Butane, 1,1-dichloro-3-methyl-

Other names: 1,1-Dichloro-3-methylbutane
Inchi: InChI=1S/C5H10Cl2/c1-4(2)3-5(6)7/h4-5H,3H2,1-2H3
InchiKey: VXEMJASOVHTHLL-UHFFFAOYSA-N
Formula: C5H10Cl2
SMILES: CC(C)CC(Cl)Cl
Mol. weight [g/mol]: 141.04
CAS: 625-66-1

Physical Properties

Property code	Value	Unit	Source
gf	-37.52	kJ/mol	Joback Method
hf	-188.57	kJ/mol	Joback Method
hfus	10.05	kJ/mol	Joback Method
hvap	34.72	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.836		Crippen Method
mcvol	105.790	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	402.75 ± 0.50	K	NIST Webbook
tb	400.65 ± 3.00	K	NIST Webbook
tb	401.00 ± 3.00	K	NIST Webbook
tb	403.85 ± 2.00	K	NIST Webbook
tc	577.75	K	Joback Method
tf	175.95	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.68	J/mol×K	387.78	Joback Method
cpg	185.11	J/mol×K	419.44	Joback Method
cpg	194.11	J/mol×K	451.10	Joback Method
cpg	202.69	J/mol×K	482.77	Joback Method
cpg	210.87	J/mol×K	514.43	Joback Method

cpg	218.66	J/mol×K	546.09	Joback Method
cpg	226.08	J/mol×K	577.75	Joback Method
dvisc	0.0132129	Pa×s	175.95	Joback Method
dvisc	0.0042286	Pa×s	211.25	Joback Method
dvisc	0.0018754	Pa×s	246.56	Joback Method
dvisc	0.0010197	Pa×s	281.87	Joback Method
dvisc	0.0006349	Pa×s	317.17	Joback Method
dvisc	0.0004347	Pa×s	352.48	Joback Method
dvisc	0.0003189	Pa×s	387.78	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34681e+01
Coeff. B	-2.71235e+03
Coeff. C	-9.62620e+01
Temperature range (K), min.	302.05
Temperature range (K), max.	428.80

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=C625661&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume