Hexachlorocyclopropane

Inchi: InChI=1S/C3Cl6/c4-1(5)2(6,7)3(1,8)9
InchiKey: AVFQBLKYJWKKJP-UHFFFAOYSA-N
Formula: C3Cl6
SMILES: ClC1(Cl)C(Cl)(Cl)C1(Cl)Cl
Mol. weight [g/mol]: 248.75
CAS: 2065-35-2

Physical Properties

Property code	Value	Unit	Source
gf	-68.34	kJ/mol	Joback Method
hf	-121.85	kJ/mol	Joback Method
hfus	10.09	kJ/mol	Joback Method
hvap	44.42	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.522		Crippen Method
mcvol	115.710	ml/mol	McGowan Method
pc	4277.45	kPa	Joback Method
tb	490.74	K	Joback Method
tc	753.55	K	Joback Method
tf	384.25	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.52	J/mol×K	490.74	Joback Method
cpg	178.26	J/mol×K	534.54	Joback Method
cpg	180.70	J/mol×K	578.34	Joback Method
cpg	182.34	J/mol×K	622.14	Joback Method
cpg	183.70	J/mol×K	665.95	Joback Method
cpg	185.28	J/mol×K	709.75	Joback Method
cpg	187.61	J/mol×K	753.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2065352&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume