2,2,6,6-Tetrachlorocyclohexanol

Other names: Cyclohexanol, 2,2,6,6-tetrachloro-
Inchi: InChI=1S/C6H8Cl4O/c7-5(8)2-1-3-6(9,10)4(5)11/h4,11H,1-3H2
InchiKey: RORBTKDJFQCFMD-UHFFFAOYSA-N
Formula: C6H8Cl4O
SMILES: OC1C(Cl)(Cl)CCCC1(Cl)Cl
Mol. weight [g/mol]: 237.94
CAS: 56207-45-5

Physical Properties

Property code	Value	Unit	Source
gf	-186.85	kJ/mol	Joback Method
hf	-338.24	kJ/mol	Joback Method
hfus	13.55	kJ/mol	Joback Method
hvap	60.68	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.879		Crippen Method
mcvol	139.370	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
tb	589.27	K	Joback Method
tc	821.77	K	Joback Method
tf	384.58	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.07	J/mol×K	589.27	Joback Method
cpg	299.80	J/mol×K	628.02	Joback Method
cpg	308.89	J/mol×K	666.77	Joback Method
cpg	317.56	J/mol×K	705.52	Joback Method
cpg	326.04	J/mol×K	744.27	Joback Method
cpg	334.56	J/mol×K	783.02	Joback Method
cpg	343.34	J/mol×K	821.77	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56207455&Units=SI

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