

1-Butene, 4-chloro-3-methyl-

Other names:	4-Chloro-3-methyl-1-butene
Inchi:	InChI=1S/C5H9Cl/c1-3-5(2)4-6/h3,5H,1,4H2,2H3
InchiKey:	ZFXHRKNMXMGZNU-UHFFFAOYSA-N
Formula:	C5H9Cl
SMILES:	C=CC(C)CCl
Mol. weight [g/mol]:	104.58
CAS:	10524-01-3

Physical Properties

Property code	Value	Unit	Source
gf	64.69	kJ/mol	Joback Method
hf	-42.12	kJ/mol	Joback Method
hfus	8.10	kJ/mol	Joback Method
hvap	30.05	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	2.047		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
rinpol	664.00		NIST Webbook
rinpol	667.00		NIST Webbook
tb	347.47	K	Joback Method
tc	528.00	K	Joback Method
tf	159.27	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.93	J/molxK	347.47	Joback Method
cpg	146.57	J/molxK	377.56	Joback Method
cpg	154.83	J/molxK	407.65	Joback Method
cpg	162.72	J/molxK	437.74	Joback Method
cpg	170.25	J/molxK	467.83	Joback Method
cpg	177.44	J/molxK	497.91	Joback Method

cpg	184.29	J/mol×K	528.00	Joback Method
dvisc	0.0062892	Paxs	159.27	Joback Method
dvisc	0.0024182	Paxs	190.64	Joback Method
dvisc	0.0012181	Paxs	222.00	Joback Method
dvisc	0.0007271	Paxs	253.37	Joback Method
dvisc	0.0004863	Paxs	284.74	Joback Method
dvisc	0.0003523	Paxs	316.10	Joback Method
dvisc	0.0002705	Paxs	347.47	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38365e+01
Coeff. B	-3.08181e+03
Coeff. C	-4.26620e+01
Temperature range (K), min.	270.12
Temperature range (K), max.	404.16

Sources

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=C10524013&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/ci9903071

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

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