Butane, 1,1-dichloro-

Other names:	1,1-Dichlorobutane
	Butylidene chloride
Inchi:	InChI=1S/C4H8Cl2/c1-2-3-4(5)6/h4H,2-3H2,1H3
InchiKey:	SEQRDAAUNCRFIT-UHFFFAOYSA-N
Formula:	C4H8Cl2
SMILES:	CCCC(Cl)Cl
Mol. weight [g/mol]:	127.01
CAS:	541-33-3

Physical Properties

Property code	Value	Unit	Source
gf	-43.50	kJ/mol	Joback Method
hf	-162.65	kJ/mol	Joback Method
hfus	10.99	kJ/mol	Joback Method
hvap	39.40 ± 0.60	kJ/mol	NIST Webbook
hvap	39.50	kJ/mol	NIST Webbook
log10ws	-2.40		Aqueous Solubility Prediction Method
logp	2.590		Crippen Method
mcvol	91.700	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	755.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	787.00		NIST Webbook
tb	387.00 ± 4.00	K	NIST Webbook
tb	387.00	K	NIST Webbook
tc	551.71	K	Joback Method
tf	179.68	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	182.54	J/mol×K	551.71	Joback Method
cpg	141.59	J/mol×K	365.34	Joback Method
cpg	149.22	J/mol×K	396.40	Joback Method
cpg	156.51	J/mol×K	427.46	Joback Method
cpg	163.48	J/mol×K	458.52	Joback Method
cpg	170.14	J/mol×K	489.58	Joback Method
cpg	176.48	J/mol×K	520.65	Joback Method
dvisc	0.0003376	Pa×s	365.34	Joback Method
dvisc	0.0069129	Pa×s	179.68	Joback Method
dvisc	0.0028879	Pa×s	210.62	Joback Method
dvisc	0.0015088	Pa×s	241.57	Joback Method
dvisc	0.0009135	Pa×s	272.51	Joback Method
dvisc	0.0006126	Pa×s	303.45	Joback Method
dvisc	0.0004424	Pa×s	334.40	Joback Method
hvapt	38.70	kJ/mol	345.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42047e+01
Coeff. B	-3.17500e+03
Coeff. C	-5.58020e+01
Temperature range (K), min.	283.94
Temperature range (K), max.	412.81

Sources

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C541333&Units=SI

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
pvap:	Vapor 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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