Hexachloropropene

Other names:	1,1,2,3,3,3-Hexachloro-1-propene
	1-Propene, 1,1,2,3,3,3-hexachloro-
	1-Propene, hexachloro-
	Hexachloropropylene
	NSC 7297
	Perchloropropene
	Perchloropropylene
	Propene, hexachloro-
	Rcra waste number U243
Inchi:	InChI=1S/C3Cl6/c4-1(2(5)6)3(7,8)9
InchiKey:	VFDYKPARTDCDCU-UHFFFAOYSA-N
Formula:	C3Cl6
SMILES:	ClC(Cl)=C(Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	248.75
CAS:	1888-71-7

Physical Properties

Property code	Value	Unit	Source
gf	-31.24	kJ/mol	Joback Method
hf	-110.80	kJ/mol	Joback Method
hfus	18.88	kJ/mol	Joback Method
hvap	54.80 ± 0.40	kJ/mol	NIST Webbook
log10ws	-4.44		Crippen Method
logp	4.242		Crippen Method
mcvol	122.270	ml/mol	McGowan Method
pc	2500.00 ± 200.00	kPa	NIST Webbook
rhoc	485.06 ± 14.92	kg/m3	NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	203.65		NIST Webbook
rinpol	203.60		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	203.65		NIST Webbook
tb	484.80 ± 0.80	K	NIST Webbook
tb	482.70	K	NIST Webbook
tc	680.00 ± 5.00	K	NIST Webbook
tf	272.51	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.42	J/mol×K	700.24	Joback Method
cpg	171.04	J/mol×K	493.31	Joback Method
cpg	175.11	J/mol×K	534.70	Joback Method
cpg	178.49	J/mol×K	576.08	Joback Method
cpg	181.28	J/mol×K	617.47	Joback Method
cpg	183.56	J/mol×K	658.85	Joback Method
cpg	186.94	J/mol×K	741.63	Joback Method
hvapt	49.30	kJ/mol	461.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46815e+01
Coeff. B	-4.17631e+03
Coeff. C	-6.76880e+01
Temperature range (K), min.	357.83
Temperature range (K), max.	513.40

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1888717&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
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
rhoc:	Critical density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume