Butane, 1,3-dibromo-

Other names: 1,3-Dibromobutane
Inchi: InChI=1S/C4H8Br2/c1-4(6)2-3-5/h4H,2-3H2,1H3
InchiKey: XZNGUVQDFJHPLU-UHFFFAOYSA-N
Formula: C4H8Br2
SMILES: CC(Br)CCBr
Mol. weight [g/mol]: 215.91
CAS: 107-80-2

Physical Properties

Property code	Value	Unit	Source
gf	9.00	kJ/mol	Joback Method
hf	-97.28	kJ/mol	NIST Webbook
hfl	-147.80 ± 5.10	kJ/mol	NIST Webbook
hfus	13.16	kJ/mol	Joback Method
hvap	49.50	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	964.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	987.00		NIST Webbook
tb	448.15 ± 1.50	K	NIST Webbook
tb	447.20	K	NIST Webbook
tb	447.65 ± 2.00	K	NIST Webbook
tc	634.29	K	Joback Method
tf	239.44	K	Joback Method
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	0.0043966	Pa×s	239.44	Joback Method
dvisc	0.0023844	Pa×s	270.00	Joback Method
dvisc	0.0014644	Pa×s	300.56	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	44.70	kJ/mol	400.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43406e+01
Coeff. B	-3.27841e+03
Coeff. C	-1.09992e+02
Temperature range (K), min.	343.28
Temperature range (K), max.	473.09

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C107802&Units=SI

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

Legend

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume