1H-Pentachloropropene

Other names: 1-Propene, 1,1,2,3,3-pentachloro-
1,1,2,3,3-pentachloropropene
Inchi: InChI=1S/C3HCl5/c4-1(2(5)6)3(7)8/h2H
InchiKey: MAXQCYDCBHPIAB-UHFFFAOYSA-N
Formula: C3HCl5
SMILES: ClC(Cl)=C(Cl)C(Cl)Cl
Mol. weight [g/mol]: 214.31
CAS: 1600-37-9

Physical Properties

Property code	Value	Unit	Source
gf	-24.59	kJ/mol	Joback Method
hf	-91.59	kJ/mol	Joback Method
hfus	18.57	kJ/mol	Joback Method
hvap	43.93	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.676		Crippen Method
mcvol	110.030	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	1041.00		NIST Webbook
rinpol	1044.00		NIST Webbook
tb	458.67	K	Joback Method
tc	690.20	K	Joback Method
tf	225.17	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.74	J/mol×K	458.67	Joback Method
cpg	155.08	J/mol×K	497.26	Joback Method
cpg	158.96	J/mol×K	535.85	Joback Method
cpg	162.42	J/mol×K	574.43	Joback Method
cpg	165.51	J/mol×K	613.02	Joback Method

cpg	168.27	J/mol×K	651.61	Joback Method
cpg	170.73	J/mol×K	690.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1600379&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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