Butane, 1,1-dichloro-3,3-dimethyl-

Other names: 1,1-dichloro-3,3-dimethylbutane
Inchi: InChI=1S/C6H12Cl2/c1-6(2,3)4-5(7)8/h5H,4H2,1-3H3
InchiKey: BLRPQFOUUPCTED-UHFFFAOYSA-N
Formula: C6H12Cl2
SMILES: CC(C)(C)CC(Cl)Cl
Mol. weight [g/mol]: 155.06
CAS: 6130-96-7

Physical Properties

Property code	Value	Unit	Source
gf	-23.82	kJ/mol	Joback Method
hf	-212.68	kJ/mol	Joback Method
hfus	8.75	kJ/mol	Joback Method
hvap	36.04	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	3.226		Crippen Method
mcvol	119.880	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
rinpol	871.00		NIST Webbook
rinpol	871.00		NIST Webbook
tb	420.20	K	NIST Webbook
tb	423.00 ± 2.00	K	NIST Webbook
tc	604.68	K	Joback Method
tf	217.00 ± 4.00	K	NIST Webbook
tf	212.85 ± 0.60	K	NIST Webbook
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.30	J/mol×K	407.87	Joback Method
cpg	226.11	J/mol×K	440.67	Joback Method
cpg	237.23	J/mol×K	473.47	Joback Method
cpg	247.69	J/mol×K	506.27	Joback Method

cpg	257.53	J/mol×K	539.07	Joback Method
cpg	266.77	J/mol×K	571.88	Joback Method
cpg	275.45	J/mol×K	604.68	Joback Method
dvisc	0.0130916	Pa×s	204.64	Joback Method
dvisc	0.0046345	Pa×s	238.51	Joback Method
dvisc	0.0021241	Pa×s	272.38	Joback Method
dvisc	0.0011569	Pa×s	306.25	Joback Method
dvisc	0.0007112	Pa×s	340.13	Joback Method
dvisc	0.0004775	Pa×s	374.00	Joback Method
dvisc	0.0003425	Pa×s	407.87	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62320e+01
Coeff. B	-4.20398e+03
Coeff. C	-5.82160e+01
Temperature range (K), min.	321.88
Temperature range (K), max.	443.18

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=C6130967&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume