Butane, 1,2,2-tribromo-

Other names: 1,2,2-Tribromobutane
Inchi: InChI=1S/C4H7Br3/c1-2-4(6,7)3-5/h2-3H2,1H3
InchiKey: LMTXANJNYFUPOZ-UHFFFAOYSA-N
Formula: C4H7Br3
SMILES: CCC(Br)(Br)CBr
Mol. weight [g/mol]: 294.81
CAS: 3675-69-2

Physical Properties

Property code	Value	Unit	Source
gf	28.60	kJ/mol	Joback Method
hf	-55.65	kJ/mol	Joback Method
hfus	14.56	kJ/mol	Joback Method
hvap	42.51	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.277		Crippen Method
mcvol	119.720	ml/mol	McGowan Method
pc	5281.57	kPa	Joback Method
tb	487.00	K	NIST Webbook
tc	726.33	K	Joback Method
tf	316.66	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.74	J/mol×K	686.30	Joback Method
cpg	227.56	J/mol×K	726.33	Joback Method
cpg	189.99	J/mol×K	486.17	Joback Method
cpg	197.96	J/mol×K	526.20	Joback Method
cpg	205.14	J/mol×K	566.22	Joback Method
cpg	211.61	J/mol×K	606.25	Joback Method
cpg	217.45	J/mol×K	646.28	Joback Method
dvisc	0.0004204	Pa×s	486.17	Joback Method

dvisc	0.0005270	Pa×s	457.92	Joback Method
dvisc	0.0029905	Pa×s	316.66	Joback Method
dvisc	0.0018861	Pa×s	344.91	Joback Method
dvisc	0.0012755	Pa×s	373.16	Joback Method
dvisc	0.0009115	Pa×s	401.41	Joback Method
dvisc	0.0006807	Pa×s	429.67	Joback Method
hvapt	50.70	kJ/mol	400.00	NIST Webbook
hvapt	48.40	kJ/mol	421.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51089e+01
Coeff. B	-4.30616e+03
Coeff. C	-7.65220e+01
Temperature range (K), min.	367.06
Temperature range (K), max.	516.04

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3675692&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

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