«beta»-Chlordene

Other names:	1,6-Methano-1H-indene, 2,3,3a,4,5,7-hexachloro-3a,6,7,7a-tetrahydro-, (1«alpha»,3a«beta»,6«alpha»,7«alpha»,7a«beta»)- 2,3,3a,4,5,7-Hexachloro-3a,6,7,7a-tetrahydro-1,6-methano-1H-indene-, (1«alpha»,3a«beta»,6«alpha»,7«alpha»,7a«beta»)- 1,6-Methano-1H-indene, 2,3,3a,4,5,7-hexachloro-3a,6,7,7a-tetrahydro-, (1R,3aR,6S,7S,7aR)-rel- 2,3,3a,4,5,7-Hexachloro-3a,6,7,7a-tetrahydro-1,6-methano-1H-indene
Inchi:	InChI=1S/C10H6Cl6/c11-5-3-1-2-4(5)10(16,8(14)6(2)12)9(15)7(3)13/h2-5H,1H2
InchiKey:	OSFPUJNCRLXHDW-UHFFFAOYSA-N
Formula:	C10H6Cl6
SMILES:	ClC1=C(Cl)C2(Cl)C(Cl)=C(Cl)C3CC1C(Cl)C32
Mol. weight [g/mol]:	338.87
CAS:	56534-03-3

Physical Properties

Property code	Value	Unit	Source
gf	132.38	kJ/mol	Joback Method
hf	-87.69	kJ/mol	Joback Method
hfus	35.88	kJ/mol	Joback Method
hvap	65.54	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.229		Crippen Method
mcvol	184.020	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1925.80		NIST Webbook
rinpol	1898.00		NIST Webbook
rinpol	1925.80		NIST Webbook
rinpol	1964.80		NIST Webbook
rinpol	1898.00		NIST Webbook
tb	686.41	K	Joback Method
tc	943.87	K	Joback Method
tf	499.30	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	395.62	J/mol×K	686.41	Joback Method
cpg	405.84	J/mol×K	729.32	Joback Method
cpg	415.64	J/mol×K	772.23	Joback Method
cpg	425.29	J/mol×K	815.14	Joback Method
cpg	435.06	J/mol×K	858.05	Joback Method
cpg	445.23	J/mol×K	900.96	Joback Method
cpg	456.08	J/mol×K	943.87	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56534033&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume