1-Propene, 1,1-dichloro-

Other names: 1,1-Dichloro-1-propene
1,1-Dichloropropene
1,1-Dichloropropylene
Propene, 1,1-dichloro-
Inchi: InChI=1S/C3H4Cl2/c1-2-3(4)5/h2H,1H3
InchiKey: ZAIDIVBQUMFXEC-UHFFFAOYSA-N
Formula: C3H4Cl2
SMILES: CC=C(Cl)Cl
Mol. weight [g/mol]: 110.97
CAS: 563-58-6

Physical Properties

Property code	Value	Unit	Source
gf	22.19	kJ/mol	Joback Method
hf	-29.30	kJ/mol	Joback Method
hfus	10.81	kJ/mol	Joback Method
hvap	31.08	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.325		Crippen Method
mcvol	73.310	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
rinpol	642.00		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	642.00		NIST Webbook
tb	349.70	K	NIST Webbook
tc	543.75	K	Joback Method
tf	164.37	K	Joback Method
vc	0.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	95.67	J/mol×K	346.94	Joback Method
cpg	101.09	J/mol×K	379.74	Joback Method

cpg	106.16	J/mol×K	412.54	Joback Method
cpg	110.90	J/mol×K	445.35	Joback Method
cpg	115.33	J/mol×K	478.15	Joback Method
cpg	119.47	J/mol×K	510.95	Joback Method
cpg	123.34	J/mol×K	543.75	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51080e+01
Coeff. B	-3.26594e+03
Coeff. C	-3.83530e+01
Temperature range (K), min.	258.72
Temperature range (K), max.	371.73

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
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535
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=C563586&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
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