Butane, 1,2-dichloro-

Other names: 1,2-Butylene chloride
1,2-Dichlorobutane
Inchi: InChI=1S/C4H8Cl2/c1-2-4(6)3-5/h4H,2-3H2,1H3
InchiKey: PQBOTZNYFQWRHU-UHFFFAOYSA-N
Formula: C4H8Cl2
SMILES: CCC(Cl)CCl
Mol. weight [g/mol]: 127.01
CAS: 616-21-7

Physical Properties

Property code	Value	Unit	Source
chl	-2533.30 ± 1.60	kJ/mol	NIST Webbook
gf	-43.50	kJ/mol	Joback Method
hf	-191.20 ± 1.70	kJ/mol	NIST Webbook
hfl	-231.40 ± 1.70	kJ/mol	NIST Webbook
hfl	-232.20	kJ/mol	NIST Webbook
hfus	10.99	kJ/mol	Joback Method
hvap	32.88	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	2.243		Crippen Method
mcvol	91.700	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	785.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	785.00		NIST Webbook
tb	387.85	K	NIST Webbook
tb	397.20	K	NIST Webbook
tb	397.15 ± 2.00	K	NIST Webbook
tb	395.15 ± 2.00	K	NIST Webbook
tb	397.00 ± 5.00	K	NIST Webbook
tb	397.15 ± 2.00	K	NIST Webbook
tb	397.20 ± 0.50	K	NIST Webbook
tb	397.20	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	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
cpg	182.54	J/mol×K	551.71	Joback Method
cpl	195.60	J/mol×K	298.15	NIST Webbook
dvisc	0.0028879	Pa×s	210.62	Joback Method
dvisc	0.0069129	Pa×s	179.68	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
dvisc	0.0003376	Pa×s	365.34	Joback Method
hvapt	33.90	kJ/mol	397.20	NIST Webbook
hvapt	39.00	kJ/mol	353.00	NIST Webbook
hvapt	38.10	kJ/mol	323.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51007e+01
Coeff. B	-3.98019e+03
Coeff. C	-1.62960e+01
Temperature range (K), min.	284.99
Temperature range (K), max.	422.89

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C616217&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1603
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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