2-exo,3-endo,6-exo,8b,9c,10a-hexachlorobornane

Inchi: InChI=1S/C10H12Cl6/c11-2-9(3-12)5-1-6(14)10(9,4-13)8(16)7(5)15/h5-8H,1-4H2/t5?,6-,7

InchiKey: FFKWIAYHUUWFCB-SZAGHJGMSA-N

Formula: C10H12Cl6

SMILES: ClCC1(CCl)C2CC(Cl)C1(CCl)C(Cl)C2Cl

Mol. weight [g/mol]: 344.92

Physical Properties

Property code	Value	Unit	Source
gf	29.32	kJ/mol	Joback Method
hf	-255.61	kJ/mol	Joback Method
hfus	32.70	kJ/mol	Joback Method
hvap	60.62	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.531		Crippen Method
mcvol	203.480	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	2088.30		NIST Webbook
tb	652.33	K	Joback Method
tc	894.30	K	Joback Method
tf	445.18	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.20	J/mol×K	652.33	Joback Method
cpg	479.91	J/mol×K	692.66	Joback Method
cpg	493.01	J/mol×K	732.99	Joback Method
cpg	505.82	J/mol×K	773.32	Joback Method
cpg	518.64	J/mol×K	813.65	Joback Method
cpg	531.81	J/mol×K	853.98	Joback Method
cpg	545.65	J/mol×K	894.30	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=R502562&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