Butane, 2-chloro-3,3-dimethyl

Other names: (dl) 2-chloro-3,3-dimethylbutane
Inchi: InChI=1S/C6H13Cl/c1-5(7)6(2,3)4/h5H,1-4H3
InchiKey: COVFMDKBWYLRSV-UHFFFAOYSA-N
Formula: C6H13Cl
SMILES: CC(Cl)C(C)(C)C
Mol. weight [g/mol]: 120.62
CAS: 5750-00-5

Physical Properties

Property code	Value	Unit	Source
gf	-11.89	kJ/mol	Joback Method
hf	-196.94	kJ/mol	Joback Method
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	752.00		NIST Webbook
rinpol	752.00		NIST Webbook
tb	371.00 ± 4.00	K	NIST Webbook
tb	383.15 ± 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	362.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5750005&Units=SI
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
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume