

Bicyclo[2.2.1]hepta-2,5-diene, 1,2,3,4,7,7-hexachloro-

Other names:	2,5-Norbornadiene, 1,2,3,4,7,7-hexachloro-Hexachloronorbornadiene 1,2,3,4,7,7-Hexachlorobicyclo[2.2.1]hepta-2,5-diene 1,2,3,4,7,7-Hexachloronorbornadiene 1,2,3,4,7,7-Hexachloro-2,5-norbornadiene
Inchi:	InChI=1S/C7H2Cl6/c8-3-4(9)6(11)2-1-5(3,10)7(6,12)13/h1-2H
InchiKey:	IHAXIFZOERJWDF-UHFFFAOYSA-N
Formula:	C7H2Cl6
SMILES:	C1C=C(Cl)C2(Cl)C=CC1(Cl)C2(Cl)Cl
Mol. weight [g/mol]:	298.81
CAS:	3389-71-7

Physical Properties

Property code	Value	Unit	Source
gf	62.36	kJ/mol	Joback Method
hf	-24.81	kJ/mol	Joback Method
hfus	17.08	kJ/mol	Joback Method
hvap	55.63	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.388		Crippen Method
mvol	152.610	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
tb	606.22	K	Joback Method
tc	883.92	K	Joback Method
tf	474.55	K	Joback Method
vc	0.593	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.62	J/mol×K	606.22	Joback Method
cpg	275.74	J/mol×K	652.50	Joback Method
cpg	280.57	J/mol×K	698.79	Joback Method
cpg	285.79	J/mol×K	745.07	Joback Method

cpg	292.06	J/mol×K	791.35	Joback Method
cpg	300.05	J/mol×K	837.63	Joback Method
cpg	310.42	J/mol×K	883.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C3389717&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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