1-Butene, 4-chloro-2-methyl-

Other names: 4-Chloro-2-methyl-1-butene
Inchi: InChI=1S/C5H9Cl/c1-5(2)3-4-6/h1,3-4H2,2H3
InchiKey: LGMPVUDVTHHFDR-UHFFFAOYSA-N
Formula: C5H9Cl
SMILES: C=C(C)CCCl
Mol. weight [g/mol]: 104.58
CAS: 10523-96-3

Physical Properties

Property code	Value	Unit	Source
gf	58.58	kJ/mol	Joback Method
hf	-46.63	kJ/mol	Joback Method
hfus	10.31	kJ/mol	Joback Method
hvap	30.52	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	2.191		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
rinpol	694.00		NIST Webbook
rinpol	696.00		NIST Webbook
rinpol	694.00		NIST Webbook
tb	347.79	K	Joback Method
tc	527.66	K	Joback Method
tf	160.31	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.14	J/mol×K	347.79	Joback Method
cpg	146.61	J/mol×K	377.77	Joback Method
cpg	154.71	J/mol×K	407.75	Joback Method
cpg	162.44	J/mol×K	437.72	Joback Method
cpg	169.84	J/mol×K	467.70	Joback Method

cpg	176.89	J/mol×K	497.68	Joback Method
cpg	183.63	J/mol×K	527.66	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48111e+01
Coeff. B	-3.37931e+03
Coeff. C	-4.54420e+01
Temperature range (K), min.	278.12
Temperature range (K), max.	401.17

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=C10523963&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume