2,2,5-endo,6-exo,8c,9b,9c,10a,10b-nonachlorobor

Inchi: InChI=1S/C10H9Cl9/c11-2-8-5(13)4(12)3(1-9(8,18)19)10(8,6(14)15)7(16)17/h3-7H,1-2H2
InchiKey: UCIHQSZARDUKEB-KTGYALDVSA-N
Formula: C10H9Cl9
SMILES: ClCC12C(Cl)C(Cl)C(CC1(Cl)Cl)C2(C(Cl)Cl)C(Cl)Cl
Mol. weight [g/mol]: 448.25

Physical Properties

Property code	Value	Unit	Source
gf	-16.84	kJ/mol	Joback Method
hf	-298.15	kJ/mol	Joback Method
hfus	31.94	kJ/mol	Joback Method
hvap	71.85	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	6.228		Crippen Method
mcvol	240.200	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	2505.80		NIST Webbook
rinpol	2505.80		NIST Webbook
tb	763.98	K	Joback Method
tc	1032.37	K	Joback Method
tf	528.84	K	Joback Method
vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.94	J/mol×K	763.98	Joback Method
cpg	543.31	J/mol×K	808.71	Joback Method
cpg	557.80	J/mol×K	853.44	Joback Method
cpg	574.01	J/mol×K	898.18	Joback Method
cpg	592.57	J/mol×K	942.91	Joback Method
cpg	614.09	J/mol×K	987.64	Joback Method
cpg	639.16	J/mol×K	1032.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R502468&Units=SI
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

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