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

Other names: 2-Chloro-3-methyl-1-butene
CH2=C(Cl)CH(CH3)2
Inchi: InChI=1S/C5H9Cl/c1-4(2)5(3)6/h4H,3H2,1-2H3
InchiKey: RBSYGFLXVMWYGD-UHFFFAOYSA-N
Formula: C5H9Cl
SMILES: C=C(Cl)C(C)C
Mol. weight [g/mol]: 104.58
CAS: 17773-64-7

Physical Properties

Property code	Value	Unit	Source
gf	56.14	kJ/mol	Joback Method
hf	-51.91	kJ/mol	Joback Method
hfus	6.79	kJ/mol	Joback Method
hvap	30.13	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.395		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
rinpol	626.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	626.00		NIST Webbook
tb	347.35	K	Joback Method
tc	531.71	K	Joback Method
tf	145.31	K	Joback Method
vc	0.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.98	J/mol×K	347.35	Joback Method
cpg	146.76	J/mol×K	378.08	Joback Method
cpg	155.15	J/mol×K	408.80	Joback Method
cpg	163.16	J/mol×K	439.53	Joback Method

cpg	170.79	J/mol×K	470.26	Joback Method
cpg	178.07	J/mol×K	500.99	Joback Method
cpg	185.00	J/mol×K	531.71	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36588e+01
Coeff. B	-3.02744e+03
Coeff. C	-4.21060e+01
Temperature range (K), min.	268.52
Temperature range (K), max.	404.79

Sources

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=C17773647&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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