Butane, 1-chloro-3,3-dimethyl-

Other names:	1-Chloro-3,3-dimethylbutane
	Neohexyl chloride
Inchi:	InChI=1S/C6H13Cl/c1-6(2,3)4-5-7/h4-5H2,1-3H3
InchiKey:	XGCKOSFYXBAPQM-UHFFFAOYSA-N
Formula:	C6H13Cl
SMILES:	CC(C)(C)CCCl
Mol. weight [g/mol]:	120.62
CAS:	2855-08-5

Physical Properties

Property code	Value	Unit	Source
gf	-9.45	kJ/mol	Joback Method
hf	-191.66	kJ/mol	Joback Method
hfus	8.08	kJ/mol	Joback Method
hvap	32.04	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.661		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	832.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	841.00		NIST Webbook
ripol	936.00		NIST Webbook
ripol	945.00		NIST Webbook
ripol	936.00		NIST Webbook
ripol	936.00		NIST Webbook
tb	388.20	K	NIST Webbook
tb	388.15 ± 3.00	K	NIST Webbook
tb	390.65 ± 3.00	K	NIST Webbook
tb	391.15 ± 3.00	K	NIST Webbook
tc	554.85	K	Joback Method
tf	189.72	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.00	J/mol×K	370.88	Joback Method
cpg	198.88	J/mol×K	401.54	Joback Method
cpg	210.15	J/mol×K	432.20	Joback Method
cpg	220.83	J/mol×K	462.87	Joback Method
cpg	230.95	J/mol×K	493.53	Joback Method
cpg	240.54	J/mol×K	524.19	Joback Method
cpg	249.61	J/mol×K	554.85	Joback Method
dvisc	0.0092209	Pa×s	189.72	Joback Method
dvisc	0.0036325	Pa×s	219.91	Joback Method
dvisc	0.0017919	Pa×s	250.11	Joback Method
dvisc	0.0010293	Pa×s	280.30	Joback Method
dvisc	0.0006585	Pa×s	310.49	Joback Method
dvisc	0.0004561	Pa×s	340.69	Joback Method
dvisc	0.0003353	Pa×s	370.88	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	314.20	K	6.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57097e+01
Coeff. B	-3.75542e+03
Coeff. C	-4.96120e+01
Temperature range (K), min.	293.12
Temperature range (K), max.	410.77

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=C2855085&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume