2-Butene, 1-chloro-3-methyl-

Other names:	1-Chloro-3-methyl-2-butene
	1-chloro-3-methylbut-2-ene
	3,3-Dimethylallyl chloride
	3-Methyl-2-butenyl chloride
	3-Methylcrotyl chloride
	Isoprenyl chloride
	Prenyl chloride
	«gamma»,«gamma»-Dimethylallyl chloride
	Â«gammaÂ»,Â«gammaÂ»-Dimethylallyl chloride
Inchi:	InChI=1S/C5H9Cl/c1-5(2)3-4-6/h3H,4H2,1-2H3
InchiKey:	JKXQKGNGJVZKFA-UHFFFAOYSA-N
Formula:	C5H9Cl
SMILES:	CC(C)=CCCl
Mol. weight [g/mol]:	104.58
CAS:	503-60-6

Physical Properties

Property code	Value	Unit	Source
gf	50.96	kJ/mol	Joback Method
hf	-54.84	kJ/mol	Joback Method
hfus	11.79	kJ/mol	Joback Method
hvap	31.15	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	2.191		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
rinpol	760.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	726.00		NIST Webbook
tb	382.20	K	NIST Webbook
tc	541.10	K	Joback Method
tf	156.99	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.97	J/mol×K	355.27	Joback Method
cpg	145.84	J/mol×K	386.24	Joback Method
cpg	154.27	J/mol×K	417.21	Joback Method
cpg	162.28	J/mol×K	448.19	Joback Method
cpg	169.87	J/mol×K	479.16	Joback Method
cpg	177.09	J/mol×K	510.13	Joback Method
cpg	183.93	J/mol×K	541.10	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	331.70	K	16.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51195e+01
Coeff. B	-3.51300e+03
Coeff. C	-4.76660e+01
Temperature range (K), min.	284.52
Temperature range (K), max.	405.84

Sources

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=C503606&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume