

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	39.50	kJ/mol	NIST Webbook
hvap	39.40 ± 0.60	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	756.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	755.00		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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	182.54	J/molxK	551.71	Joback Method
cpg	141.59	J/molxK	365.34	Joback Method
cpg	149.22	J/molxK	396.40	Joback Method
cpg	156.51	J/molxK	427.46	Joback Method
cpg	163.48	J/molxK	458.52	Joback Method
cpg	170.14	J/molxK	489.58	Joback Method
cpg	176.48	J/molxK	520.65	Joback Method
dvisc	0.0003376	Paxs	365.34	Joback Method
dvisc	0.0069129	Paxs	179.68	Joback Method
dvisc	0.0028879	Paxs	210.62	Joback Method
dvisc	0.0015088	Paxs	241.57	Joback Method
dvisc	0.0009135	Paxs	272.51	Joback Method
dvisc	0.0006126	Paxs	303.45	Joback Method
dvisc	0.0004424	Paxs	334.40	Joback Method
hvapt	38.70	kJ/mol	345.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C541333&Units=SI>

The Yaws Handbook of Vapor

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Pressure:

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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>

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
mccvol:	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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