Butane, 2-chloro-3-methyl-

Other names: (+/-)-2-Chloro-3-methyl-butane
2-Chloro-3-methylbutane
Inchi: InChI=1S/C5H11Cl/c1-4(2)5(3)6/h4-5H,1-3H3
InchiKey: JMTRCXPSDMMAGM-UHFFFAOYSA-N
Formula: C5H11Cl
SMILES: CC(C)C(C)Cl
Mol. weight [g/mol]: 106.59
CAS: 631-65-2

Physical Properties

Property code	Value	Unit	Source
gf	-25.59	kJ/mol	Joback Method
hf	-172.83	kJ/mol	Joback Method
hfus	5.86	kJ/mol	Joback Method
hvap	30.33	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	2.270		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
rinpol	672.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	662.00		NIST Webbook
rinpol	668.00		NIST Webbook
tb	366.15 ± 1.00	K	NIST Webbook
tc	531.42	K	Joback Method
tf	146.03	K	Joback Method
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.02	J/mol×K	531.42	Joback Method
cpg	195.21	J/mol×K	501.24	Joback Method
cpg	187.07	J/mol×K	471.06	Joback Method

cpg	178.56	J/mol×K	440.88	Joback Method
cpg	169.69	J/mol×K	410.71	Joback Method
cpg	160.45	J/mol×K	380.53	Joback Method
cpg	150.82	J/mol×K	350.35	Joback Method
dvisc	0.0167571	Pa×s	146.03	Joback Method
dvisc	0.0002760	Pa×s	350.35	Joback Method
dvisc	0.0003785	Pa×s	316.30	Joback Method
dvisc	0.0005603	Pa×s	282.24	Joback Method
dvisc	0.0009237	Pa×s	248.19	Joback Method
dvisc	0.0017850	Pa×s	214.14	Joback Method
dvisc	0.0044255	Pa×s	180.08	Joback Method
hvapt	35.90	kJ/mol	345.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54405e+01
Coeff. B	-3.49844e+03
Coeff. C	-4.28840e+01
Temperature range (K), min.	273.76
Temperature range (K), max.	388.27

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=C631652&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

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
hvapt:	Enthalpy of vaporization at a given temperature
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