Butane, 1-chloro-2,3-dimethyl

Other names: 1-chloro-2,3-dimethylbutane
Inchi: InChI=1S/C6H13Cl/c1-5(2)6(3)4-7/h5-6H,4H2,1-3H3
InchiKey: UMJSXTUELCDYKZ-UHFFFAOYSA-N
Formula: C6H13Cl
SMILES: CC(C)C(C)CCl
Mol. weight [g/mol]: 120.62
CAS: 600-06-6

Physical Properties

Property code	Value	Unit	Source
gf	-17.17	kJ/mol	Joback Method
hf	-193.47	kJ/mol	Joback Method
hfus	8.45	kJ/mol	Joback Method
hvap	32.56	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	2.517		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
rinpol	787.00		NIST Webbook
rinpol	787.00		NIST Webbook
tb	397.15 ± 4.00	K	NIST Webbook
tc	553.82	K	Joback Method
tf	157.30	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.75	J/mol×K	373.23	Joback Method
cpg	196.81	J/mol×K	403.33	Joback Method
cpg	207.42	J/mol×K	433.43	Joback Method
cpg	217.60	J/mol×K	463.52	Joback Method
cpg	227.35	J/mol×K	493.62	Joback Method
cpg	236.69	J/mol×K	523.72	Joback Method

cpg	245.63	J/mol×K	553.82	Joback Method
dvisc	0.0170744	Pa×s	157.30	Joback Method
dvisc	0.0045226	Pa×s	193.29	Joback Method
dvisc	0.0018178	Pa×s	229.28	Joback Method
dvisc	0.0009357	Pa×s	265.26	Joback Method
dvisc	0.0005644	Pa×s	301.25	Joback Method
dvisc	0.0003793	Pa×s	337.24	Joback Method
dvisc	0.0002752	Pa×s	373.23	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52598e+01
Coeff. B	-3.68493e+03
Coeff. C	-5.10020e+01
Temperature range (K), min.	297.12
Temperature range (K), max.	421.41

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=C600066&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
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