Butane, 2,3-dibromo-

Other names:	2,3-Dibromobutane
	«beta»-Butylene bromide
	Â«betaÂ»-Butylene bromide
Inchi:	InChI=1S/C4H8Br2/c1-3(5)4(2)6/h3-4H,1-2H3
InchiKey:	BXXWFOGWXLJPPA-UHFFFAOYSA-N
Formula:	C4H8Br2
SMILES:	CC(Br)C(C)Br
Mol. weight [g/mol]:	215.91
CAS:	5408-86-6

Physical Properties

Property code	Value	Unit	Source
gf	6.56	kJ/mol	Joback Method
hf	-83.79	kJ/mol	Joback Method
hfus	9.64	kJ/mol	Joback Method
hvap	36.59	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.553		Crippen Method
mcvol	102.220	ml/mol	McGowan Method
pc	4769.39	kPa	Joback Method
rinpol	904.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	904.00		NIST Webbook
tb	431.15 ± 1.50	K	NIST Webbook
tb	431.00 ± 2.00	K	NIST Webbook
tc	639.11	K	Joback Method
tf	224.44	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.26	J/mol×K	422.36	Joback Method

cpg	166.58	J/mol×K	458.48	Joback Method
cpg	174.37	J/mol×K	494.61	Joback Method
cpg	181.67	J/mol×K	530.73	Joback Method
cpg	188.50	J/mol×K	566.86	Joback Method
cpg	194.90	J/mol×K	602.98	Joback Method
cpg	200.90	J/mol×K	639.11	Joback Method
dvisc	0.0065317	Pa×s	224.44	Joback Method
dvisc	0.0030527	Pa×s	257.43	Joback Method
dvisc	0.0016958	Pa×s	290.41	Joback Method
dvisc	0.0010621	Pa×s	323.40	Joback Method
dvisc	0.0007254	Pa×s	356.39	Joback Method
dvisc	0.0005285	Pa×s	389.37	Joback Method
dvisc	0.0004045	Pa×s	422.36	Joback Method
hvapt	37.70	kJ/mol	295.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.70	K	21.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53443e+01
Coeff. B	-3.95955e+03
Coeff. C	-6.18440e+01
Temperature range (K), min.	324.82
Temperature range (K), max.	456.50

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=C5408866&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume