Butane, 1-chloro-2-methyl-

Other names: (dl) 1-chloro-2-methylbutane
1-Chloro-2-methylbutane
Inchi: InChI=1S/C5H11Cl/c1-3-5(2)4-6/h5H,3-4H2,1-2H3
InchiKey: IWAKWOFEHSYKSI-UHFFFAOYSA-N
Formula: C5H11Cl
SMILES: CCC(C)CCl
Mol. weight [g/mol]: 106.59
CAS: 616-13-7

Physical Properties

Property code	Value	Unit	Source
gf	-23.15	kJ/mol	Joback Method
hf	-167.55	kJ/mol	Joback Method
hfus	9.38	kJ/mol	Joback Method
hvap	30.72	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	2.271		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
rinpol	718.00		NIST Webbook
rinpol	696.00		NIST Webbook
rinpol	699.00		NIST Webbook
ripol	898.00		NIST Webbook
ripol	900.00		NIST Webbook
ripol	891.00		NIST Webbook
tb	370.35 ± 3.00	K	NIST Webbook
tb	373.05 ± 0.60	K	NIST Webbook
tb	373.15 ± 0.60	K	NIST Webbook
tc	527.49	K	Joback Method
tf	161.03	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.54	J/mol×K	527.49	Joback Method
cpg	150.99	J/mol×K	350.79	Joback Method
cpg	160.28	J/mol×K	380.24	Joback Method
cpg	169.22	J/mol×K	409.69	Joback Method
cpg	177.80	J/mol×K	439.14	Joback Method
cpg	186.05	J/mol×K	468.59	Joback Method
cpg	193.96	J/mol×K	498.04	Joback Method
dvisc	0.0002823	Pa×s	350.79	Joback Method
dvisc	0.0078623	Pa×s	161.03	Joback Method
dvisc	0.0028647	Pa×s	192.66	Joback Method
dvisc	0.0013876	Pa×s	224.28	Joback Method
dvisc	0.0008040	Pa×s	255.91	Joback Method
dvisc	0.0005253	Pa×s	287.54	Joback Method
dvisc	0.0003734	Pa×s	319.16	Joback Method
hvapt	35.40	kJ/mol	337.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55462e+01
Coeff. B	-3.58448e+03
Coeff. C	-4.50360e+01
Temperature range (K), min.	279.95
Temperature range (K), max.	395.26

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=C616137&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume