4,7-Methanoindan, 3a,4,7,7a-tetrahydro-1,2-epoxy-4,5,6,7,8,8-hexachl

Other names: Chlordene epoxide

2,5-Methano-2H-indeno(1,2-b)oxirene, 2,3,4,5,7,7-hexachloro-1a,1b,5,5a,6,6a-hexahydro-

3a,4,7,7a-Tetrahydro-1,2-epoxy-4,5,6,7,8,8-hexachloro-4,7-methanoindan

Inchi: InChI=1S/C10H6Cl6O/c11-6-7(12)9(14)4-2(1-3-5(4)17-3)8(6,13)10(9,15)16/h2-5H,1H2

InchiKey: VMNNMBZKONGDDQ-UHFFFAOYSA-N

Formula: C10H6Cl6O

SMILES: ClC1=C(Cl)C2(Cl)C3C4OC4CC3C1(Cl)C2(Cl)Cl

Mol. weight [g/mol]: 354.87

CAS: 6058-23-7

Physical Properties

Property code	Value	Unit	Source
gf	101.82	kJ/mol	Joback Method
hf	-159.27	kJ/mol	Joback Method
hfus	34.22	kJ/mol	Joback Method
hvap	65.39	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.235		Crippen Method
mcvol	183.330	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
tb	698.25	K	Joback Method
tc	968.59	K	Joback Method
tf	568.61	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.70	J/mol×K	698.25	Joback Method
cpg	433.89	J/mol×K	743.31	Joback Method
cpg	444.73	J/mol×K	788.36	Joback Method
cpg	456.93	J/mol×K	833.42	Joback Method
cpg	471.25	J/mol×K	878.48	Joback Method
cpg	488.41	J/mol×K	923.53	Joback Method

cpg	509.16	J/mol×K	968.59	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=C6058237&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume