Butane, 2,2-dichloro-

Other names: 2,2-Dichlorobutane
Inchi: InChI=1S/C4H8Cl2/c1-3-4(2,5)6/h3H2,1-2H3
InchiKey: BSRTYNDWQXVCKR-UHFFFAOYSA-N
Formula: C4H8Cl2
SMILES: CCC(C)(Cl)Cl
Mol. weight [g/mol]: 127.01
CAS: 4279-22-5

Physical Properties

Property code	Value	Unit	Source
gf	-38.22	kJ/mol	Joback Method
hf	-166.12	kJ/mol	Joback Method
hfus	7.10	kJ/mol	Joback Method
hvap	33.70 ± 0.60	kJ/mol	NIST Webbook
hvap	36.30 ± 0.10	kJ/mol	NIST Webbook
hvap	36.70	kJ/mol	NIST Webbook
log10ws	-2.41		Crippen Method
logp	2.590		Crippen Method
mcvol	91.700	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
rinpol	724.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	724.00		NIST Webbook
tb	376.15 ± 0.50	K	NIST Webbook
tb	376.00 ± 4.00	K	NIST Webbook
tb	374.00 ± 4.00	K	NIST Webbook
tb	377.20	K	NIST Webbook
tc	557.27	K	Joback Method
tf	197.10	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.80	J/mol×K	557.27	Joback Method
cpg	181.49	J/mol×K	524.81	Joback Method
cpg	174.74	J/mol×K	492.36	Joback Method
cpg	167.53	J/mol×K	459.91	Joback Method
cpg	159.83	J/mol×K	427.46	Joback Method
cpg	151.62	J/mol×K	395.00	Joback Method
cpg	142.86	J/mol×K	362.55	Joback Method
dvisc	0.0076660	Pa×s	197.10	Joback Method
dvisc	0.0004048	Pa×s	362.55	Joback Method
dvisc	0.0005402	Pa×s	334.98	Joback Method
dvisc	0.0007591	Pa×s	307.40	Joback Method
dvisc	0.0011406	Pa×s	279.82	Joback Method
dvisc	0.0018734	Pa×s	252.25	Joback Method
dvisc	0.0034758	Pa×s	224.68	Joback Method
hvapt	36.40	kJ/mol	334.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38948e+01
Coeff. B	-3.02068e+03
Coeff. C	-5.15700e+01
Temperature range (K), min.	273.56
Temperature range (K), max.	403.50

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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=C4279225&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

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