1-Butene, 3-chloro-

Other names:	1-METHYLALLYL CHLORIDE
	2-Chloro-3-butene
	3-CHLORO-1-BUTENE
	3-chlorobut-1-ene
	ALPHA-METHALLYL CHLORIDE
	«alpha»-Methallyl chloride
	«alpha»-Methylallyl chloride
	«gamma»-Chloro-«alpha»-butylene
	Â«alphaÂ»-Methallyl chloride
	Â«alphaÂ»-Methylallyl chloride
	Â«gammaÂ»-Chloro-Â«alphaÂ»-butylene
Inchi:	InChI=1S/C4H7Cl/c1-3-4(2)5/h3-4H,1H2,2H3
InchiKey:	VZGLVCFVUREVDP-UHFFFAOYSA-N
Formula:	C4H7Cl
SMILES:	C=CC(C)Cl
Mol. weight [g/mol]:	90.55
CAS:	563-52-0

Physical Properties

Property code	Value	Unit	Source
gf	56.27	kJ/mol	Joback Method
hf	-45.61	kJ/mol	NIST Webbook
hfus	5.51	kJ/mol	Joback Method
hvap	27.83	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.800		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
rinpol	576.00		NIST Webbook
tb	324.59	K	Joback Method
tc	505.07	K	Joback Method
tf	148.00	K	Joback Method
vc	0.283	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	106.50	J/mol×K	324.59	Joback Method
cpg	113.56	J/mol×K	354.67	Joback Method
cpg	120.31	J/mol×K	384.75	Joback Method
cpg	126.76	J/mol×K	414.83	Joback Method
cpg	132.91	J/mol×K	444.91	Joback Method
cpg	138.77	J/mol×K	474.99	Joback Method
cpg	144.37	J/mol×K	505.07	Joback Method
dvisc	0.0054737	Pa×s	148.00	Joback Method
dvisc	0.0021566	Pa×s	177.43	Joback Method
dvisc	0.0011075	Pa×s	206.86	Joback Method
dvisc	0.0006715	Pa×s	236.30	Joback Method
dvisc	0.0004548	Pa×s	265.73	Joback Method
dvisc	0.0003330	Pa×s	295.16	Joback Method
dvisc	0.0002580	Pa×s	324.59	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43521e+01
Coeff. B	-2.99395e+03
Coeff. C	-2.94150e+01
Temperature range (K), min.	242.29
Temperature range (K), max.	360.78

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1754

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C563520&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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