Chlorbicyclen

Other names:	Bicyclo[2.2.1]hept-2-ene, 1,2,3,4,7,7-hexachloro-5,6-bis(chloromethyl)- AC 12402 Alodan Cyclodan Hercules 426 Hercules 12402 2-Norbornene, 1,2,3,4,7,7-Hexachloro-5,6-bis(chloromethyl)- 5,6-Bis-(chloromethyl)-1,2,3,4,7,7-hexachlorobicyclo-(2,2,1)-2-heptene Nodon Allodan 2,3-Bis(chloromethyl)-1,4,5,6,7,7-hexachlorobicyclo(2.2.1)hept-4-ene 1,2,3,4,7,7-Hexachloro-5,6-bis(chloromethyl)-2-norbornene Alodan (pesticide) NSC 41891
Inchi:	InChI=1S/C9H6Cl8/c10-1-3-4(2-11)8(15)6(13)5(12)7(3,14)9(8,16)17/h3-4H,1-2H2
InchiKey:	FUZORIOHZSVKAW-UHFFFAOYSA-N
Formula:	C9H6Cl8
SMILES:	ClCC1C(CCl)C2(Cl)C(Cl)=C(Cl)C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]:	397.77
CAS:	2550-75-6

Physical Properties

Property code	Value	Unit	Source
gf	9.96	kJ/mol	Joback Method
hf	-196.03	kJ/mol	Joback Method
hfus	31.57	kJ/mol	Joback Method
hvap	67.94	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.542		Crippen Method
mcvol	209.570	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
rinpol	2013.70		NIST Webbook
rinpol	1979.90		NIST Webbook
tb	718.34	K	Joback Method
tc	984.40	K	Joback Method
tf	547.69	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.61	J/mol×K	718.34	Joback Method
cpg	435.34	J/mol×K	762.68	Joback Method
cpg	445.90	J/mol×K	807.03	Joback Method
cpg	457.86	J/mol×K	851.37	Joback Method
cpg	471.79	J/mol×K	895.71	Joback Method
cpg	488.28	J/mol×K	940.06	Joback Method
cpg	507.90	J/mol×K	984.40	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2550756&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

Latest version available from:
https://www.chemeo.com/cid/32-563-1/Chlorbicyclen.pdf
Generated by Cheméo on 2025-12-05 11:56:15.025110274 +0000 UTC m=+4683972.555150938.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.