Butane, 1,2-dibromo-

Other names:	1,2-DIBROMOBUTANE
	ALPHA-BUTYLENE DIBROMIDE
	«alpha»-Butylene bromide
	«alpha»-Butylene dibromide
	Â«alphaÂ»-Butylene bromide
	Â«alphaÂ»-Butylene dibromide
Inchi:	InChI=1S/C4H8Br2/c1-2-4(6)3-5/h4H,2-3H2,1H3
InchiKey:	CZWSZZHGSNZRMW-UHFFFAOYSA-N
Formula:	C4H8Br2
SMILES:	CCC(Br)CBr
Mol. weight [g/mol]:	215.91
CAS:	533-98-2

Physical Properties

Property code	Value	Unit	Source
chl	-2570.10 ± 2.20	kJ/mol	NIST Webbook
gf	9.00	kJ/mol	Joback Method
hf	-102.20 ± 2.40	kJ/mol	NIST Webbook
hf	-92.93	kJ/mol	NIST Webbook
hfl	-140.80	kJ/mol	NIST Webbook
hfl	-146.90 ± 2.10	kJ/mol	NIST Webbook
hfus	13.16	kJ/mol	Joback Method
hvap	45.90	kJ/mol	NIST Webbook
hvap	47.86	kJ/mol	NIST Webbook
hvap	45.60 ± 0.70	kJ/mol	NIST Webbook
log10ws	-2.47		Crippen Method
logp	2.555		Crippen Method
mcvol	102.220	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
rinpol	960.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	944.00		NIST Webbook
tb	439.15 ± 1.50	K	NIST Webbook
tb	439.50 ± 0.50	K	NIST Webbook

tb	433.15 ± 6.00	K	NIST Webbook
tc	634.29	K	Joback Method
tf	207.70 ± 0.30	K	NIST Webbook
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.15	J/mol×K	422.80	Joback Method
cpg	166.17	J/mol×K	458.05	Joback Method
cpg	173.70	J/mol×K	493.30	Joback Method
cpg	180.76	J/mol×K	528.54	Joback Method
cpg	187.39	J/mol×K	563.79	Joback Method
cpg	193.62	J/mol×K	599.04	Joback Method
cpg	199.46	J/mol×K	634.29	Joback Method
dvisc	0.0014644	Pa×s	300.56	Joback Method
dvisc	0.0023844	Pa×s	270.00	Joback Method
dvisc	0.0043966	Pa×s	239.44	Joback Method
dvisc	0.0009841	Pa×s	331.12	Joback Method
dvisc	0.0007073	Pa×s	361.68	Joback Method
dvisc	0.0005352	Pa×s	392.24	Joback Method
dvisc	0.0004216	Pa×s	422.80	Joback Method
hvapt	43.50	kJ/mol	381.50	NIST Webbook
hvapt	42.80	kJ/mol	360.00	NIST Webbook
hvapt	45.19	kJ/mol	300.00	NIST Webbook
hvapt	45.10	kJ/mol	303.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	332.70	K	2.70	NIST Webbook
tbrp	333.00	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61960e+01
Coeff. B	-5.10156e+03
Coeff. C	1.51800e+00
Temperature range (K), min.	319.17
Temperature range (K), max.	467.18

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.57712e+01
Coeff. B	-7.27878e+03
Coeff. C	-7.50551e+00
Coeff. D	5.71307e-06
Temperature range (K), min.	273.15
Temperature range (K), max.	659.28

Sources

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=1601

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C533982&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1601

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume