1-Propene, 1-chloro-2-methyl-

Other names:	1-Chloro-2-methyl-1-propene
	1-Chloro-2-methylpropene
	1-Chloroisobutylene
	2,2-Dimethylvinyl chloride
	2-Methyl-1-chloropropene
	2-Methyl-1-propenyl chloride
	Dimethylvinylchloride
	Isocrotyl chloride
	NCI-C54819
	Propene, 1-chloro-2-methyl-
	«alpha»-Chloroisobutylene
	«beta»,«beta»-Dimethylvinyl chloride
	Â«alphaÂ»-Chloroisobutylene
	Â«betaÂ»,Â«betaÂ»-Dimethylvinyl chloride
Inchi:	InChI=1S/C4H7Cl/c1-4(2)3-5/h3H,1-2H3
InchiKey:	KWISWUFGPUHDRY-UHFFFAOYSA-N
Formula:	C4H7Cl
SMILES:	CC(C)=CCl
Mol. weight [g/mol]:	90.55
CAS:	513-37-1

Physical Properties

Property code	Value	Unit	Source
gf	42.54	kJ/mol	Joback Method
hf	-34.20	kJ/mol	Joback Method
hfus	9.21	kJ/mol	Joback Method
hvap	28.92	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	2.149		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
rinpol	601.00		NIST Webbook
tb	341.25 ± 1.00	K	NIST Webbook
tb	341.15 ± 2.00	K	NIST Webbook
tb	341.20	K	NIST Webbook
tc	518.49	K	Joback Method
tf	145.72	K	Joback Method

vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.99	J/mol×K	487.47	Joback Method
cpg	105.03	J/mol×K	332.39	Joback Method
cpg	112.34	J/mol×K	363.41	Joback Method
cpg	119.28	J/mol×K	394.42	Joback Method
cpg	125.86	J/mol×K	425.44	Joback Method
cpg	132.09	J/mol×K	456.45	Joback Method
cpg	143.59	J/mol×K	518.49	Joback Method
hvapt	33.20	kJ/mol	314.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.32574e+01
Coeff. B	-2.22725e+03
Coeff. C	-8.33900e+01
Temperature range (K), min.	255.12
Temperature range (K), max.	363.76

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=C513371&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume