2,2,3-exo,5,5,8c,9b,10a,10b-nonachlorobornane

Inchi: InChI=1S/C10H9Cl9/c11-2-7-1-9(16,17)4(5(13)10(7,18)19)8(7,3-12)6(14)15/h4-6H,1-3H2
InchiKey: ZCLDZZOUNCBYOC-USLBLKDFSA-N
Formula: C10H9Cl9
SMILES: ClCC1(C(Cl)Cl)C2C(Cl)C(Cl)(Cl)C1(CCl)CC2(Cl)Cl
Mol. weight [g/mol]: 448.25

Physical Properties

Property code	Value	Unit	Source
gf	-19.89	kJ/mol	Joback Method
hf	-277.63	kJ/mol	Joback Method
hfus	29.17	kJ/mol	Joback Method
hvap	71.09	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	6.229		Crippen Method
mcvol	240.200	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	2498.20		NIST Webbook
rinpol	2498.20		NIST Webbook
tb	764.66	K	Joback Method
tc	1037.61	K	Joback Method
tf	567.74	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.44	J/mol×K	764.66	Joback Method
cpg	538.40	J/mol×K	810.15	Joback Method
cpg	554.36	J/mol×K	855.64	Joback Method
cpg	573.11	J/mol×K	901.14	Joback Method
cpg	595.48	J/mol×K	946.63	Joback Method
cpg	622.27	J/mol×K	992.12	Joback Method
cpg	654.30	J/mol×K	1037.61	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=R502364&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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