2,3,4,4,5,5,6,6-Octachloro cyclohex-2-ene-1-one

Inchi: InChI=1S/C6Cl8O/c7-1-2(8)4(9,10)6(13,14)5(11,12)3(1)15
InchiKey: CZLVPINBLDRZCJ-UHFFFAOYSA-N
Formula: C6Cl8O
SMILES: O=C1C(Cl)=C(Cl)C(Cl)(Cl)C(Cl)(Cl)C1(Cl)Cl
Mol. weight [g/mol]: 371.69
CAS: 4024-81-1

Physical Properties

Property code	Value	Unit	Source
gf	-215.13	kJ/mol	Joback Method
hf	-336.59	kJ/mol	Joback Method
hfus	19.91	kJ/mol	Joback Method
hvap	66.25	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.780		Crippen Method
mcvol	179.730	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
tb	723.99	K	Joback Method
tc	1021.67	K	Joback Method
tf	561.36	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.25	J/mol×K	723.99	Joback Method
cpg	317.70	J/mol×K	773.60	Joback Method
cpg	326.45	J/mol×K	823.22	Joback Method
cpg	337.09	J/mol×K	872.83	Joback Method
cpg	350.22	J/mol×K	922.45	Joback Method
cpg	366.45	J/mol×K	972.06	Joback Method
cpg	386.37	J/mol×K	1021.67	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=C4024811&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