1-Propene, 3-chloro-2-methyl-

Other names:	1-Chloro-2-methyl-2-propene
	2-Methallyl chloride
	2-Methyl-2-propenyl chloride
	2-Methyl-allylchlorid
	2-Methylallyl chloride
	3-Chlor-2-methyl-prop-1-en
	3-Chloro-2-methyl-1-propene
	3-Chloro-2-methylpropene
	3-Chloro-2-methylpropene-1
	3-Cloro-2-metil-prop-1-ene
	Chlorure de methallyle
	Cloruro di metallile
	Isobutenyl chloride
	Methallyl chloride
	Methylallyl chloride
	NCI-C54820
	NSC 7303
	Propene, 3-chloro-2-methyl-
	UN 2554
	«beta»-Methallyl chloride
	«beta»-Methylallyl chloride
	«gamma»-Chloroisobutylene
	Â«betaÂ»-Methallyl chloride
	Â«betaÂ»-Methylallyl chloride
	Â«gammaÂ»-Chloroisobutylene
Inchi:	InChI=1S/C4H7Cl/c1-4(2)3-5/h1,3H2,2H3
InchiKey:	OHXAOPZTJOUYKM-UHFFFAOYSA-N
Formula:	C4H7Cl
SMILES:	C=C(C)CCl
Mol. weight [g/mol]:	90.55
CAS:	563-47-3

Physical Properties

Property code	Value	Unit	Source
gf	50.16	kJ/mol	Joback Method
hf	-25.99	kJ/mol	Joback Method

hfus	7.72	kJ/mol	Joback Method
hvap	28.29	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.801		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
rinpol	626.00		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	598.00		NIST Webbook
rinpol	598.00		NIST Webbook
tb	344.10 ± 0.70	K	NIST Webbook
tb	345.25 ± 0.70	K	NIST Webbook
tb	344.70	K	NIST Webbook
tb	345.55 ± 0.60	K	NIST Webbook
tb	431.00 ± 5.00	K	NIST Webbook
tc	504.71	K	Joback Method
tf	194.50 ± 5.00	K	NIST Webbook
vc	0.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.32	J/mol×K	474.75	Joback Method
cpg	106.79	J/mol×K	324.91	Joback Method
cpg	113.69	J/mol×K	354.88	Joback Method
cpg	120.28	J/mol×K	384.84	Joback Method
cpg	126.57	J/mol×K	414.81	Joback Method
cpg	132.58	J/mol×K	444.78	Joback Method
cpg	143.79	J/mol×K	504.71	Joback Method
hvapt	33.30	kJ/mol	316.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40704e+01
Coeff. B	-2.80114e+03

Coeff. C	-4.83490e+01
Temperature range (K), min.	251.58
Temperature range (K), max.	369.03

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=C563473&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
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