2-endo,3-exo,5-endo,6-exo,8b,8c,9c,10a,10c-nona

Inchi: InChI=1S/C10H9Cl9/c11-1-9(7(16)17)2-3(12)5(14)10(9,8(18)19)6(15)4(2)13/h2-8H,1H2/t
InchiKey: ICTWAJXDCVGTJO-DHTDEGTBSA-N
Formula: C10H9Cl9
SMILES: ClCC1(C(Cl)Cl)C2C(Cl)C(Cl)C1(C(Cl)Cl)C(Cl)C2Cl
Mol. weight [g/mol]: 448.25

Physical Properties

Property code	Value	Unit	Source
gf	-19.06	kJ/mol	Joback Method
hf	-333.73	kJ/mol	Joback Method
hfus	39.31	kJ/mol	Joback Method
hvap	72.69	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	5.878		Crippen Method
mcvol	240.200	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	2415.10		NIST Webbook
rinpol	2415.10		NIST Webbook
tb	759.07	K	Joback Method
tc	1018.11	K	Joback Method
tf	500.70	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.89	J/mol×K	759.07	Joback Method
cpg	551.83	J/mol×K	802.24	Joback Method
cpg	564.99	J/mol×K	845.42	Joback Method
cpg	578.77	J/mol×K	888.59	Joback Method
cpg	593.57	J/mol×K	931.76	Joback Method
cpg	609.76	J/mol×K	974.93	Joback Method
cpg	627.75	J/mol×K	1018.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R502517&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