Butane, 2-chloro-2,3-dimethyl-

Other names: 2-Chloro-2,3-dimethylbutane
Inchi: InChI=1S/C6H13Cl/c1-5(2)6(3,4)7/h5H,1-4H3
InchiKey: HEMQRALQJLCVBR-UHFFFAOYSA-N
Formula: C6H13Cl
SMILES: CC(C)C(C)(C)Cl
Mol. weight [g/mol]: 120.62
CAS: 594-57-0

Physical Properties

Property code	Value	Unit	Source
gf	-11.89	kJ/mol	Joback Method
hf	-196.94	kJ/mol	Joback Method
hfl	-262.00 ± 2.00	kJ/mol	NIST Webbook
hfus	4.56	kJ/mol	Joback Method
hvap	31.65	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.660		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
rinpol	830.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	831.00		NIST Webbook
ripol	916.00		NIST Webbook
ripol	927.00		NIST Webbook
ripol	919.00		NIST Webbook
tb	385.15 ± 1.50	K	NIST Webbook
tb	385.20	K	NIST Webbook
tb	382.65 ± 3.00	K	NIST Webbook
tb	381.65 ± 1.50	K	NIST Webbook
tc	558.94	K	Joback Method
tf	174.72	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.87	J/mol×K	370.44	Joback Method
cpg	199.15	J/mol×K	401.86	Joback Method
cpg	210.77	J/mol×K	433.27	Joback Method
cpg	221.78	J/mol×K	464.69	Joback Method
cpg	232.19	J/mol×K	496.11	Joback Method
cpg	242.02	J/mol×K	527.53	Joback Method
cpg	251.32	J/mol×K	558.94	Joback Method
dvisc	0.0179295	Pa×s	174.72	Joback Method
dvisc	0.0054373	Pa×s	207.34	Joback Method
dvisc	0.0022808	Pa×s	239.96	Joback Method
dvisc	0.0011778	Pa×s	272.58	Joback Method
dvisc	0.0007005	Pa×s	305.20	Joback Method
dvisc	0.0004606	Pa×s	337.82	Joback Method
dvisc	0.0003261	Pa×s	370.44	Joback Method
hvapt	38.00	kJ/mol	363.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54766e+01
Coeff. B	-3.65901e+03
Coeff. C	-4.82220e+01
Temperature range (K), min.	262.75
Temperature range (K), max.	408.18

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C594570&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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

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