2,2,5,5,8c,9b,9c,10a,10b-nonachlorobornane

Inchi: InChI=1S/C10H9Cl9/c11-3-7-2-8(16,17)4(1-9(7,18)19)10(7,5(12)13)6(14)15/h4-6H,1-3H2
InchiKey: BUWMNBVKPBVDPO-UHFFFAOYSA-N
Formula: C10H9Cl9
SMILES: ClCC12CC(Cl)(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	-14.62	kJ/mol	Joback Method
hf	-262.57	kJ/mol	Joback Method
hfus	24.57	kJ/mol	Joback Method
hvap	71.01	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	6.577		Crippen Method
mcvol	240.200	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	2539.40		NIST Webbook
rinpol	2539.40		NIST Webbook
tb	768.89	K	Joback Method
tc	1047.16	K	Joback Method
tf	556.98	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.92	J/mol×K	768.89	Joback Method
cpg	534.94	J/mol×K	815.27	Joback Method
cpg	551.16	J/mol×K	861.65	Joback Method
cpg	570.47	J/mol×K	908.02	Joback Method
cpg	593.73	J/mol×K	954.40	Joback Method
cpg	621.82	J/mol×K	1000.78	Joback Method
cpg	655.61	J/mol×K	1047.16	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=R502408&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

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