Butane, 2-chloro-2-methyl-

Other names:	1,1-DIMETHYLPROPYL CHLORIDE
	2-Chloro-2-methylbutane
	2-Methyl-2-chlorobutane
	TERT-AMYL CHLORIDE
	TERT-PENTYL CHLORIDE
	Tertiary pentyl chloride
Inchi:	InChI=1S/C5H11Cl/c1-4-5(2,3)6/h4H2,1-3H3
InchiKey:	CRNIHJHMEQZAAS-UHFFFAOYSA-N
Formula:	C5H11Cl
SMILES:	CCC(C)(C)Cl
Mol. weight [g/mol]:	106.59
CAS:	594-36-5

Physical Properties

Property code	Value	Unit	Source
chl	-3327.50 ± 8.40	kJ/mol	NIST Webbook
gf	-17.87	kJ/mol	Joback Method
hf	-171.02	kJ/mol	Joback Method
hfl	-235.00 ± 2.00	kJ/mol	NIST Webbook
hfus	5.49	kJ/mol	Joback Method
hvap	29.81	kJ/mol	Joback Method
log10ws	-2.51		Aqueous Solubility Prediction Method
log10ws	-2.51		Estimated Solubility Method
logp	2.414		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
rinpol	657.00		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	647.88		NIST Webbook
rinpol	657.00		NIST Webbook

rinpol	648.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	647.89		NIST Webbook
ripol	826.00		NIST Webbook
ripol	837.00		NIST Webbook
ripol	849.00		NIST Webbook
tb	358.75 ± 0.50	K	NIST Webbook
tb	358.15 ± 2.00	K	NIST Webbook
tb	358.00 ± 2.00	K	NIST Webbook
tb	358.80	K	NIST Webbook
tb	358.80 ± 0.20	K	NIST Webbook
tc	532.51	K	Joback Method
tf	200.45 ± 0.50	K	NIST Webbook
tf	200.00 ± 5.00	K	NIST Webbook
tf	199.77	K	Aqueous Solubility Prediction Method
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.01	J/mol×K	501.76	Joback Method
cpg	190.56	J/mol×K	471.01	Joback Method
cpg	181.62	J/mol×K	440.25	Joback Method
cpg	172.18	J/mol×K	409.50	Joback Method
cpg	162.20	J/mol×K	378.75	Joback Method
cpg	151.66	J/mol×K	348.00	Joback Method
cpg	207.00	J/mol×K	532.51	Joback Method
dvisc	0.0090043	Pa×s	178.45	Joback Method
dvisc	0.0003465	Pa×s	348.00	Joback Method
dvisc	0.0004692	Pa×s	319.74	Joback Method
dvisc	0.0006737	Pa×s	291.48	Joback Method
dvisc	0.0010454	Pa×s	263.23	Joback Method
dvisc	0.0018032	Pa×s	234.97	Joback Method
dvisc	0.0036100	Pa×s	206.71	Joback Method
hvapt	35.00	kJ/mol	338.00	NIST Webbook
hvapt	33.50 ± 0.84	kJ/mol	356.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54520e+01
Coeff. B	-3.44417e+03
Coeff. C	-4.08850e+01
Temperature range (K), min.	268.01
Temperature range (K), max.	380.53

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.20848e+01
Coeff. B	-6.87078e+03
Coeff. C	-1.00577e+01
Coeff. D	6.64130e-06
Temperature range (K), min.	280.15
Temperature range (K), max.	548.97

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C594365&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

KDB: https://www.cheric.org/files/research/kdb/mol/mol1623.mol

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1623

Joback Method: https://en.wikipedia.org/wiki/Joback_method

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl:	Standard liquid enthalpy of combustion
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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