s	trichloroethene	S	CH	1.15	-1.24	0.89	0.74	trichloroethene_don_03_h2s
h2s	1,3-dibromobenzene	S	CH	1.15	-1.03	1.18	0.96	1,3-dibromobenzene_don_04_h2s
h2s	1-nitropropane1	S	CH	1.15	-1.14	1.03	0.94	1-nitropropane1_don_04_h2s
h2s	aceticacid0	S	OH	1.15	-1.99	-1.10	-0.88	aceticacid0_don_04_h2s
h2s	aceticacid1	S	OH	1.15	-2.12	-1.40	-1.23	aceticacid1_don_04_h2s
h2s	aziridine	S	NH	1.15	-1.25	0.80	0.25	aziridine_don_04_h2s
h2s	butyricacid0	S	OH	1.15	-1.97	-1.06	-0.83	butyricacid0_don_04_h2s
h2s	butyricacid1	S	OH	1.15	-2.12	-1.40	-1.19	butyricacid1_don_04_h2s
h2s	ch2br2	S	CH	1.15	-1.17	0.99	0.61	ch2br2_don_04_h2s
h2s	chcl2br	S	CH	1.15	-1.4	0.66	0.50	chcl2br_don_04_h2s
h2s	dimethylamine	S	NH	1.15	-1.17	0.93	0.36	dimethylamine_don_04_h2s
h2s	dimethylsulfoxide	S	CH	1.15	-0.95	1.29	1.04	dimethylsulfoxide_don_04_h2s
h2s	ethine	S	CH	1.15	-1.45	0.59	0.62	ethine_don_04_h2s
h2s	nitroethane0	S	CH	1.15	-1.1	1.08	0.79	nitroethane0_don_04_h2s
h2s	nitromethane	S	CH	1.15	-1.3	0.80	0.81	nitromethane_don_04_h2s
h2s	propionicacid0	S	OH	1.15	-1.97	-1.06	-0.84	propionicacid0_don_04_h2s

h2s	propionicacid1	S	OH	1.15	-2.12	-1.40	-1.20	propionicacid1_don_04_h2s
h2s	1,1-difluoroethene	S	CH	1.15	-1.01	1.21	0.69	1,1-difluoroethene_don_05_h2s
h2s	2-propanol0	S	OH	1.15	-1.7	-0.44	-0.53	2-propanol0_don_05_h2s
h2s	2-propanol1	S	OH	1.15	-1.7	-0.44	-0.35	2-propanol1_don_05_h2s
h2s	2-propenenitrile	S	CH	1.15	-1.09	1.10	0.74	2-propenenitrile_don_05_h2s
h2s	acetamide	S	NH	1.15	-1.69	0.08	0.22	acetamide_don_05_h2s
h2s	ch2clbr	S	CH	1.15	-1.16	1.00	0.68	ch2clbr_don_05_h2s
h2s	ch2fcl	S	CH	1.15	-1.09	1.10	0.73	ch2fcl_don_05_h2s
h2s	chbr3	S	CH	1.15	-1.39	0.68	0.38	chbr3_don_05_h2s
h2s	chf2cl	S	CH	1.15	-1.34	0.75	0.87	chf2cl_don_05_h2s
h2s	chfcl2	S	CH	1.15	-1.36	0.72	0.79	chfcl2_don_05_h2s
h2s	formamide	S	NH	1.15	-1.69	0.08	0.21	formamide_don_05_h2s
h2s	formicacid	S	CH	1.15	-1.06	1.14	0.75	formicacid_don_05_h2s
h2s	methylurethane	S	NH	1.15	-1.69	0.08	0.36	methylurethane_don_05_h2s
h2s	1,2-diaminoethane1	S	NH	1.15	-1.17	0.93	0.39	1,2-diaminoethane1_don_06_h2s
h2s	1,2-dibromoethane1	S	CH	1.15	-1	1.22	0.79	1,2-dibromoethane1_don_06_h2s
h2s	1,3,5-tribromobenzene	S	CH	1.15	-1.08	1.11	0.94	1,3,5-tribromobenzene_don_06_h2s
h2s	2-butanol0	S	OH	1.15	-1.69	-0.41	-0.31	2-butanol0_don_06_h2s
h2s	2-butanol1	S	OH	1.15	-1.69	-0.41	-0.45	2-butanol1_don_06_h2s
h2s	2-butanol2	S	OH	1.15	-1.7	-0.44	-0.52	2-butanol2_don_06_h2s
h2s	2-butanol3	S	OH	1.15	-1.7	-0.44	-0.39	2-butanol3_don_06_h2s
h2s	acetamide	S	NH	1.15	-1.62	0.20	0.50	acetamide_don_06_h2s
h2s	cis-1,2-dichloroethene	S	CH	1.15	-1.15	1.01	0.73	cis-1,2-dichloroethene_don_06_h2s
h2s	dibutylamine	S	NH	1.15	-1.13	1.00	0.59	dibutylamine_don_06_h2s
h2s	diethylamine0	S	NH	1.15	-1.13	1.00	0.70	diethylamine0_don_06_h2s
h2s	diethylamine1	S	NH	1.15	-1.13	1.00	0.63	diethylamine1_don_06_h2s
h2s	dipropylamine	S	NH	1.15	-1.13	1.00	0.63	dipropylamine_don_06_h2s
h2s	formamide	S	NH	1.15	-1.66	0.13	0.42	formamide_don_06_h2s
h2s	furane	S	CH	1.15	-1.04	1.17	0.68	furane_don_06_h2s
h2s	glycol0	S	OH	1.15	-1.76	-0.57	-0.71	glycol0_don_06_h2s

h2s	glycol3	S	OH	1.15	-1.76	-0.57	-0.92	glycol3_don_06_h2s
h2s	imidazole	S	CH	1.15	-1.04	1.17	0.77	imidazole_don_06_h2s
h2s	isobutanol0	S	OH	1.15	-1.71	-0.46	-0.64	isobutanol0_don_06_h2s
h2s	isobutanol2	S	OH	1.15	-1.71	-0.46	-0.80	isobutanol2_don_06_h2s
h2s	methanol	S	OH	1.15	-1.73	-0.50	-0.85	methanol_don_06_h2s
h2s	methylamine	S	NH	1.15	-1.15	0.96	0.34	methylamine_don_06_h2s
h2s	methylformamide	S	NH	1.15	-1.66	0.13	0.18	methylformamide_don_06_h2s
h2s	methylimidazol	S	CH	1.15	-1.01	1.21	0.71	methylimidazol_don_06_h2s
h2s	methylurethane	S	NH	1.15	-1.69	0.08	0.27	methylurethane_don_06_h2s
h2s	n-methylacetamide	S	NH	1.15	-1.66	0.13	0.20	n-methylacetamide_don_06_h2s
h2s	thiophene	S	CH	1.15	-0.99	1.24	0.72	thiophene_don_06_h2s
h2s	trans-1,2-dichloroethene	S	CH	1.15	-1.18	0.97	0.78	trans-1,2-dichloroethene_don_06_h2s
h2s	3-cyano-1-nitrobenzene	S	CH	1.15	-1.09	1.10	0.91	3-cyano-1-nitrobenzene_don_07_h2s
h2s	butyricacid1	S	CH	1.15	-0.99	1.24	1.05	butyricacid1_don_07_h2s
h2s	dicyanomethane	S	CH	1.15	-1.46	0.58	0.73	dicyanomethane_don_07_h2s
h2s	ethanol1	S	OH	1.15	-1.71	-0.46	-0.81	ethanol1_don_07_h2s
h2s	methylindole	S	NH	1.15	-1.73	0.02	0.25	methylindole_don_07_h2s
h2s	pentyne	S	CH	1.15	-1.35	0.73	0.58	pentyne_don_07_h2s
h2s	piperidine	S	NH	1.15	-1.16	0.95	0.38	piperidine_don_07_h2s
h2s	1,2,3,5-tetrafluorobenzene	S	CH	1.15	-1.16	1.00	0.78	1,2,3,5-tetrafluorobenzene_don_08_h2s
h2s	2-propen-1-ol0	S	OH	1.15	-1.75	-0.55	-0.53	2-propen-1-ol0_don_08_h2s
h2s	2-propen-1-ol1	S	OH	1.15	-1.76	-0.57	-0.89	2-propen-1-ol1_don_08_h2s
h2s	2-propen-1-ol2	S	OH	1.15	-1.74	-0.53	-0.91	2-propen-1-ol2_don_08_h2s
h2s	aceticacid1	S	CH	1.15	-1.04	1.17	0.86	aceticacid1_don_08_h2s
h2s	chinone	S	CH	1.15	-1.01	1.21	0.89	chinone_don_08_h2s
h2s	dimethylsulfoxide	S	CH	1.15	-0.95	1.29	0.97	dimethylsulfoxide_don_08_h2s
h2s	furfural0	S	CH	1.15	-1	1.22	0.71	furfural0_don_08_h2s
h2s	furfural1	S	CH	1.15	-1	1.22	0.70	furfural1_don_08_h2s
h2s	hexyne	S	CH	1.15	-1.35	0.73	0.56	hexyne_don_08_h2s
h2s	imidazole	S	CH	1.15	-1.01	1.21	0.73	imidazole_don_08_h2s

h2s	octyne	S	CH	1.15	-1.35	0.73	0.56	octyne_don_08_h2s
h2s	propanol0	S	OH	1.15	-1.73	-0.50	-0.65	propanol0_don_08_h2s
h2s	propynol0	S	OH	1.15	-1.83	-0.73	-0.81	propynol0_don_08_h2s
h2s	1-bromo-2-nitrobenzene	S	CH	1.15	-1.02	1.19	0.84	1-bromo-2-nitrobenzene_don_09_h2s
h2s	1-butylamine	S	NH	1.15	-1.14	0.98	0.47	1-butylamine_don_09_h2s
h2s	3-cyano-1-nitrobenzene	S	CH	1.15	-1.19	0.96	1.14	3-cyano-1-nitrobenzene_don_09_h2s
h2s	ethanethiol0	S	SH	1.15	-1.04	0.97	0.37	ethanethiol0_don_09_h2s
h2s	ethanethiol1	S	SH	1.15	-1.04	0.97	0.23	ethanethiol1_don_09_h2s
h2s	ethanol0	S	OH	1.15	-1.72	-0.48	-0.60	ethanol0_don_09_h2s
h2s	ethylamine2	S	NH	1.15	-1.15	0.96	0.37	ethylamine2_don_09_h2s
h2s	furfural0	S	CH	1.15	-1.18	0.97	0.76	furfural0_don_09_h2s
h2s	furfural1	S	CH	1.15	-1.17	0.99	0.75	furfural1_don_09_h2s
h2s	imidazole	S	NH	1.15	-1.81	-0.11	0.20	imidazole_don_09_h2s
h2s	1,2-diaminoethane3	S	NH	1.15	-1.17	0.93	0.34	1,2-diaminoethane3_don_10_h2s
h2s	3-cyanophenol	S	OH	1.15	-2.05	-1.24	-1.03	3-cyanophenol_don_10_h2s
h2s	butyne	S	CH	1.15	-1.35	0.73	0.58	butyne_don_10_h2s
h2s	dimethylsulfone	S	CH	1.15	-1.06	1.14	1.20	dimethylsulfone_don_10_h2s
h2s	ethylamine0	S	NH	1.15	-1.14	0.98	0.47	ethylamine0_don_10_h2s
h2s	ethylamine1	S	NH	1.15	-1.14	0.98	0.48	ethylamine1_don_10_h2s
h2s	furfural0	S	CH	1.15	-1.06	1.14	0.82	furfural0_don_10_h2s
h2s	glycol1	S	OH	1.15	-1.77	-0.60	-0.90	glycol1_don_10_h2s
h2s	glycol3	S	OH	1.15	-1.77	-0.60	-0.84	glycol3_don_10_h2s
h2s	hexylamine	S	NH	1.15	-1.14	0.98	0.46	hexylamine_don_10_h2s
h2s	methylimidazol	S	NH	1.15	-1.79	-0.08	0.21	methylimidazol_don_10_h2s
h2s	n-pentylamine	S	NH	1.15	-1.14	0.98	0.47	n-pentylamine_don_10_h2s
h2s	n-propylamine	S	NH	1.15	-1.14	0.98	0.47	n-propylamine_don_10_h2s
h2s	pyrrole	S	NH	1.15	-1.71	0.05	0.17	pyrrole_don_10_h2s
h2s	1,2-diaminoethane2	S	NH	1.15	-1.17	0.93	0.42	1,2-diaminoethane2_don_11_h2s
h2s	1,2-diaminoethane3	S	NH	1.15	-1.17	0.93	0.65	1,2-diaminoethane3_don_11_h2s
h2s	1,2-dibromopropane1	S	CH	1.15	-1	1.22	0.84	1,2-dibromopropane1_don_11_h2s

h2s	2-amino-2-methylpropane0	S	NH	1.15	-1.13	1.00	0.59	2-amino-2-methylpropane0_don_11_h2s
h2s	3-cyano-1-nitrobenzene	S	CH	1.15	-1.02	1.19	0.97	3-cyano-1-nitrobenzene_don_11_h2s
h2s	morpholine	S	NH	1.15	-1.21	0.87	0.40	morpholine_don_11_h2s
h2s	1,2-diaminoethane0	S	NH	1.15	-1.15	0.96	0.53	1,2-diaminoethane0_don_12_h2s
h2s	1,2-diaminoethane2	S	NH	1.15	-1.15	0.96	0.34	1,2-diaminoethane2_don_12_h2s
h2s	1-propanethiol0	S	SH	1.15	-1.04	0.97	0.35	1-propanethiol0_don_12_h2s
h2s	1-propanethiol1	S	SH	1.15	-1.04	0.97	0.23	1-propanethiol1_don_12_h2s
h2s	isopropylamine	S	NH	1.15	-1.13	1.00	0.45	isopropylamine_don_12_h2s
h2s	propanol1	S	OH	1.15	-1.71	-0.46	-0.82	propanol1_don_12_h2s
h2s	2-methylphenol0	S	OH	1.15	-1.95	-1.01	-0.80	2-methylphenol0_don_13_h2s
h2s	4-bromophenol0	S	OH	1.15	-2.01	-1.15	-0.92	4-bromophenol0_don_13_h2s
h2s	4-methylphenol	S	OH	1.15	-1.96	-1.03	-0.82	4-methylphenol_don_13_h2s
h2s	aniline	S	NH	1.15	-1.46	0.46	0.35	aniline_don_13_h2s
h2s	phenol	S	OH	1.15	-1.98	-1.08	-0.84	phenol_don_13_h2s
h2s	3-hydroxybenzaldehyde0	S	OH	1.15	-2.02	-1.17	-0.86	3-hydroxybenzaldehyde0_don_14_h2s
h2s	3-hydroxybenzaldehyde1	S	OH	1.15	-2.03	-1.19	-0.94	3-hydroxybenzaldehyde1_don_14_h2s
h2s	3-hydroxybenzaldehyde2	S	OH	1.15	-2.02	-1.17	-1.00	3-hydroxybenzaldehyde2_don_14_h2s
h2s	4-cyanophenol	S	OH	1.15	-2.06	-1.26	-1.14	4-cyanophenol_don_14_h2s
h2s	pyrrolidin	S	NH	1.15	-1.18	0.92	0.41	pyrrolidin_don_14_h2s
h2s	1-butanol0	S	OH	1.15	-1.72	-0.48	-0.63	1-butanol0_don_15_h2s
h2s	1-butanol1	S	OH	1.15	-1.71	-0.46	-0.80	1-butanol1_don_15_h2s
h2s	3-nitrophenol	S	OH	1.15	-2.07	-1.28	-0.96	3-nitrophenol_don_15_h2s
h2s	tert-butanol	S	OH	1.15	-1.69	-0.41	-0.32	tert-butanol_don_15_h2s
h2s	2-amino-2-methylpropane1	S	NH	1.15	-1.13	1.00	0.57	2-amino-2-methylpropane1_don_16_h2s
h2s	benzylamine0	S	NH	1.15	-1.21	0.87	0.52	benzylamine0_don_16_h2s
h2s	benzylamine1	S	NH	1.15	-1.18	0.92	0.40	benzylamine1_don_16_h2s
h2s	benzylamine2	S	NH	1.15	-1.18	0.92	0.37	benzylamine2_don_16_h2s
h2s	ethoxyethanol4	S	OH	1.15	-1.77	-0.60	-0.81	ethoxyethanol4_don_16_h2s
h2s	ethoxyethanol5	S	OH	1.15	-1.76	-0.57	-0.92	ethoxyethanol5_don_16_h2s
h2s	ethoxyethanol6	S	OH	1.15	-1.75	-0.55	-0.59	ethoxyethanol6_don_16_h2s

h2s	ethoxyethanol7	S	OH	1.15	-1.75	-0.55	-0.62	ethoxyethanol7_don_16_h2s
h2s	ethoxyethanol8	S	OH	1.15	-1.73	-0.50	-0.89	ethoxyethanol8_don_16_h2s
h2s	benzylamine2	S	NH	1.15	-1.18	0.92	0.48	benzylamine2_don_17_h2s
h2s	1-pentanol0	S	OH	1.15	-1.73	-0.50	-0.63	1-pentanol0_don_18_h2s
h2s	1-pentanol1	S	OH	1.15	-1.71	-0.46	-0.82	1-pentanol1_don_18_h2s
h2s	cyclohexanol0	S	OH	1.15	-1.71	-0.46	-0.41	cyclohexanol0_don_19_h2s
h2s	cyclohexanol1	S	OH	1.15	-1.68	-0.39	-0.50	cyclohexanol1_don_19_h2s
h2s	1-heptanol0	S	OH	1.15	-1.72	-0.48	-0.63	1-heptanol0_don_24_h2s
h2s	1-heptanol1	S	OH	1.15	-1.71	-0.46	-0.83	1-heptanol1_don_24_h2s
h2s	1-octanol0	S	OH	1.15	-1.72	-0.48	-0.62	1-octanol0_don_27_h2s
h2s	1-octanol1	S	OH	1.15	-1.71	-0.46	-0.82	1-octanol1_don_27_h2s
ph3	propyne	P	CH	1.25	-1.35	0.77	0.75	propyne_don_01_ph3
ph3	propynol0	P	CH	1.25	-1.41	0.69	0.79	propynol0_don_01_ph3
ph3	1-bromo-2-nitrobenzene	P	CH	1.25	-1.06	1.15	1.13	1-bromo-2-nitrobenzene_don_02_ph3
ph3	1-nitropropane0	P	CH	1.25	-1.14	1.05	1.03	1-nitropropane0_don_02_ph3
ph3	butanethiol0	P	SH	1.25	-1.04	0.99	0.47	butanethiol0_don_02_ph3
ph3	butanethiol1	P	SH	1.25	-1.04	0.99	0.38	butanethiol1_don_02_ph3
ph3	ch2cl2	P	CH	1.25	-1.14	1.05	0.83	ch2cl2_don_02_ph3
ph3	chcl3	P	CH	1.25	-1.38	0.73	0.90	chcl3_don_02_ph3
ph3	dimethylsulfone	P	CH	1.25	-1.05	1.16	1.13	dimethylsulfone_don_02_ph3
ph3	h2o	P	OH	1.25	-1.74	-0.40	-0.58	h2o_don_02_ph3
ph3	methanethiol	P	SH	1.25	-1.04	0.99	0.40	methanethiol_don_02_ph3
ph3	nitroethane0	P	CH	1.25	-1.1	1.10	0.94	nitroethane0_don_02_ph3
ph3	1,1-dichloroethane	P	CH	1.25	-1.13	1.06	0.91	1,1-dichloroethane_don_03_ph3
ph3	1,1-dichloroethylene	P	CH	1.25	-1.01	1.22	0.84	1,1-dichloroethylene_don_03_ph3
ph3	butenyne	P	CH	1.25	-1.41	0.69	0.77	butenyne_don_03_ph3
ph3	diiodomethane	P	CH	1.25	-1.11	1.08	0.71	diiodomethane_don_03_ph3
ph3	ethine	P	CH	1.25	-1.45	0.64	0.82	ethine_don_03_ph3
ph3	hcn	P	CH	1.25	-1.81	0.17	0.86	hcn_don_03_ph3
ph3	trichloroethene	P	CH	1.25	-1.24	0.92	0.89	trichloroethene_don_03_ph3

ph3	1,2-dibromoethane1	P	CH	1.25	-1	1.23	0.90	1,2-dibromoethane1_don_04_ph3
ph3	1,3-dibromobenzene	P	CH	1.25	-1.03	1.19	0.97	1,3-dibromobenzene_don_04_ph3
ph3	1-nitropropane1	P	CH	1.25	-1.14	1.05	1.09	1-nitropropane1_don_04_ph3
ph3	aceticacid0	P	OH	1.25	-1.99	-0.94	-0.62	aceticacid0_don_04_ph3
ph3	aceticacid1	P	OH	1.25	-2.12	-1.22	-1.13	aceticacid1_don_04_ph3
ph3	aziridine	P	NH	1.25	-1.25	0.84	0.35	aziridine_don_04_ph3
ph3	butyricacid1	P	OH	1.25	-2.12	-1.22	-1.10	butyricacid1_don_04_ph3
ph3	ch2br2	P	CH	1.25	-1.17	1.01	0.75	ch2br2_don_04_ph3
ph3	chcl2br	P	CH	1.25	-1.4	0.71	0.72	chcl2br_don_04_ph3
ph3	dimethylamine	P	NH	1.25	-1.17	0.96	0.47	dimethylamine_don_04_ph3
ph3	dimethylsulfone	P	CH	1.25	-1.06	1.15	1.25	dimethylsulfone_don_04_ph3
ph3	h2o2	P	OH	1.25	-1.89	-0.73	-1.33	h2o2_don_04_ph3
ph3	methylformate	P	CH	1.25	-1.02	1.20	0.83	methylformate_don_04_ph3
ph3	nh3	P	NH	1.25	-1.18	0.94	0.44	nh3_don_04_ph3
ph3	nitromethane	P	CH	1.25	-1.3	0.84	1.04	nitromethane_don_04_ph3
ph3	propionicacid0	P	OH	1.25	-1.97	-0.90	-0.57	propionicacid0_don_04_ph3
ph3	propionicacid1	P	OH	1.25	-2.12	-1.22	-1.07	propionicacid1_don_04_ph3
ph3	1,1-difluoroethene	P	CH	1.25	-1.01	1.22	0.81	1,1-difluoroethene_don_05_ph3
ph3	2-propanol0	P	OH	1.25	-1.7	-0.32	-0.39	2-propanol0_don_05_ph3
ph3	2-propanol1	P	OH	1.25	-1.7	-0.32	-0.25	2-propanol1_don_05_ph3
ph3	2-propenenitrile	P	CH	1.25	-1.09	1.11	0.90	2-propenenitrile_don_05_ph3
ph3	acetamide	P	NH	1.25	-1.69	0.17	0.48	acetamide_don_05_ph3
ph3	ch2clbr	P	CH	1.25	-1.16	1.02	0.80	ch2clbr_don_05_ph3
ph3	ch2fcl	P	CH	1.25	-1.09	1.11	0.87	ch2fcl_don_05_ph3
ph3	chbr3	P	CH	1.25	-1.39	0.72	0.52	chbr3_don_05_ph3
ph3	chf2cl	P	CH	1.25	-1.34	0.79	1.07	chf2cl_don_05_ph3
ph3	chfcl2	P	CH	1.25	-1.36	0.76	0.95	chfcl2_don_05_ph3
ph3	formamide	P	NH	1.25	-1.69	0.17	0.54	formamide_don_05_ph3
ph3	formicacid	P	CH	1.25	-1.06	1.15	0.89	formicacid_don_05_ph3
ph3	methylurethane	P	NH	1.25	-1.69	0.17	0.63	methylurethane_don_05_ph3

ph3	1,2-diaminoethane2	P	NH	1.25	-1.17	0.96	0.49	1,2-diaminoethane2_don_06_ph3
ph3	2-butanol0	P	OH	1.25	-1.69	-0.30	-0.21	2-butanol0_don_06_ph3
ph3	2-butanol2	P	OH	1.25	-1.7	-0.32	-0.40	2-butanol2_don_06_ph3
ph3	2-butanol3	P	OH	1.25	-1.7	-0.32	-0.28	2-butanol3_don_06_ph3
ph3	acetamide	P	NH	1.25	-1.62	0.27	0.76	acetamide_don_06_ph3
ph3	cis-1,2-dichloroethene	P	CH	1.25	-1.15	1.03	0.89	cis-1,2-dichloroethene_don_06_ph3
ph3	dibutylamine	P	NH	1.25	-1.13	1.02	0.59	dibutylamine_don_06_ph3
ph3	dicyanomethane	P	CH	1.25	-1.46	0.63	1.01	dicyanomethane_don_06_ph3
ph3	diethylamine0	P	NH	1.25	-1.13	1.02	0.71	diethylamine0_don_06_ph3
ph3	diethylamine1	P	NH	1.25	-1.13	1.02	0.70	diethylamine1_don_06_ph3
ph3	dipropylamine	P	NH	1.25	-1.13	1.02	0.64	dipropylamine_don_06_ph3
ph3	formamide	P	NH	1.25	-1.66	0.21	0.71	formamide_don_06_ph3
ph3	furane	P	CH	1.25	-1.04	1.18	0.79	furane_don_06_ph3
ph3	glycol0	P	OH	1.25	-1.76	-0.45	-0.57	glycol0_don_06_ph3
ph3	glycol3	P	OH	1.25	-1.76	-0.45	-0.73	glycol3_don_06_ph3
ph3	imidazole	P	CH	1.25	-1.04	1.18	0.86	imidazole_don_06_ph3
ph3	isobutanol0	P	OH	1.25	-1.71	-0.34	-0.49	isobutanol0_don_06_ph3
ph3	isobutanol2	P	OH	1.25	-1.71	-0.34	-0.61	isobutanol2_don_06_ph3
ph3	methanol	P	OH	1.25	-1.73	-0.38	-0.67	methanol_don_06_ph3
ph3	methylformamide	P	NH	1.25	-1.66	0.21	0.46	methylformamide_don_06_ph3
ph3	methylimidazol	P	CH	1.25	-1.01	1.22	0.83	methylimidazol_don_06_ph3
ph3	methylurethane	P	NH	1.25	-1.69	0.17	0.50	methylurethane_don_06_ph3
ph3	n-methylacetamide	P	NH	1.25	-1.66	0.21	0.42	n-methylacetamide_don_06_ph3
ph3	thiophene	P	CH	1.25	-0.99	1.24	0.80	thiophene_don_06_ph3
ph3	trans-1,2-dichloroethene	P	CH	1.25	-1.18	0.99	0.90	trans-1,2-dichloroethene_don_06_ph3
ph3	3-cyano-1-nitrobenzene	P	CH	1.25	-1.09	1.11	1.01	3-cyano-1-nitrobenzene_don_07_ph3
ph3	butyricacid1	P	CH	1.25	-0.99	1.24	1.08	butyricacid1_don_07_ph3
ph3	ethanol1	P	OH	1.25	-1.71	-0.34	-0.61	ethanol1_don_07_ph3
ph3	methylamine	P	NH	1.25	-1.15	0.99	0.48	methylamine_don_07_ph3
ph3	methylindole	P	NH	1.25	-1.73	0.11	0.52	methylindole_don_07_ph3

ph3	pentyne	P	CH	1.25	-1.35	0.77	0.73	pentyne_don_07_ph3
ph3	piperidine	P	NH	1.25	-1.16	0.97	0.48	piperidine_don_07_ph3
ph3	1,2,4,5-tetrafluorobenzene	P	CH	1.25	-1.19	0.98	0.93	1,2,4,5-tetrafluorobenzene_don_08_ph3
ph3	2-propen-1-ol0	P	OH	1.25	-1.75	-0.43	-0.43	2-propen-1-ol0_don_08_ph3
ph3	2-propen-1-ol1	P	OH	1.25	-1.76	-0.45	-0.69	2-propen-1-ol1_don_08_ph3
ph3	2-propen-1-ol2	P	OH	1.25	-1.74	-0.40	-0.71	2-propen-1-ol2_don_08_ph3
ph3	aceticacid1	P	CH	1.25	-1.04	1.18	0.99	aceticacid1_don_08_ph3
ph3	dimethylsulfoxide	P	CH	1.25	-0.95	1.29	1.01	dimethylsulfoxide_don_08_ph3
ph3	furfural0	P	CH	1.25	-1	1.23	0.82	furfural0_don_08_ph3
ph3	furfural1	P	CH	1.25	-1	1.23	0.82	furfural1_don_08_ph3
ph3	hexyne	P	CH	1.25	-1.35	0.77	0.74	hexyne_don_08_ph3
ph3	imidazole	P	CH	1.25	-1.01	1.22	0.85	imidazole_don_08_ph3
ph3	octyne	P	CH	1.25	-1.35	0.77	0.74	octyne_don_08_ph3
ph3	propanol0	P	OH	1.25	-1.73	-0.38	-0.53	propanol0_don_08_ph3
ph3	propynol0	P	OH	1.25	-1.83	-0.60	-0.65	propynol0_don_08_ph3
ph3	propynol1	P	OH	1.25	-1.8	-0.53	-0.73	propynol1_don_08_ph3
ph3	1-bromo-2-nitrobenzene	P	CH	1.25	-1.02	1.20	0.94	1-bromo-2-nitrobenzene_don_09_ph3
ph3	1-butylamine	P	NH	1.25	-1.14	1.00	0.56	1-butylamine_don_09_ph3
ph3	3-cyano-1-nitrobenzene	P	CH	1.25	-1.19	0.98	1.15	3-cyano-1-nitrobenzene_don_09_ph3
ph3	chinone	P	CH	1.25	-1.01	1.22	0.97	chinone_don_09_ph3
ph3	ethanethiol0	P	SH	1.25	-1.04	0.99	0.48	ethanethiol0_don_09_ph3
ph3	ethanethiol1	P	SH	1.25	-1.04	0.99	0.40	ethanethiol1_don_09_ph3
ph3	ethanol0	P	OH	1.25	-1.72	-0.36	-0.47	ethanol0_don_09_ph3
ph3	ethylamine1	P	NH	1.25	-1.14	1.00	0.57	ethylamine1_don_09_ph3
ph3	ethylamine2	P	NH	1.25	-1.15	0.99	0.49	ethylamine2_don_09_ph3
ph3	furfural0	P	CH	1.25	-1.18	0.99	0.89	furfural0_don_09_ph3
ph3	furfural1	P	CH	1.25	-1.17	1.01	0.90	furfural1_don_09_ph3
ph3	imidazole	P	NH	1.25	-1.81	-0.02	0.55	imidazole_don_09_ph3
ph3	1,2-diaminoethane1	P	NH	1.25	-1.14	1.00	0.55	1,2-diaminoethane1_don_10_ph3
ph3	1,2-diaminoethane3	P	NH	1.25	-1.17	0.96	0.49	1,2-diaminoethane3_don_10_ph3

ph3	1,3,5-tribromobenzene	P	CH	1.25	-1.08	1.12	0.97	1,3,5-tribromobenzene_don_10_ph3
ph3	3-cyanophenol	P	OH	1.25	-2.05	-1.07	-0.72	3-cyanophenol_don_10_ph3
ph3	butyne	P	CH	1.25	-1.35	0.77	0.74	butyne_don_10_ph3
ph3	ethylamine0	P	NH	1.25	-1.14	1.00	0.57	ethylamine0_don_10_ph3
ph3	furfural0	P	CH	1.25	-1.06	1.15	0.91	furfural0_don_10_ph3
ph3	furfural1	P	CH	1.25	-1.07	1.14	1.04	furfural1_don_10_ph3
ph3	glycol1	P	OH	1.25	-1.77	-0.47	-0.69	glycol1_don_10_ph3
ph3	hexylamine	P	NH	1.25	-1.14	1.00	0.54	hexylamine_don_10_ph3
ph3	methylimidazol	P	NH	1.25	-1.79	0.01	0.55	methylimidazol_don_10_ph3
ph3	n-pentylamine	P	NH	1.25	-1.14	1.00	0.55	n-pentylamine_don_10_ph3
ph3	n-propylamine	P	NH	1.25	-1.14	1.00	0.54	n-propylamine_don_10_ph3
ph3	pyrrole	P	NH	1.25	-1.71	0.14	0.49	pyrrole_don_10_ph3
ph3	1,2-diaminoethane0	P	NH	1.25	-1.15	0.99	0.64	1,2-diaminoethane0_don_11_ph3
ph3	1,2-diaminoethane2	P	NH	1.25	-1.17	0.96	0.55	1,2-diaminoethane2_don_11_ph3
ph3	1,2-diaminoethane3	P	NH	1.25	-0.51	1.30	0.76	1,2-diaminoethane3_don_11_ph3
ph3	1,2-dibromopropane1	P	CH	1.25	-1	1.23	0.90	1,2-dibromopropane1_don_11_ph3
ph3	2-amino-2-methylpropane0	P	NH	1.25	-1.13	1.02	0.66	2-amino-2-methylpropane0_don_11_ph3
ph3	2-amino-2-methylpropane1	P	NH	1.25	-1.13	1.02	0.64	2-amino-2-methylpropane1_don_11_ph3
ph3	3-cyano-1-nitrobenzene	P	CH	1.25	-1.02	1.20	1.03	3-cyano-1-nitrobenzene_don_11_ph3
ph3	morpholine	P	NH	1.25	-1.21	0.90	0.54	morpholine_don_11_ph3
ph3	1,2,3,5-tetrafluorobenzene	P	CH	1.25	-1.16	1.02	0.91	1,2,3,5-tetrafluorobenzene_don_12_ph3
ph3	1,2-diaminoethane2	P	NH	1.25	-1.15	0.99	0.48	1,2-diaminoethane2_don_12_ph3
ph3	1-propanethiol0	P	SH	1.25	-1.04	0.99	0.47	1-propanethiol0_don_12_ph3
ph3	1-propanethiol1	P	SH	1.25	-1.04	0.99	0.40	1-propanethiol1_don_12_ph3
ph3	isopropylamine	P	NH	1.25	-1.13	1.02	0.56	isopropylamine_don_12_ph3
ph3	propanol1	P	OH	1.25	-1.71	-0.34	-0.62	propanol1_don_12_ph3
ph3	2-methylphenol0	P	OH	1.25	-1.95	-0.85	-0.58	2-methylphenol0_don_13_ph3
ph3	4-bromophenol0	P	OH	1.25	-2.01	-0.98	-0.68	4-bromophenol0_don_13_ph3
ph3	4-methylphenol	P	OH	1.25	-1.96	-0.87	-0.60	4-methylphenol_don_13_ph3
ph3	aniline	P	NH	1.25	-1.46	0.52	0.53	aniline_don_13_ph3

ph3	phenol	P	OH	1.25	-1.98	-0.92	-0.61	phenol_don_13_ph3
ph3	3-hydroxybenzaldehyde0	P	OH	1.25	-2.02	-1.00	-0.68	3-hydroxybenzaldehyde0_don_14_ph3
ph3	3-hydroxybenzaldehyde1	P	OH	1.25	-2.03	-1.02	-0.69	3-hydroxybenzaldehyde1_don_14_ph3
ph3	3-hydroxybenzaldehyde2	P	OH	1.25	-2.02	-1.00	-0.69	3-hydroxybenzaldehyde2_don_14_ph3
ph3	4-cyanophenol	P	OH	1.25	-2.06	-1.09	-0.79	4-cyanophenol_don_14_ph3
ph3	pyrrolidin	P	NH	1.25	-1.18	0.94	0.46	pyrrolidin_don_14_ph3
ph3	1-butanol0	P	OH	1.25	-1.72	-0.36	-0.50	1-butanol0_don_15_ph3
ph3	1-butanol1	P	OH	1.25	-1.71	-0.34	-0.62	1-butanol1_don_15_ph3
ph3	3-nitrophenol	P	OH	1.25	-2.07	-1.11	-0.66	3-nitrophenol_don_15_ph3
ph3	tert-butanol	P	OH	1.25	-1.69	-0.30	-0.23	tert-butanol_don_15_ph3
ph3	benzylamine0	P	NH	1.25	-1.21	0.90	0.67	benzylamine0_don_16_ph3
ph3	benzylamine2	P	NH	1.25	-1.18	0.94	0.51	benzylamine2_don_16_ph3
ph3	ethoxyethanol4	P	OH	1.25	-1.77	-0.47	-0.71	ethoxyethanol4_don_16_ph3
ph3	ethoxyethanol5	P	OH	1.25	-1.76	-0.45	-0.72	ethoxyethanol5_don_16_ph3
ph3	ethoxyethanol8	P	OH	1.25	-1.73	-0.38	-0.70	ethoxyethanol8_don_16_ph3
ph3	benzylamine1	P	NH	1.25	-1.18	0.94	0.49	benzylamine1_don_17_ph3
ph3	benzylamine2	P	NH	1.25	-1.18	0.94	0.56	benzylamine2_don_17_ph3
ph3	1-pentanol0	P	OH	1.25	-1.73	-0.38	-0.49	1-pentanol0_don_18_ph3
ph3	1-pentanol1	P	OH	1.25	-1.71	-0.34	-0.63	1-pentanol1_don_18_ph3
ph3	cyclohexanol0	P	OH	1.25	-1.71	-0.34	-0.33	cyclohexanol0_don_19_ph3
ph3	1-heptanol1	P	OH	1.25	-1.71	-0.34	-0.64	1-heptanol1_don_24_ph3
ph3	1-octanol1	P	OH	1.25	-1.71	-0.34	-0.63	1-octanol1_don_27_ph3
NH3	propyne	N	CH	2.43	-1.35	-0.69	0.02	propyne_don_01
NH3	propynol0	N	CH	2.43	-1.41	-0.98	-0.26	propynol0_don_01
NH3	propynol1	N	CH	2.43	-1.42	-1.03	-0.30	propynol1_don_01
NH3	propynol2	N	CH	2.43	-1.41	-0.98	-0.25	propynol2_don_01
NH3	1-bromo-2-nitrobenzene	N	CH	2.43	-1.06	0.73	1.95	1-bromo-2-nitrobenzene_don_02
NH3	1-nitropropane0	N	CH	2.43	-1.14	0.34	0.97	1-nitropropane0_don_02
NH3	butanethiol0	N	SH	2.43	-1.04	0.12	-0.67	butanethiol0_don_02
NH3	butanethiol1	N	SH	2.43	-1.04	0.12	-0.94	butanethiol1_don_02

NH3	ch2fcl	N	CH	2.43	-1.09	0.58	0.82	ch2fcl_don_02
NH3	chcl3	N	CH	2.43	-1.38	-0.84	-0.84	chcl3_don_02
NH3	dimethylsulfone	N	CH	2.43	-1.05	0.78	1.43	dimethylsulfone_don_02
NH3	methanethiol	N	SH	2.43	-1.04	0.12	-0.93	methanethiol_don_02
NH3	1,1-dichloroethane	N	CH	2.43	-1.13	0.39	0.63	1,1-dichloroethane_don_03
NH3	butenyne	N	CH	2.43	-1.41	-0.98	-0.31	butenyne_don_03
NH3	ch2cl2	N	CH	2.43	-1.14	0.34	0.50	ch2cl2_don_03
NH3	diiodomethane	N	CH	2.43	-1.11	0.48	0.34	diiodomethane_don_03
NH3	ethine	N	CH	2.43	-1.45	-1.18	-0.39	ethine_don_03
NH3	h2o	N	OH	2.43	-1.74	-5.10	-5.16	h2o_don_03
NH3	nh3	N	NH	2.43	-1.18	-0.05	-0.32	nh3_don_03
NH3	trichloroethene	N	CH	2.43	-1.24	-0.15	0.37	trichloroethene_don_03
NH3	1,1-dichloroethylene	N	CH	2.43	-1.01	0.97	1.21	1,1-dichloroethylene_don_04
NH3	1,3-dibromobenzene	N	CH	2.43	-1.03	0.87	1.54	1,3-dibromobenzene_don_04
NH3	aceticacid0	N	OH	2.43	-1.99	-7.11	-8.84	aceticacid0_don_04
NH3	aceticacid1	N	OH	2.43	-2.12	-8.15	-9.93	aceticacid1_don_04
NH3	aziridine	N	NH	2.43	-1.25	-0.45	-0.91	aziridine_don_04
NH3	butyricacid0	N	OH	2.43	-1.97	-6.95	-8.51	butyricacid0_don_04
NH3	chcl2br	N	CH	2.43	-1.4	-0.93	-1.01	chcl2br_don_04
NH3	dimethylamine	N	NH	2.43	-1.17	0.00	-0.29	dimethylamine_don_04
NH3	dimethylsulfoxide	N	CH	2.43	-0.95	1.27	1.55	dimethylsulfoxide_don_04
NH3	h2o2	N	OH	2.43	-1.89	-6.31	-7.59	h2o2_don_04
NH3	methylformate	N	CH	2.43	-1.02	0.92	0.88	methylformate_don_04
NH3	nitroethane0	N	CH	2.43	-1.1	0.53	0.93	nitroethane0_don_04
NH3	nitromethane	N	CH	2.43	-1.3	-0.44	0.71	nitromethane_don_04
NH3	propionicacid0	N	OH	2.43	-1.97	-6.95	-8.46	propionicacid0_don_04
NH3	2-propanol0	N	OH	2.43	-1.7	-4.78	-4.49	2-propanol0_don_05
NH3	2-propanol1	N	OH	2.43	-1.7	-4.78	-4.03	2-propanol1_don_05
NH3	2-propenenitrile	N	CH	2.43	-1.09	0.58	0.71	2-propenenitrile_don_05
NH3	acetamide	N	NH	2.43	-1.69	-2.96	-2.59	acetamide_don_05

NH3	ch2br2	N	CH	2.43	-1.17	0.19	0.28	ch2br2_don_05
NH3	ch2clbr	N	CH	2.43	-1.16	0.24	0.39	ch2clbr_don_05
NH3	chbr3	N	CH	2.43	-1.39	-0.88	-1.22	chbr3_don_05
NH3	chf2cl	N	CH	2.43	-1.34	-0.64	-0.02	chf2cl_don_05
NH3	chfcl2	N	CH	2.43	-1.36	-0.74	-0.43	chfcl2_don_05
NH3	formamide	N	NH	2.43	-1.69	-2.96	-2.88	formamide_don_05
NH3	formicacid	N	CH	2.43	-1.06	0.73	0.78	formicacid_don_05
NH3	1,1-difluoroethene	N	CH	2.43	-1.01	0.97	1.18	1,1-difluoroethene_don_06
NH3	1,2-diaminoethane2	N	NH	2.43	-1.17	0.00	-0.18	1,2-diaminoethane2_don_06
NH3	1,2-dibromoethane1	N	CH	2.43	-1	1.02	1.03	1,2-dibromoethane1_don_06
NH3	2-butanol0	N	OH	2.43	-1.69	-4.70	-3.82	2-butanol0_don_06
NH3	2-butanol1	N	OH	2.43	-1.69	-4.70	-4.43	2-butanol1_don_06
NH3	2-butanol2	N	OH	2.43	-1.7	-4.78	-4.39	2-butanol2_don_06
NH3	2-butanol3	N	OH	2.43	-1.7	-4.78	-4.03	2-butanol3_don_06
NH3	acetamide	N	NH	2.43	-1.62	-2.56	-1.89	acetamide_don_06
NH3	cis-1,2-dichloroethene	N	CH	2.43	-1.15	0.29	0.61	cis-1,2-dichloroethene_don_06
NH3	dibutylamine	N	NH	2.43	-1.13	0.23	0.43	dibutylamine_don_06
NH3	dicyanomethane	N	CH	2.43	-1.46	-1.23	-1.38	dicyanomethane_don_06
NH3	diethylamine0	N	NH	2.43	-1.13	0.23	0.51	diethylamine0_don_06
NH3	diethylamine1	N	NH	2.43	-1.13	0.23	0.48	diethylamine1_don_06
NH3	dipropylamine	N	NH	2.43	-1.13	0.23	0.47	dipropylamine_don_06
NH3	formamide	N	NH	2.43	-1.69	-2.96	-2.27	formamide_don_06
NH3	furane	N	CH	2.43	-1.04	0.83	0.99	furane_don_06
NH3	glycol0	N	OH	2.43	-1.76	-5.26	-5.33	glycol0_don_06
NH3	glycol3	N	OH	2.43	-1.76	-5.26	-5.58	glycol3_don_06
NH3	isobutanol0	N	OH	2.43	-1.71	-4.86	-4.67	isobutanol0_don_06
NH3	isobutanol1	N	OH	2.43	-1.71	-4.86	-4.73	isobutanol1_don_06
NH3	isobutanol2	N	OH	2.43	-1.71	-4.86	-4.95	isobutanol2_don_06
NH3	methanol	N	OH	2.43	-1.73	-5.02	-5.22	methanol_don_06
NH3	methylformamide	N	NH	2.43	-1.66	-2.79	-2.90	methylformamide_don_06

NH3	methylimidazol	N	CH	2.43	-1.01	0.97	1.07	methylimidazol_don_06
NH3	methylurethane	N	NH	2.43	-1.69	-2.96	-2.46	methylurethane_don_06
NH3	n-methylacetamide	N	NH	2.43	-1.66	-2.79	-2.55	n-methylacetamide_don_06
NH3	trans-1,2-dichloroethene	N	CH	2.43	-1.18	0.14	0.75	trans-1,2-dichloroethene_don_06
NH3	3-cyano-1-nitrobenzene	N	CH	2.43	-1.09	0.58	1.12	3-cyano-1-nitrobenzene_don_07
NH3	aceticacid1	N	CH	2.43	-1.04	0.83	1.46	aceticacid1_don_07
NH3	butyricacid1	N	CH	2.43	-0.99	1.07	1.92	butyricacid1_don_07
NH3	ethanol1	N	OH	2.43	-1.71	-4.86	-5.00	ethanol1_don_07
NH3	methylamine	N	NH	2.43	-1.15	0.12	-0.19	methylamine_don_07
NH3	methylindole	N	NH	2.43	-1.73	-3.19	-2.97	methylindole_don_07
NH3	pentyne	N	CH	2.43	-1.35	-0.69	-0.01	pentyne_don_07
NH3	piperidine	N	NH	2.43	-1.16	0.06	-0.18	piperidine_don_07
NH3	propionicacid1	N	OH	2.43	-2.12	-8.15	-9.50	propionicacid1_don_07
NH3	1,2,4,5-tetrafluorobenzene	N	CH	2.43	-1.19	0.09	0.78	1,2,4,5-tetrafluorobenzene_don_08
NH3	2-propen-1-ol0	N	OH	2.43	-1.75	-5.18	-4.85	2-propen-1-ol0_don_08
NH3	2-propen-1-ol1	N	OH	2.43	-1.76	-5.26	-5.49	2-propen-1-ol1_don_08
NH3	2-propen-1-ol2	N	OH	2.43	-1.74	-5.10	-5.50	2-propen-1-ol2_don_08
NH3	aceticacid1	N	CH	2.43	-1.04	0.83	1.53	aceticacid1_don_08
NH3	butyricacid1	N	OH	2.43	-2.12	-8.15	-9.50	butyricacid1_don_08
NH3	dimethylsulfoxide	N	CH	2.43	-0.97	1.17	1.53	dimethylsulfoxide_don_08
NH3	furfural0	N	CH	2.43	-1	1.02	1.11	furfural0_don_08
NH3	furfural1	N	CH	2.43	-1	1.02	1.13	furfural1_don_08
NH3	hexyne	N	CH	2.43	-1.35	-0.69	-0.01	hexyne_don_08
NH3	imidazole	N	CH	2.43	-1.01	0.97	1.13	imidazole_don_08
NH3	isopropylamine	N	NH	2.43	-1.13	0.23	0.08	isopropylamine_don_08
NH3	octyne	N	CH	2.43	-1.35	-0.69	-0.02	octyne_don_08
NH3	propanol0	N	OH	2.43	-1.73	-5.02	-4.84	propanol0_don_08
NH3	propynol0	N	OH	2.43	-1.83	-5.82	-5.85	propynol0_don_08
NH3	propynol1	N	OH	2.43	-1.8	-5.58	-6.09	propynol1_don_08
NH3	propynol2	N	OH	2.43	-1.83	-5.82	-5.86	propynol2_don_08

NH3	1-bromo-2-nitrobenzene	N	CH	2.43	-1.02	0.92	1.29	1-bromo-2-nitrobenzene_don_09
NH3	3-cyano-1-nitrobenzene	N	CH	2.43	-1.19	0.09	1.51	3-cyano-1-nitrobenzene_don_09
NH3	ethanethiol0	N	SH	2.43	-1.04	0.12	-0.61	ethanethiol0_don_09
NH3	ethanethiol1	N	SH	2.43	-1.04	0.12	-0.90	ethanethiol1_don_09
NH3	ethanol0	N	OH	2.43	-1.72	-4.94	-4.75	ethanol0_don_09
NH3	ethylamine2	N	NH	2.43	-1.15	0.12	-0.14	ethylamine2_don_09
NH3	furfural0	N	CH	2.43	-1.18	0.14	0.65	furfural0_don_09
NH3	furfural1	N	CH	2.43	-1.17	0.19	0.67	furfural1_don_09
NH3	imidazole	N	NH	2.43	-1.81	-3.65	-3.94	imidazole_don_09
NH3	thiophene	N	CH	2.43	-0.99	1.07	1.11	thiophene_don_09
NH3	1,2-diaminoethane0	N	NH	2.43	-1.18	-0.05	0.05	1,2-diaminoethane0_don_10
NH3	1,2-diaminoethane1	N	NH	2.43	-1.14	0.17	0.03	1,2-diaminoethane1_don_10
NH3	1,2-diaminoethane3	N	NH	2.43	-1.17	0.00	-0.25	1,2-diaminoethane3_don_10
NH3	1,3,5-tribromobenzene	N	CH	2.43	-1.08	0.63	1.36	1,3,5-tribromobenzene_don_10
NH3	1-butylamine	N	NH	2.43	-1.14	0.17	0.06	1-butylamine_don_10
NH3	butyne	N	CH	2.43	-1.35	-0.69	0.00	butyne_don_10
NH3	ethylamine0	N	NH	2.43	-1.14	0.17	0.10	ethylamine0_don_10
NH3	ethylamine1	N	NH	2.43	-1.14	0.17	0.11	ethylamine1_don_10
NH3	ethylamine2	N	NH	2.43	-1.13	0.23	0.08	ethylamine2_don_10
NH3	furfural0	N	CH	2.43	-1.06	0.73	1.08	furfural0_don_10
NH3	furfural1	N	CH	2.43	-1.07	0.68	1.46	furfural1_don_10
NH3	glycol1	N	OH	2.43	-1.77	-5.34	-5.62	glycol1_don_10
NH3	glycol2	N	OH	2.43	-1.77	-5.34	-5.63	glycol2_don_10
NH3	glycol3	N	OH	2.43	-1.77	-5.34	-5.51	glycol3_don_10
NH3	hexylamine	N	NH	2.43	-1.14	0.17	0.06	hexylamine_don_10
NH3	methylimidazol	N	NH	2.43	-1.79	-3.53	-3.71	methylimidazol_don_10
NH3	n-pentylamine	N	NH	2.43	-1.14	0.17	0.06	n-pentylamine_don_10
NH3	n-propylamine	N	NH	2.43	-1.14	0.17	0.06	n-propylamine_don_10
NH3	pyrrole	N	NH	2.43	-1.71	-3.08	-3.09	pyrrole_don_10
NH3	1,2-diaminoethane1	N	NH	2.43	-1.17	0.00	0.06	1,2-diaminoethane1_don_11

NH3	1,2-diaminoethane2	N	NH	2.43	-1.17	0.00	0.07	1,2-diaminoethane2_don_11
NH3	1,2-dibromopropane1	N	CH	2.43	-1	1.02	1.11	1,2-dibromopropane1_don_11
NH3	2-amino-2-methylpropane0	N	NH	2.43	-1.13	0.23	0.39	2-amino-2-methylpropane0_don_11
NH3	3-cyano-1-nitrobenzene	N	CH	2.43	-1.02	0.92	1.53	3-cyano-1-nitrobenzene_don_11
NH3	chinone	N	CH	2.43	-1.01	0.97	1.37	chinone_don_11
NH3	dimethylsulfone	N	CH	2.43	-1.06	0.73	1.51	dimethylsulfone_don_11
NH3	morpholine	N	NH	2.43	-1.21	-0.23	-0.41	morpholine_don_11
NH3	1,2,3,5-tetrafluorobenzene	N	CH	2.43	-1.16	0.24	0.91	1,2,3,5-tetrafluorobenzene_don_12
NH3	1,2-diaminoethane2	N	NH	2.43	-1.15	0.12	-0.16	1,2-diaminoethane2_don_12
NH3	1-propanethiol0	N	SH	2.43	-1.04	0.12	-0.64	1-propanethiol0_don_12
NH3	1-propanethiol1	N	SH	2.43	-1.04	0.12	-0.93	1-propanethiol1_don_12
NH3	propanol1	N	OH	2.43	-1.71	-4.86	-5.02	propanol1_don_12
NH3	2-methylphenol0	N	OH	2.43	-1.95	-6.79	-6.92	2-methylphenol0_don_13
NH3	4-methylphenol	N	OH	2.43	-1.96	-6.87	-7.00	4-methylphenol_don_13
NH3	phenol	N	OH	2.43	-1.98	-7.03	-7.22	phenol_don_13
NH3	3-cyanophenol	N	OH	2.43	-2.05	-7.59	-8.23	3-cyanophenol_don_14
NH3	3-hydroxybenzaldehyde0	N	OH	2.43	-2.02	-7.35	-7.90	3-hydroxybenzaldehyde0_don_14
NH3	3-hydroxybenzaldehyde1	N	OH	2.43	-2.03	-7.43	-7.91	3-hydroxybenzaldehyde1_don_14
NH3	3-hydroxybenzaldehyde2	N	OH	2.43	-2.02	-7.35	-7.93	3-hydroxybenzaldehyde2_don_14
NH3	4-cyanophenol	N	OH	2.43	-2.06	-7.67	-8.74	4-cyanophenol_don_14
NH3	aniline	N	NH	2.43	-1.46	-1.65	-1.29	aniline_don_14
NH3	pyrrolidin	N	NH	2.43	-1.18	-0.05	-0.14	pyrrolidin_don_14
NH3	1-butanol0	N	OH	2.43	-1.72	-4.94	-4.78	1-butanol0_don_15
NH3	1-butanol1	N	OH	2.43	-1.71	-4.86	-5.03	1-butanol1_don_15
NH3	3-nitrophenol	N	OH	2.43	-2.07	-7.75	-8.43	3-nitrophenol_don_15
NH3	tert-butanol	N	OH	2.43	-1.69	-4.70	-3.88	tert-butanol_don_15
NH3	2-amino-2-methylpropane1	N	NH	2.43	-1.13	0.23	0.36	2-amino-2-methylpropane1_don_16
NH3	benzylamine1	N	NH	2.43	-1.18	-0.05	-0.27	benzylamine1_don_16
NH3	benzylamine2	N	NH	2.43	-1.18	-0.05	-0.36	benzylamine2_don_16
NH3	ethoxyethanol2	N	OH	2.43	-1.75	-5.18	-4.75	ethoxyethanol2_don_16

NH3	ethoxyethanol4	N	OH	2.43	-1.77	-5.34	-5.49	ethoxyethanol4_don_16
NH3	ethoxyethanol5	N	OH	2.43	-1.76	-5.26	-5.58	ethoxyethanol5_don_16
NH3	ethoxyethanol6	N	OH	2.43	-1.75	-5.18	-5.03	ethoxyethanol6_don_16
NH3	ethoxyethanol7	N	OH	2.43	-1.75	-5.18	-4.85	ethoxyethanol7_don_16
NH3	ethoxyethanol8	N	OH	2.43	-1.73	-5.02	-5.21	ethoxyethanol8_don_16
NH3	benzylamine0	N	NH	2.43	-1.21	-0.23	0.17	benzylamine0_don_17
NH3	benzylamine1	N	NH	2.43	-1.18	-0.05	0.02	benzylamine1_don_17
NH3	benzylamine2	N	NH	2.43	-1.18	-0.05	0.10	benzylamine2_don_17
NH3	1-pentanol0	N	OH	2.43	-1.73	-5.02	-4.81	1-pentanol0_don_18
NH3	1-pentanol1	N	OH	2.43	-1.71	-4.86	-5.04	1-pentanol1_don_18
NH3	cyclohexanol0	N	OH	2.43	-1.71	-4.86	-4.06	cyclohexanol0_don_19
NH3	cyclohexanol1	N	OH	2.43	-1.68	-4.62	-4.19	cyclohexanol1_don_19
NH3	1-heptanol0	N	OH	2.43	-1.72	-4.94	-4.79	1-heptanol0_don_24
NH3	1-heptanol1	N	OH	2.43	-1.71	-4.86	-5.03	1-heptanol1_don_24
NH3	4-(1,1-dimethylethyl)-phenol	N	OH	2.43	-1.96	-6.87	-7.56	4-(1,1-dimethylethyl)-phenol_don_25
NH3	1-octanol0	N	OH	2.43	-1.72	-4.94	-4.77	1-octanol0_don_27
NH3	1-octanol1	N	OH	2.43	-1.71	-4.86	-5.02	1-octanol1_don_27
HCN	propyne	N	CH	1.34	-1.35	0.53	0.45	propyne_donw_10
HCN	propynol0	N	CH	1.34	-1.41	0.42	0.41	propynol0_donw_10
HCN	propynol1	N	CH	1.34	-1.42	0.40	0.40	propynol1_donw_10
HCN	propynol2	N	CH	1.34	-1.41	0.42	0.41	propynol2_donw_10
HCN	1-bromo-2-nitrobenzene	N	CH	1.34	-1.06	1.08	1.40	1-bromo-2-nitrobenzene_donw_20
HCN	1-nitropropane0	N	CH	1.34	-1.14	0.93	1.01	1-nitropropane0_donw_20
HCN	butanethiol0	N	SH	1.34	-1.04	0.85	0.63	butanethiol0_donw_20
HCN	butanethiol1	N	SH	1.34	-1.04	0.85	0.54	butanethiol1_donw_20
HCN	ch2fcl	N	CH	1.34	-1.09	1.02	0.83	ch2fcl_donw_20
HCN	chcl3	N	CH	1.34	-1.38	0.48	0.73	chcl3_donw_20
HCN	diiodomethane	N	CH	1.34	-1.11	0.99	0.66	diiodomethane_donw_20
HCN	h2o	N	OH	1.34	-1.74	-1.17	-1.24	h2o_donw_20
HCN	h2s	N	SH	1.34	-1.18	0.19	0.34	h2s_donw_20

HCN	methanethiol	N	SH	1.34	-1.04	0.85	0.54	methanethiol_donw_20
HCN	1,1-dichloroethane	N	CH	1.34	-1.13	0.95	0.90	1,1-dichloroethane_donw_30
HCN	butenyne	N	CH	1.34	-1.41	0.42	0.38	butenyne_donw_30
HCN	ch2cl2	N	CH	1.34	-1.14	0.93	0.75	ch2cl2_donw_30
HCN	ethine	N	CH	1.34	-1.45	0.34	0.39	ethine_donw_30
HCN	h2o2	N	OH	1.34	-1.89	-1.64	-2.02	h2o2_donw_30
HCN	hcn	N	CH	1.34	-1.81	-0.34	-0.13	hcn_donw_30
HCN	nitromethane	N	CH	1.34	-1.3	0.63	0.94	nitromethane_donw_30
HCN	trichloroethene	N	CH	1.34	-1.24	0.74	0.74	trichloroethene_donw_30
HCN	1,1-dichloroethylene	N	CH	1.34	-1.01	1.18	0.83	1,1-dichloroethylene_donw_40
HCN	1,3-dibromobenzene	N	CH	1.34	-1.03	1.14	1.09	1,3-dibromobenzene_donw_40
HCN	1-nitropropane1	N	CH	1.34	-1.08	1.04	1.03	1-nitropropane1_donw_40
HCN	aceticacid0	N	OH	1.34	-1.99	-1.95	-1.76	aceticacid0_donw_40
HCN	aceticacid1	N	OH	1.34	-2.12	-2.35	-2.45	aceticacid1_donw_40
HCN	aziridine	N	NH	1.34	-1.25	0.62	0.23	aziridine_donw_40
HCN	butyricacid0	N	OH	1.34	-1.97	-1.89	-1.69	butyricacid0_donw_40
HCN	butyricacid1	N	OH	1.34	-2.12	-2.35	-2.34	butyricacid1_donw_40
HCN	ch2br2	N	CH	1.34	-1.17	0.87	0.66	ch2br2_donw_40
HCN	chcl2br	N	CH	1.34	-1.4	0.44	0.66	chcl2br_donw_40
HCN	cis-1,2-dichloroethene	N	CH	1.34	-1.15	0.91	0.75	cis-1,2-dichloroethene_donw_40
HCN	dimethylamine	N	NH	1.34	-1.17	0.80	0.36	dimethylamine_donw_40
HCN	dimethylsulfone	N	CH	1.34	-1.05	1.10	1.17	dimethylsulfone_donw_40
HCN	formicacid	N	OH	1.34	-2.06	-2.17	-2.09	formicacid_donw_40
HCN	methylformate	N	CH	1.34	-1.02	1.16	0.75	methylformate_donw_40
HCN	HCN	N	NH	1.34	-1.18	0.78	0.27	HCN_donw_40
HCN	nitroethane0	N	CH	1.34	-1.1	1.01	0.92	nitroethane0_donw_40
HCN	nitromethane	N	CH	1.34	-1.01	1.18	0.93	nitromethane_donw_40
HCN	propionicacid0	N	OH	1.34	-1.97	-1.89	-1.68	propionicacid0_donw_40
HCN	propionicacid1	N	OH	1.34	-2.12	-2.35	-2.35	propionicacid1_donw_40
HCN	2-propanol0	N	OH	1.34	-1.7	-1.05	-0.96	2-propanol0_donw_50

HCN	2-propanol1	N	OH	1.34	-1.7	-1.05	-0.80	2-propanol1_donw_50
HCN	2-propenenitrile	N	CH	1.34	-1.09	1.02	0.80	2-propenenitrile_donw_50
HCN	acetamide	N	NH	1.34	-1.69	-0.35	-0.28	acetamide_donw_50
HCN	ch2clbr	N	CH	1.34	-1.16	0.89	0.70	ch2clbr_donw_50
HCN	chbr3	N	CH	1.34	-1.39	0.46	0.38	chbr3_donw_50
HCN	chf2cl	N	CH	1.34	-1.34	0.55	0.86	chf2cl_donw_50
HCN	chfcl2	N	CH	1.34	-1.36	0.51	0.75	chfcl2_donw_50
HCN	formamide	N	NH	1.34	-1.69	-0.35	-0.29	formamide_donw_50
HCN	formicacid	N	CH	1.34	-1.06	1.08	0.80	formicacid_donw_50
HCN	methylurethane	N	NH	1.34	-1.69	-0.35	-0.12	methylurethane_donw_50
HCN	1,1-difluoroethene	N	CH	1.34	-1.01	1.18	0.79	1,1-difluoroethene_donw_60
HCN	1,2-diaminoethane0	N	NH	1.34	-1.18	0.78	0.48	1,2-diaminoethane0_donw_60
HCN	1,2-diaminoethane1	N	NH	1.34	-1.17	0.80	0.37	1,2-diaminoethane1_donw_60
HCN	1,2-diaminoethane2	N	NH	1.34	-1.17	0.80	0.36	1,2-diaminoethane2_donw_60
HCN	1,2-dibromoethane1	N	CH	1.34	-1	1.19	0.83	1,2-dibromoethane1_donw_60
HCN	2-butanol0	N	OH	1.34	-1.69	-1.02	-0.73	2-butanol0_donw_60
HCN	2-butanol1	N	OH	1.34	-1.69	-1.02	-0.93	2-butanol1_donw_60
HCN	2-butanol2	N	OH	1.34	-1.7	-1.05	-0.96	2-butanol2_donw_60
HCN	2-butanol3	N	OH	1.34	-1.7	-1.05	-0.81	2-butanol3_donw_60
HCN	acetamide	N	NH	1.34	-1.62	-0.19	0.12	acetamide_donw_60
HCN	dibutylamine	N	NH	1.34	-1.13	0.89	0.64	dibutylamine_donw_60
HCN	dicyanomethane	N	CH	1.34	-1.46	0.33	0.67	dicyanomethane_donw_60
HCN	diethylamine0	N	NH	1.34	-1.13	0.89	0.73	diethylamine0_donw_60
HCN	diethylamine1	N	NH	1.34	-1.13	0.89	0.69	diethylamine1_donw_60
HCN	dipropylamine	N	NH	1.34	-1.13	0.89	0.68	dipropylamine_donw_60
HCN	formamide	N	NH	1.34	-1.66	-0.28	-0.01	formamide_donw_60
HCN	glycol0	N	OH	1.34	-1.76	-1.24	-1.24	glycol0_donw_60
HCN	glycol2	N	OH	1.34	-1.77	-1.27	-1.38	glycol2_donw_60
HCN	glycol3	N	OH	1.34	-1.76	-1.24	-1.38	glycol3_donw_60
HCN	imidazole	N	CH	1.34	-1.04	1.12	0.77	imidazole_donw_60

HCN	isobutanol0	N	OH	1.34	-1.71	-1.08	-1.05	isobutanol0_donw_60
HCN	isobutanol1	N	OH	1.34	-1.71	-1.08	-0.97	isobutanol1_donw_60
HCN	isobutanol2	N	OH	1.34	-1.71	-1.08	-1.19	isobutanol2_donw_60
HCN	methanol	N	OH	1.34	-1.73	-1.14	-1.27	methanol_donw_60
HCN	methylamine	N	NH	1.34	-1.15	0.84	0.35	methylamine_donw_60
HCN	methylformamide	N	NH	1.34	-1.66	-0.28	-0.27	methylformamide_donw_60
HCN	methylimidazol	N	CH	1.34	-1.01	1.18	0.77	methylimidazol_donw_60
HCN	methylurethane	N	NH	1.34	-1.69	-0.35	-0.25	methylurethane_donw_60
HCN	n-methylacetamide	N	NH	1.34	-1.66	-0.28	-0.24	n-methylacetamide_donw_60
HCN	trans-1,2-dichloroethene	N	CH	1.34	-1.18	0.85	0.81	trans-1,2-dichloroethene_donw_60
HCN	3-cyano-1-nitrobenzene	N	CH	1.34	-1.09	1.02	0.95	3-cyano-1-nitrobenzene_donw_70
HCN	ethanol1	N	OH	1.34	-1.71	-1.08	-1.20	ethanol1_donw_70
HCN	methylindole	N	NH	1.34	-1.73	-0.44	-0.32	methylindole_donw_70
HCN	pentyne	N	CH	1.34	-1.35	0.53	0.43	pentyne_donw_70
HCN	piperidine	N	NH	1.34	-1.16	0.82	0.36	piperidine_donw_70
HCN	1,2,4,5-tetrafluorobenzene	N	CH	1.34	-1.19	0.84	0.84	1,2,4,5-tetrafluorobenzene_donw_80
HCN	2-propen-1-ol0	N	OH	1.34	-1.75	-1.20	-1.00	2-propen-1-ol0_donw_80
HCN	2-propen-1-ol1	N	OH	1.34	-1.76	-1.24	-1.34	2-propen-1-ol1_donw_80
HCN	2-propen-1-ol2	N	OH	1.34	-1.74	-1.17	-1.30	2-propen-1-ol2_donw_80
HCN	aceticacid1	N	CH	1.34	-1.04	1.12	0.98	aceticacid1_donw_80
HCN	butyricacid1	N	CH	1.34	-0.99	1.21	1.18	butyricacid1_donw_80
HCN	dimethylsulfoxide	N	CH	1.34	-0.97	1.25	1.00	dimethylsulfoxide_donw_80
HCN	furfural0	N	CH	1.34	-1	1.19	0.72	furfural0_donw_80
HCN	furfural1	N	CH	1.34	-1	1.19	0.72	furfural1_donw_80
HCN	hexyne	N	CH	1.34	-1.35	0.53	0.44	hexyne_donw_80
HCN	imidazole	N	CH	1.34	-1.01	1.18	0.76	imidazole_donw_80
HCN	octyne	N	CH	1.34	-1.35	0.53	0.44	octyne_donw_80
HCN	propanol0	N	OH	1.34	-1.73	-1.14	-1.08	propanol0_donw_80
HCN	propynol0	N	OH	1.34	-1.83	-1.45	-1.31	propynol0_donw_80
HCN	propynol1	N	OH	1.34	-1.8	-1.36	-1.43	propynol1_donw_80

HCN	propynol2	N	OH	1.34	-1.78	-1.30	-1.01	propynol2_donw_80
HCN	trifluoroaceticacid0	N	OH	1.34	-2.23	-2.69	-3.22	trifluoroaceticacid0_donw_80
HCN	trifluoroaceticacid1	N	OH	1.34	-2.29	-2.88	-2.72	trifluoroaceticacid1_donw_80
HCN	1-bromo-2-nitrobenzene	N	CH	1.34	-1.02	1.16	0.89	1-bromo-2-nitrobenzene_donw_90
HCN	1-butylamine	N	NH	1.34	-1.14	0.87	0.45	1-butylamine_donw_90
HCN	3-cyano-1-nitrobenzene	N	CH	1.34	-1.19	0.84	1.28	3-cyano-1-nitrobenzene_donw_90
HCN	ethanethiol0	N	SH	1.34	-1.04	0.85	0.63	ethanethiol0_donw_90
HCN	ethanethiol1	N	SH	1.34	-1.04	0.85	0.55	ethanethiol1_donw_90
HCN	ethanol0	N	OH	1.34	-1.72	-1.11	-1.04	ethanol0_donw_90
HCN	ethylamine2	N	NH	1.34	-1.15	0.84	0.37	ethylamine2_donw_90
HCN	furane	N	CH	1.34	-1.04	1.12	0.72	furane_donw_90
HCN	furfural0	N	CH	1.34	-1.18	0.85	0.69	furfural0_donw_90
HCN	furfural1	N	CH	1.34	-1.17	0.87	0.69	furfural1_donw_90
HCN	imidazole	N	NH	1.34	-1.81	-0.61	-0.48	imidazole_donw_90
HCN	thiophene	N	CH	1.34	-0.99	1.21	0.76	thiophene_donw_90
HCN	1,2-diaminoethane3	N	NH	1.34	-1.17	0.80	0.34	1,2-diaminoethane3_donw100
HCN	1,3,5-tribromobenzene	N	CH	1.34	-1.08	1.04	1.05	1,3,5-tribromobenzene_donw100
HCN	butyne	N	CH	1.34	-1.35	0.53	0.44	butyne_donw100
HCN	ethylamine0	N	NH	1.34	-1.14	0.87	0.50	ethylamine0_donw100
HCN	ethylamine1	N	NH	1.34	-1.14	0.87	0.49	ethylamine1_donw100
HCN	ethylamine2	N	NH	1.34	-1.13	0.89	0.47	ethylamine2_donw100
HCN	furfural0	N	CH	1.34	-1.06	1.08	0.78	furfural0_donw100
HCN	glycol0	N	OH	1.34	-1.75	-1.20	-0.91	glycol0_donw100
HCN	glycol1	N	OH	1.34	-1.77	-1.27	-1.38	glycol1_donw100
HCN	glycol3	N	OH	1.34	-1.77	-1.27	-1.35	glycol3_donw100
HCN	hexylamine	N	NH	1.34	-1.14	0.87	0.45	hexylamine_donw100
HCN	methylimidazol	N	NH	1.34	-1.79	-0.57	-0.44	methylimidazol_donw100
HCN	n-pentylamine	N	NH	1.34	-1.14	0.87	0.46	n-pentylamine_donw100
HCN	n-propylamine	N	NH	1.34	-1.14	0.87	0.46	n-propylamine_donw100
HCN	pyrrole	N	NH	1.34	-1.71	-0.39	-0.34	pyrrole_donw100

HCN	1,2-diaminoethane1	N	NH	1.34	-1.17	0.80	0.45	1,2-diaminoethane1_donw110
HCN	1,2-diaminoethane2	N	NH	1.34	-1.17	0.80	0.44	1,2-diaminoethane2_donw110
HCN	1,2-dibromopropane1	N	CH	1.34	-1	1.19	0.89	1,2-dibromopropane1_donw110
HCN	3-cyano-1-nitrobenzene	N	CH	1.34	-1.02	1.16	1.05	3-cyano-1-nitrobenzene_donw110
HCN	morpholine	N	NH	1.34	-1.21	0.71	0.35	morpholine_donw110
HCN	1,2,3,5-tetrafluorobenzene	N	CH	1.34	-1.16	0.89	0.85	1,2,3,5-tetrafluorobenzene_donw120
HCN	1,2-diaminoethane2	N	NH	1.34	-1.15	0.84	0.34	1,2-diaminoethane2_donw120
HCN	1,2-diaminoethane3	N	NH	1.34	-1.17	0.80	0.70	1,2-diaminoethane3_donw120
HCN	1-propanethiol0	N	SH	1.34	-1.04	0.85	0.62	1-propanethiol0_donw120
HCN	1-propanethiol1	N	SH	1.34	-1.04	0.85	0.55	1-propanethiol1_donw120
HCN	chinone	N	CH	1.34	-1.01	1.18	0.96	chinone_donw120
HCN	isopropylamine	N	NH	1.34	-1.13	0.89	0.46	isopropylamine_donw120
HCN	propanol1	N	OH	1.34	-1.71	-1.08	-1.20	propanol1_donw120
HCN	2-methylphenol0	N	OH	1.34	-1.95	-1.83	-1.63	2-methylphenol0_donw130
HCN	4-bromophenol0	N	OH	1.34	-2.01	-2.01	-1.85	4-bromophenol0_donw130
HCN	4-bromophenol1	N	OH	1.34	-2.01	-2.01	-1.85	4-bromophenol1_donw130
HCN	4-methylphenol	N	OH	1.34	-1.96	-1.86	-1.65	4-methylphenol_donw130
HCN	phenol	N	OH	1.34	-1.98	-1.92	-1.70	phenol_donw130
HCN	thiophenol	N	SH	1.34	-1.24	-0.09	0.57	thiophenol_donw130
HCN	3-cyanophenol	N	OH	1.34	-2.05	-2.14	-1.97	3-cyanophenol_donw140
HCN	3-hydroxybenzaldehyde0	N	OH	1.34	-2.02	-2.04	-1.83	3-hydroxybenzaldehyde0_donw140
HCN	3-hydroxybenzaldehyde1	N	OH	1.34	-2.03	-2.07	-1.89	3-hydroxybenzaldehyde1_donw140
HCN	3-hydroxybenzaldehyde2	N	OH	1.34	-2.02	-2.04	-1.90	3-hydroxybenzaldehyde2_donw140
HCN	4-cyanophenol	N	OH	1.34	-2.06	-2.17	-2.12	4-cyanophenol_donw140
HCN	aniline	N	NH	1.34	-1.46	0.16	0.10	aniline_donw140
HCN	pyrrolidin	N	NH	1.34	-1.18	0.78	0.40	pyrrolidin_donw140
HCN	1-butanol0	N	OH	1.34	-1.72	-1.11	-1.06	1-butanol0_donw150
HCN	1-butanol1	N	OH	1.34	-1.71	-1.08	-1.20	1-butanol1_donw150
HCN	3-nitrophenol	N	OH	1.34	-2.07	-2.20	-1.95	3-nitrophenol_donw150
HCN	4-nitrophenol	N	OH	1.34	-2.1	-2.29	-2.29	4-nitrophenol_donw150

HCN	benzoicacid	N	OH	1.34	-2	-1.98	-1.87	benzoicacid_donw150
HCN	tert-butanol	N	OH	1.34	-1.69	-1.02	-0.76	tert-butanol_donw150
HCN	2-amino-2-methylpropane1	N	NH	1.34	-1.13	0.89	0.61	2-amino-2-methylpropane1_donw160
HCN	2-methylphenol1	N	CH	1.34	-0.87	1.30	0.95	2-methylphenol1_donw160
HCN	benzylamine0	N	NH	1.34	-1.21	0.71	0.56	benzylamine0_donw160
HCN	benzylamine2	N	NH	1.34	-1.18	0.78	0.42	benzylamine2_donw160
HCN	ethoxyethanol4	N	OH	1.34	-1.77	-1.27	-1.33	ethoxyethanol4_donw160
HCN	ethoxyethanol5	N	OH	1.34	-1.76	-1.24	-1.37	ethoxyethanol5_donw160
HCN	ethoxyethanol6	N	OH	1.34	-1.75	-1.20	-1.10	ethoxyethanol6_donw160
HCN	ethoxyethanol7	N	OH	1.34	-1.75	-1.20	-1.12	ethoxyethanol7_donw160
HCN	ethoxyethanol8	N	OH	1.34	-1.73	-1.14	-1.33	ethoxyethanol8_donw160
HCN	benzylamine1	N	NH	1.34	-1.18	0.78	0.37	benzylamine1_donw170
HCN	1-pentanol0	N	OH	1.34	-1.73	-1.14	-1.06	1-pentanol0_donw180
HCN	1-pentanol1	N	OH	1.34	-1.71	-1.08	-1.20	1-pentanol1_donw180
HCN	cyclohexanol0	N	OH	1.34	-1.71	-1.08	-0.83	cyclohexanol0_donw190
HCN	cyclohexanol1	N	OH	1.34	-1.68	-0.99	-0.88	cyclohexanol1_donw190
HCN	1-heptanol0	N	OH	1.34	-1.72	-1.11	-1.07	1-heptanol0_donw240
HCN	1-heptanol1	N	OH	1.34	-1.71	-1.08	-1.21	1-heptanol1_donw240
HCN	4-(1,1-dimethylethyl)-phenol	N	OH	1.34	-1.96	-1.86	-2.19	4-(1,1-dimethylethyl)-phenol_donw250
HCN	1-octanol0	N	OH	1.34	-1.72	-1.11	-1.06	1-octanol0_donw270
HCN	1-octanol1	N	OH	1.34	-1.71	-1.08	-1.21	1-octanol1_donw270