2-exo,5,5,8c,9b,9c,10a,10b-octachlorobornane

Inchi: InChI=1S/C10H10Cl8/c11-3-8-2-9(17,18)4(1-5(8)12)10(8,6(13)14)7(15)16/h4-7H,1-3H2/t
InchiKey: XJZGYZQCTOFMAI-OBTXSVHCSA-N
Formula: C10H10Cl8
SMILES: ClCC12CC(Cl)(Cl)C(CC1Cl)C2(C(Cl)Cl)C(Cl)Cl
Mol. weight [g/mol]: 413.81

Physical Properties

Property code	Value	Unit	Source
gf	2.80	kJ/mol	Joback Method
hf	-262.07	kJ/mol	Joback Method
hfus	26.68	kJ/mol	Joback Method
hvap	67.78	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	6.010		Crippen Method
mcvol	227.960	ml/mol	McGowan Method
pc	2189.73	kPa	Joback Method
rinpol	2382.20		NIST Webbook
rinpol	2382.20		NIST Webbook
tb	731.22	K	Joback Method
tc	997.81	K	Joback Method
tf	503.16	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.88	J/mol×K	731.22	Joback Method
cpg	517.71	J/mol×K	775.65	Joback Method
cpg	531.24	J/mol×K	820.08	Joback Method
cpg	546.07	J/mol×K	864.52	Joback Method
cpg	562.82	J/mol×K	908.95	Joback Method
cpg	582.10	J/mol×K	953.38	Joback Method
cpg	604.51	J/mol×K	997.81	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=R502577&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