1,4-Dihydro-1,2,3,4,9,9-hexachloro-1,4-methanona

Inchi: InChI=1S/C11H4Cl6O2/c12-7-8(13)10(15)6-4(19)2-1-3(18)5(6)9(7,14)11(10,16)17/h1-2,1
InchiKey: HGWPFZAIXJHLBN-UHFFFAOYSA-N
Formula: C11H4Cl6O2
SMILES: Oc1ccc(O)c2c1C1(Cl)C(Cl)=C(Cl)C2(Cl)C1(Cl)Cl
Mol. weight [g/mol]: 380.87
CAS: 5210-87-7

Physical Properties

Property code	Value	Unit	Source
gf	-116.18	kJ/mol	Joback Method
hf	-282.39	kJ/mol	Joback Method
hfus	35.64	kJ/mol	Joback Method
hvap	92.86	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.856		Crippen Method
mcvol	201.250	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
tb	882.94	K	Joback Method
tc	1175.82	K	Joback Method
tf	788.29	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.28	J/mol×K	882.94	Joback Method
cpg	473.77	J/mol×K	931.75	Joback Method
cpg	497.53	J/mol×K	980.57	Joback Method
cpg	527.61	J/mol×K	1029.38	Joback Method
cpg	565.03	J/mol×K	1078.20	Joback Method
cpg	610.85	J/mol×K	1127.01	Joback Method
cpg	666.09	J/mol×K	1175.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5210877&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