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

Other names:	1-Chloro-2-methyl-2-butene
Inchi:	InChI=1S/C5H9Cl/c1-3-5(2)4-6/h3H,4H2,1-2H3/b5-3+
InchiKey:	ZAJKEDQTROWDDD-HWKANZROSA-N
Formula:	C5H9Cl
SMILES:	CC=C(C)CCl
Mol. weight [g/mol]:	104.58
CAS:	13417-43-1

Physical Properties

Property code	Value	Unit	Source
gf	50.96	kJ/mol	Joback Method
hf	-54.84	kJ/mol	Joback Method
hfus	11.79	kJ/mol	Joback Method
hvap	31.15	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	2.191		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
rinpol	755.00		NIST Webbook
tb	355.27	K	Joback Method
tc	541.10	K	Joback Method
tf	156.99	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.97	J/mol×K	355.27	Joback Method
cpg	145.84	J/mol×K	386.24	Joback Method
cpg	154.27	J/mol×K	417.21	Joback Method
cpg	162.28	J/mol×K	448.19	Joback Method
cpg	169.87	J/mol×K	479.16	Joback Method
cpg	177.09	J/mol×K	510.13	Joback Method
cpg	183.93	J/mol×K	541.10	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57122e+01
Coeff. B	-3.65339e+03
Coeff. C	-4.76660e+01
Temperature range (K), min.	284.52
Temperature range (K), max.	398.93

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=C13417431&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

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