

5-exo,6-endo,8,9,9,10-hexachlorocamphene

Inchi:	InChI=1S/C10H10Cl6/c11-2-6-4-1-5(8(14)7(4)13)10(6,3-12)9(15)16/h2,4-5,7-9H,1,3H2/b
InchiKey:	RKZDFGCWYYCUHL-CRKOBHGOSA-N
Formula:	C10H10Cl6
SMILES:	<chem>C1C=C1C2CC(C(Cl)C2Cl)C1(CCl)C(Cl)Cl</chem>
Mol. weight [g/mol]:	342.90

Physical Properties

Property code	Value	Unit	Source
gf	85.54	kJ/mol	Joback Method
hf	-179.76	kJ/mol	Joback Method
hfus	34.72	kJ/mol	Joback Method
hvap	62.48	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	5.003		Crippen Method
mcvol	199.180	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
tb	662.96	K	Joback Method
tc	907.70	K	Joback Method
tf	420.88	K	Joback Method
vc	0.767	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.62	J/mol×K	662.96	Joback Method
cpg	456.33	J/mol×K	703.75	Joback Method
cpg	468.28	J/mol×K	744.54	Joback Method
cpg	479.71	J/mol×K	785.33	Joback Method
cpg	490.83	J/mol×K	826.12	Joback Method
cpg	501.87	J/mol×K	866.91	Joback Method
cpg	513.04	J/mol×K	907.70	Joback Method

Sources

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=R502611&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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