1,4,5,7,8,8-Hexachloro-3a,4,7,7a-tetrahydro-1H-4,7

Inchi: InChI=1S/C10H6Cl6/c11-5-2-1-4-7(5)8(13)3-6(12)9(4,14)10(8,15)16/h1-5,7H
InchiKey: RKUDGXDTVRLFRR-UHFFFAOYSA-N
Formula: C10H6Cl6
SMILES: ClC1=CC2(Cl)C3C(Cl)C=CC3C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]: 338.87

Physical Properties

Property code	Value	Unit	Source
gf	142.58	kJ/mol	Joback Method
hf	-43.14	kJ/mol	Joback Method
hfus	25.52	kJ/mol	Joback Method
hvap	60.94	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.675		Crippen Method
mcvol	184.020	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	1778.40		NIST Webbook
rinpol	1807.10		NIST Webbook
rinpol	1778.40		NIST Webbook
tb	667.28	K	Joback Method
tc	943.85	K	Joback Method
tf	505.30	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.61	J/mol×K	667.28	Joback Method
cpg	407.08	J/mol×K	713.37	Joback Method
cpg	417.63	J/mol×K	759.47	Joback Method
cpg	428.99	J/mol×K	805.56	Joback Method
cpg	441.88	J/mol×K	851.66	Joback Method
cpg	457.00	J/mol×K	897.75	Joback Method
cpg	475.10	J/mol×K	943.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R255979&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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