Hexachlorocyclopentadiene

Other names:	1,2,3,4,5,5-Hexachloro-1,3-cyclopentadiene 1,2,3,4,5,5-Hexachloro-cyclopenta-1,3-diene 1,2,3,4,5,5-hexachlorocyclopenta-1,3-diene 1,3-Cyclopentadiene, 1,2,3,4,5,5-hexachloro- 1,3-Cyclopentadiene, hexachloro- C 56 Cyclopentadiene, hexachloro- Graphlox HCCPD HRS 1655 Hexachlorcyklopentadien Hexachloro-1,3-cyclopentadiene NCI-C55607 NSC 9235 Perchloro-1,3-cyclopentadiene Perchlorocyclopentadiene Rcra waste number U130 UN 2646
Inchi:	InChI=1S/C5Cl6/c6-1-2(7)4(9)5(10,11)3(1)8
InchiKey:	VUNCWTMEJYMOOR-UHFFFAOYSA-N
Formula:	C5Cl6
SMILES:	ClC1=C(Cl)C(Cl)(Cl)C(Cl)=C1Cl
Mol. weight [g/mol]:	272.77
CAS:	77-47-4

Physical Properties

Property code	Value	Unit	Source
chl	-2030.00 ± 3.00	kJ/mol	NIST Webbook
gf	-27.90	kJ/mol	Joback Method
hf	-11.70 ± 4.40	kJ/mol	NIST Webbook
hfl	-79.20 ± 3.10	kJ/mol	NIST Webbook
hfus	22.41	kJ/mol	Joback Method
hvap	67.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-5.18		Aqueous Solubility Prediction Method
logp	4.552		Crippen Method
mcvol	135.290	ml/mol	McGowan Method

pc	3530.46	kPa	Joback Method
rinpol	228.10		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1326.80		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1314.30		NIST Webbook
tb	572.14	K	Joback Method
tc	830.91	K	Joback Method
tf	412.03	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.40	J/mol×K	572.14	Joback Method
cpg	205.15	J/mol×K	615.27	Joback Method
cpg	208.54	J/mol×K	658.40	Joback Method
cpg	211.76	J/mol×K	701.52	Joback Method
cpg	214.97	J/mol×K	744.65	Joback Method
cpg	218.33	J/mol×K	787.78	Joback Method
cpg	222.01	J/mol×K	830.91	Joback Method
hsubt	73.60	kJ/mol	283.00	NIST Webbook
hvapt	53.70	kJ/mol	423.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	512.20	K	100.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2

Coeff. A	1.04916e+02
Coeff. B	-1.11253e+04
Coeff. C	-1.27868e+01
Coeff. D	4.60213e-06
Temperature range (K), min.	284.49
Temperature range (K), max.	746.00

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77474&Units=SI
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1755
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/files/research/kdb/mol/mol1755.mol
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
pvap: Vapor pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume