1-Propene, 1,2,3-trichloro-

Other names:	1,2,3-Trichloro-1-propene
	1,2,3-Trichloropropene
	2,3-Dichloroallyl chloride
	NSC 164001
	Propene, 1,2,3-trichloro-
Inchi:	InChI=1S/C3H3Cl3/c4-1-3(6)2-5/h1H,2H2
InchiKey:	HIILBTHBHCLUER-UHFFFAOYSA-N
Formula:	C3H3Cl3
SMILES:	ClC=C(Cl)CCl
Mol. weight [g/mol]:	145.41
CAS:	96-19-5

Physical Properties

Property code	Value	Unit	Source
chl	-1578.40	kJ/mol	NIST Webbook
gf	10.26	kJ/mol	Joback Method
hf	-45.04	kJ/mol	Joback Method
hfl	-102.00	kJ/mol	NIST Webbook
hfus	15.01	kJ/mol	Joback Method
hvap	35.47	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.544		Crippen Method
mcvol	85.550	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
tb	384.37	K	Joback Method
tc	590.66	K	Joback Method
tf	194.29	K	Joback Method
vc	0.332	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.82	J/mol×K	384.37	Joback Method
cpg	119.89	J/mol×K	418.75	Joback Method

cpg	124.59	J/mol×K	453.13	Joback Method
cpg	128.93	J/mol×K	487.51	Joback Method
cpg	132.94	J/mol×K	521.89	Joback Method
cpg	136.65	J/mol×K	556.28	Joback Method
cpg	140.07	J/mol×K	590.66	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63040e+01
Coeff. B	-3.96500e+03
Coeff. C	-5.65620e+01
Temperature range (K), min.	304.12
Temperature range (K), max.	442.88

Sources

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=C96195&Units=SI

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

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

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