2009 SAMPL Transfer energies

Selected by Peter Guthrie

These compounds fall into 3 groups:

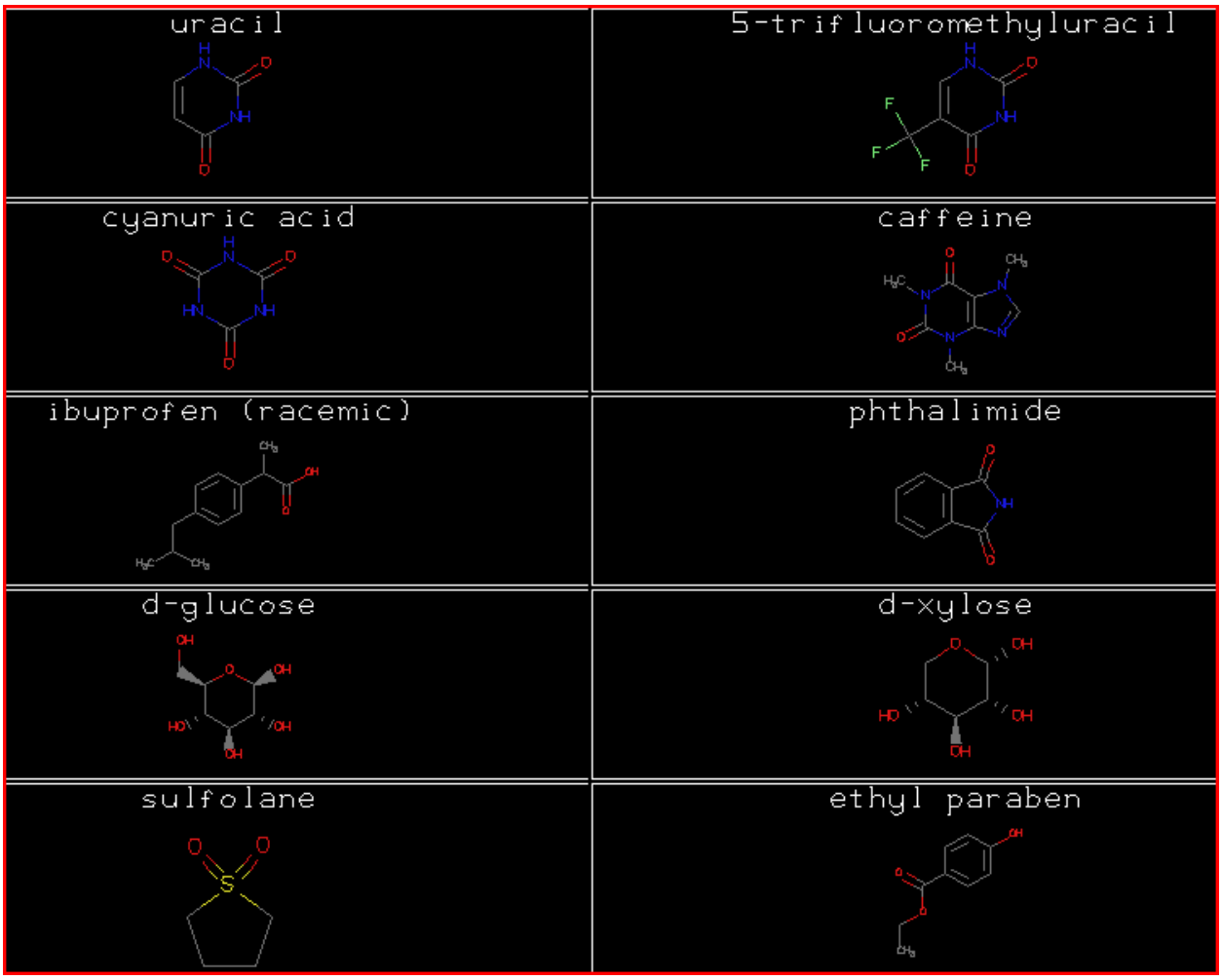
1. Obscure compounds – These compounds have been studied experimentally, but do not exist in any of the well-known large collections of Henry's Law constants. It is unlikely that they have been used in the parameterization sets of algorithms. Further, they present interesting series of polyfunctional compounds that are both pharmaceutically relevant as well as somewhat simple. This group also has a select subset that can be used alone if time does not permit calculations on the entire set.

2. Explanatory compounds – These compounds have known experimental transfer energies which will be provided (see below). They are compounds with unusual or unexpected transfer energies that we will ask participants to reproduce and explain.

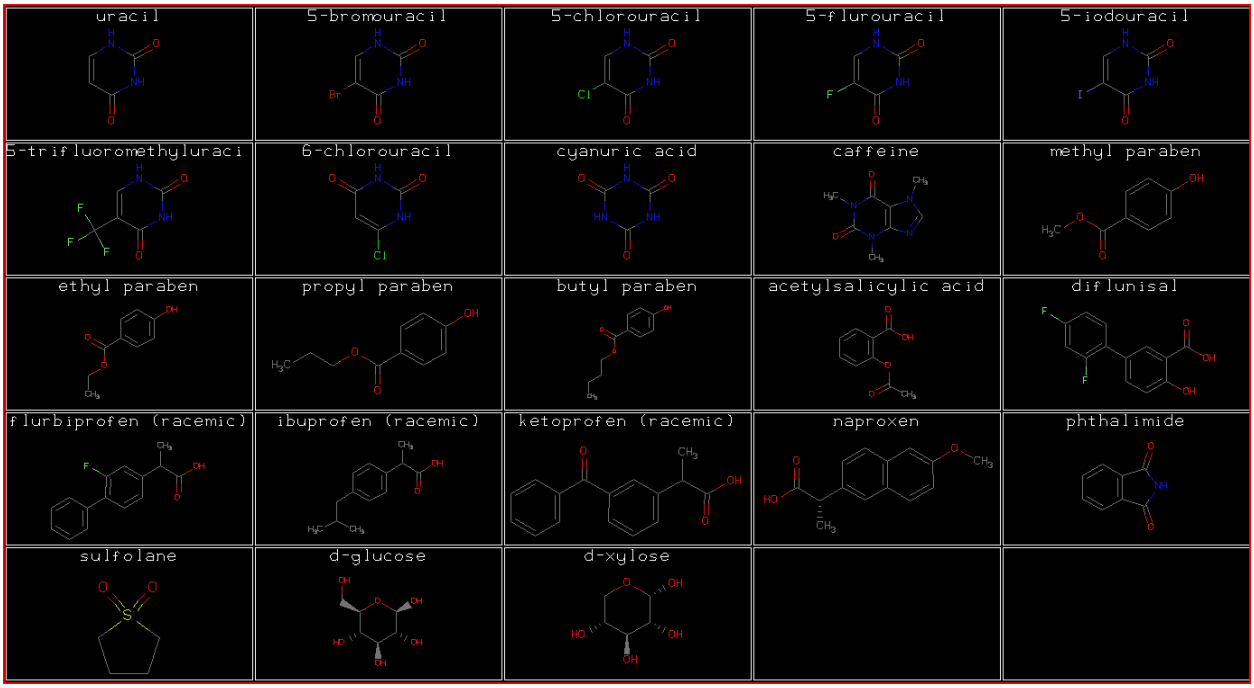
3. Investigatory compounds – These compounds do not have known experimental transfer energies. Participants will be asked to prospectively calculate transfer energies. The predictions will be compared to one another.

When you submit your results, the units will need to be kcal/mol for gas at 1M to aqueous at 1M. We hope you will submit a standard error for each of your calculations as well as the predicted value.

Obscure select (see also xfer.select.ism and xfer.select.sdf)



Obscure complete (see also xfer.ism and xfer.sdf)

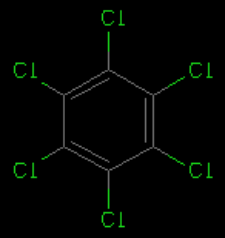


Explanatory (see also explain.ism and explain.sdf)

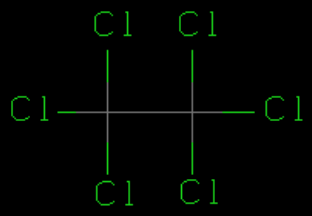
Experimental values in kcal/mol for gas at 1M to aqueous at 1M

1. Hexachlorobenzene -2.30
2. Hexachloroethane -1.41
3. Octafluorocyclobutane 3.01
4. Trimethyl orthotrifluoroacetate -0.80
5. Trimethyl phosphate -8.7
6. 4-nitroaniline -10.01
7. Glycerol -8.40
8. Pentachloronitrobenzene -5.22

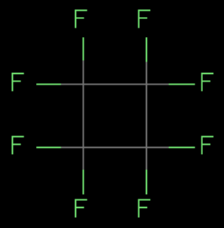
hexachlorobenzene



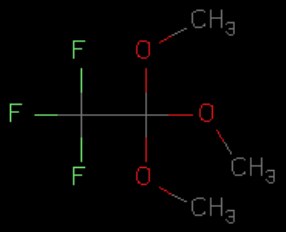
hexachloroethane



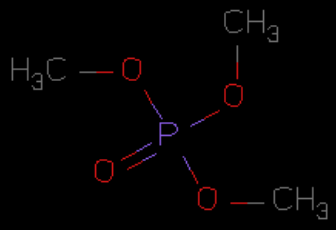
octafluorocyclobutane



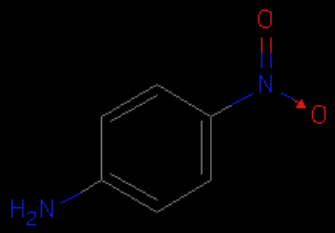
trimethyl orthotrifluoroacetate



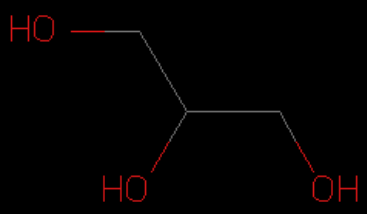
trimethyl phosphate



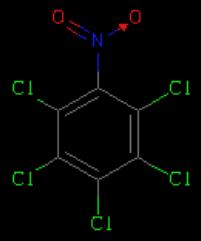
4-nitroaniline



glycerol



pentachloronitrobenzene



Investigatory (see also investigate.ism and investigate.sdf)