cis-Chlordane

Other names:	4,7-Methano-1H-indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-, (1«alpha»,2«alpha»,3a«alpha»,4«beta»,7«beta»,7a«alpha»)- 4,7-Methanoindan, 1«alpha»,2«alpha»,4«beta»,5,6,7«beta»,8,8-octachloro-3a«alpha»,4,7,7a«alpha»-tetrahy «alpha»-Chlordan «alpha»-Chlordane cis-Chlordan Chlordan, cis- 4,7-Methano-1H-indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-, (1R,2S,3aS,4S,7R,7aS)-rel-(1«alpha»,2«alpha»,3a«alpha»,4«beta»,7«beta»,7a«alpha»)-1,2,4,5,6,7,8,8-octachloro-2
Inchi:	InChI=1S/C10H6Cl8/c11-3-1-2-4(5(3)12)9(16)7(14)6(13)8(2,15)10(9,17)18/h2-5H,1H2/t2
InchiKey:	BIWJNBZANLAXMG-FZOZSSNHSA-N
Formula:	C10H6Cl8
SMILES:	ClC1=C(Cl)C2(Cl)C3C(Cl)C(Cl)CC3C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]:	409.78
CAS:	5103-71-9

Physical Properties

Property code	Value	Unit	Source
gf	71.42	kJ/mol	Joback Method
hf	-164.21	kJ/mol	Joback Method
hfus	33.37	kJ/mol	Joback Method
hvap	69.77	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	5.683		Crippen Method
mcvol	212.800	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
rinpol	2081.80		NIST Webbook
rinpol	2056.00		NIST Webbook
rinpol	2056.00		NIST Webbook
rinpol	2118.10		NIST Webbook
rinpol	2081.80		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook
ripol	2842.00		NIST Webbook
ripol	2842.00		NIST Webbook
tb	743.29	K	Joback Method
tc	1021.42	K	Joback Method
tf	381.19 ± 0.20	K	NIST Webbook

tf	377.30 ± 0.20	K	NIST Webbook
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.76	J/mol×K	928.71	Joback Method
cpg	540.74	J/mol×K	975.06	Joback Method
cpg	461.86	J/mol×K	743.29	Joback Method
cpg	473.85	J/mol×K	789.64	Joback Method
cpg	487.02	J/mol×K	836.00	Joback Method
cpg	502.09	J/mol×K	882.35	Joback Method
cpg	565.73	J/mol×K	1021.42	Joback Method
hfust	23.15	kJ/mol	379.90	NIST Webbook
hvapt	83.00	kJ/mol	366.00	NIST Webbook
hvapt	82.00	kJ/mol	398.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5103719&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
hfust: Enthalpy of fusion at a given temperature
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume