2,2,6,6-Tetrakis(chloromethyl)cyclohexanone

Inchi: InChI=1S/C10H14Cl4O/c11-4-9(5-12)2-1-3-10(6-13,7-14)8(9)15/h1-7H2
InchiKey: AQIAZQNYXUJNNC-UHFFFAOYSA-N
Formula: C10H14Cl4O
SMILES: O=C1C(CCl)(CCl)CCCC1(CCl)CCl
Mol. weight [g/mol]: 292.03

Physical Properties

Property code	Value	Unit	Source
gf	-131.23	kJ/mol	Joback Method
hf	-385.93	kJ/mol	Joback Method
hfus	18.26	kJ/mol	Joback Method
hvap	57.46	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.667		Crippen Method
mcvol	191.430	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
rinpol	2024.00		NIST Webbook
tb	661.10	K	Joback Method
tc	908.18	K	Joback Method
tf	441.30	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.19	J/mol×K	661.10	Joback Method
cpg	466.23	J/mol×K	702.28	Joback Method
cpg	480.70	J/mol×K	743.46	Joback Method
cpg	494.86	J/mol×K	784.64	Joback Method
cpg	508.97	J/mol×K	825.82	Joback Method
cpg	523.27	J/mol×K	867.00	Joback Method
cpg	538.02	J/mol×K	908.18	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=R520540&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