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

Other names:	1,1,3-Trichloro-1-propene
	1,1,3-Trichloropropene
	1,3,3-Trichloro-2-propene
	3,3-Dichloroallyl chloride
	Propene, 1,1,3-trichloro-
Inchi:	InChI=1S/C3H3Cl3/c4-2-1-3(5)6/h1H,2H2
InchiKey:	JFEVIPGMXQNRRF-UHFFFAOYSA-N
Formula:	C3H3Cl3
SMILES:	ClCC=C(Cl)Cl
Mol. weight [g/mol]:	145.41
CAS:	2567-14-8

Physical Properties

Property code	Value	Unit	Source
gf	10.26	kJ/mol	Joback Method
hf	-45.04	kJ/mol	Joback Method
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
rinpol	840.00		NIST Webbook
rinpol	840.00		NIST Webbook
tb	404.70	K	NIST Webbook
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	1.42428e+01
Coeff. B	-3.37859e+03
Coeff. C	-5.36570e+01
Temperature range (K), min.	295.76
Temperature range (K), max.	431.94

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2567148&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume