

Butane, 1-chloro-2,2-dimethyl

Inchi:	InChI=1S/C6H13Cl/c1-4-6(2,3)5-7/h4-5H2,1-3H3
InchiKey:	JRUIYWSZTLWHME-UHFFFAOYSA-N
Formula:	C6H13Cl
SMILES:	CCC(C)(C)CCl
Mol. weight [g/mol]:	120.62

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
mvol	107.640	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	773.00		NIST Webbook
rinpol	773.00		NIST Webbook
tb	370.88	K	Joback Method
tc	554.85	K	Joback Method
tf	189.72	K	Joback Method
vc	0.409	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.00	J/molxK	370.88	Joback Method
cpg	198.88	J/molxK	401.54	Joback Method
cpg	210.15	J/molxK	432.20	Joback Method
cpg	220.83	J/molxK	462.87	Joback Method
cpg	230.95	J/molxK	493.53	Joback Method
cpg	240.54	J/molxK	524.19	Joback Method
cpg	249.61	J/molxK	554.85	Joback Method
dvisc	0.0092209	Paxs	189.72	Joback Method

dvisc	0.0036325	Paxs	219.91	Joback Method
dvisc	0.0017919	Paxs	250.11	Joback Method
dvisc	0.0010293	Paxs	280.30	Joback Method
dvisc	0.0006585	Paxs	310.49	Joback Method
dvisc	0.0004561	Paxs	340.69	Joback Method
dvisc	0.0003353	Paxs	370.88	Joback Method

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=R129687&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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