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

Other names: 3-Chloro-2-methyl-1-butene
Inchi: InChI=1S/C5H9Cl/c1-4(2)5(3)6/h5H,1H2,2-3H3
InchiKey: UCUDJURUNUQAHQ-UHFFFAOYSA-N
Formula: C5H9Cl
SMILES: C=C(C)C(C)Cl
Mol. weight [g/mol]: 104.58
CAS: 5166-35-8

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	-2.03		Crippen Method
logp	2.190		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
rinpol	691.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	657.00		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	1.40010e+01
Coeff. B	-3.13211e+03
Coeff. C	-4.31620e+01
Temperature range (K), min.	271.56
Temperature range (K), max.	403.61

Sources

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=1757

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5166358&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

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