chemical sample	heat of formation (kcal/mole)	enthalpy (kcal/mole)	heat capacity (kcal/mole/Kelvin	surface area (angstromsquare)
alpha-HCH	-64.714	6.201	0.04	176.36
beta-HCH	-64.251	6.235	0.04	175.98
gamma-HCH	-63.509	6.168	0.039	176.59
delta-HCH	-64.107	6.211	0.04	176.45
epsilon-HCH	-64.092	6.162	0.039	176.29
eta-HCH	-62.962	6.157	0.039	176.7
theta-HCH	-61.663	6.156	0.039	176.56
iota-HCH	-58.247	6.13	0.039	177.32
method	MM/AM1	MM/AM1/H2O	MM/AM1/H2O	MM/AM1/H2O

chemical sample	heat of formation (kcal/mole)	enthalpy (kcal/mole)	heat capacity (kcal/mole/Kelvin	surface area (angstromsquare)
alpha-HCH	-52.855	6.62	0.042	180.77
beta-HCH	-52.424	6.683	0.042	181.14
gamma-HCH	-52.064	6.562	0.042	179.01
delta-HCH	-52.22	6.632	0.042	180.7
epsilon-HCH	-52.359	6.593	0.042	179.38
eta-HCH	-51.328	6.532	0.042	178.4
theta-HCH	-50.31	6.543	0.042	178.05
iota-HCH	-46.913	6.413	0.042	174.85
method	MM/PM3	MM/PM3/H2O	MM/PM3/H2O	MM/PM3/H2O

heat of formatio	MM/AM1	**[J. J. P. Stewart, J. Comp. Chem., 10, 221-264 (1989)]**
enthalpy	MM/AM1/H2O	**[A. Klamt and G. Schuurmann, J. Chem. Soc. Perkin Trans. 2, 799, 1993]**
heat capacity	MM/AM1/H2O	**[A. Klamt and G. Schuurmann, J. Chem. Soc. Perkin Trans. 2, 799, 1994]**
surface area	MM/AM1/H2O	**[A. Klamt and G. Schuurmann, J. Chem. Soc. Perkin Trans. 2, 799, 1995]**
heat of formatio	MM/PM3	**[J. J. P. Stewart, J. Comp. Chem., 10, 221-264 (1989)]**
enthalpy	MM/PM3/H2O	**[A. Klamt and G. Schuurmann, J. Chem. Soc. Perkin Trans. 2, 799, 1993]**
heat capacity	MM/PM3/H2O	**[A. Klamt and G. Schuurmann, J. Chem. Soc. Perkin Trans. 2, 799, 1994]**

surface area MM/PM3/H2O [A. Klamt and G. Schuurmann, J. Chem. Soc. Perkin Trans. 2, 799, 1995]

heat of formatio The energy released or used when a molecule is formed from elements in their standard states.

Procedure MM/AM1_Geo_Tab_Prop
Name Hf at MM/AM1 geometry
The heat of formation is determined after optimizing the molecular geometry
first using Augmented MM2 then using MOPAC with AM1 parameters. AM1 heats of formation
have an average unsigned difference between experimental and observed values of 22.4 kcal/mol
for 763 compounds. Excluding Al, P and S the error is 11.5 kcal/mol.
[J. J. P. Stewart, J. Comp. Chem., 10, 221-264 (1989)]

Procedure MM/PM3_Geo_Tab_Prop
Name Hf at MM/PM3 geometry
The heat of formation is determined after optimizing the molecular geometry
first using Augmented MM2 then using MOPAC with PM3 parameters. PM3 heats of formation
have an average unsigned difference between experimental and observed values of 8.6 kcal/mol
for 763 compounds. Excluding Al, P and S the error is 7.1 kcal/mol.
[J. J. P. Stewart, J. Comp. Chem., 10, 221-264 (1989)]

enthalpy Enthalpy of molecule at corresponding temperature.

Procedure MM/AM1/H2O_Geo_IR
Name enthalpy at AM1/H2O geom
Enthalpy is determined by first optimizing the molecular geometry using Augmented MM2,
followed by MOPAC with AM1 parameters and the Conductor-like Screening Model (COSMO).
[A. Klamt and G. Schuurmann, J. Chem. Soc. Perkin Trans. 2, 799, 1993]

Procedure MM/PM3/H2O_Geo_IR
Name enthalpy at PM3/H2O geom
Enthalpy is determined by first optimizing the molecular geometry using Augmented MM2,

followed by MOPAC with PM3 parameters and the Conductor-like Screening Model (COSMO).
[A. Klamt and G. Schuurmann, J. Chem. Soc. Perkin Trans. 2, 799, 1993]

heat_capacity Heat capacity at constant pressure at the corresponding temperature.
Procedure MM/AM1/H2O_Geo_IR
Name heat capacity at AM1/H2O geom
Heat capacity is determined by first optimizing the molecular geometry using Augmented MM2,
followed by MOPAC with AM1 parameters and the Conductor-like Screening Model (COSMO).
[A. Klamt and G. Schuurmann, J. Chem. Soc. Perkin Trans. 2, 799, 1993]

Procedure MM/PM3/H2O_Geo_IR
Name heat capacity at PM3/H2O geom
Heat capacity is determined by first optimizing the molecular geometry using Augmented MM2,
followed by MOPAC with PM3 parameters and the Conductor-like Screening Model (COSMO).
[A. Klamt and G. Schuurmann, J. Chem. Soc. Perkin Trans. 2, 799, 1993]

SolventAccessibleSurfaceArea The solvent accessible surface (SAS) area for the molecule when the solvent is water.
Procedure MM/AM1/H2O_Geo_Tab_Prop
Name SAS area at AM1/H2O geometry
The solvent accessible surface (SAS) area is calculated at an optimized geometry in water. The water geometry is obtained
from optimization first using Augmented MM2, then using MOPAC with AM1 parameters and the Conductor-like
Screening Model (COSMO).
[A. Klamt and G. Schuurmann, J. Chem. Soc. Perkin Trans. 2, 799, 1993]

Procedure MM/PM3/H2O_Geo_Tab_Prop
Name SAS area at PM3/H2O geometry
The solvent accessible surface (SAS) area is calculated at an optimized geometry in water. The water geometry is obtained
from optimization first using Augmented MM2, then using MOPAC with PM3 parameters and the Conductor-like
Screening Model (COSMO).
[A. Klamt and G. Schuurmann, J. Chem. Soc. Perkin Trans. 2, 799, 1993]