Butane, 1,1,2-tribromo-

Other names: 1,1,2-Tribromobutane
Inchi: InChI=1S/C4H7Br3/c1-2-3(5)4(6)7/h3-4H,2H2,1H3
InchiKey: WMGQSHQUFZATPG-UHFFFAOYSA-N
Formula: C4H7Br3
SMILES: CCC(Br)C(Br)Br
Mol. weight [g/mol]: 294.81
CAS: 3675-68-1

Physical Properties

Property code	Value	Unit	Source
gf	20.88	kJ/mol	Joback Method
hf	-57.46	kJ/mol	Joback Method
hfus	14.92	kJ/mol	Joback Method
hvap	43.03	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.276		Crippen Method
mcvol	119.720	ml/mol	McGowan Method
pc	5258.62	kPa	Joback Method
tb	489.40	K	NIST Webbook
tc	723.92	K	Joback Method
tf	284.24	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.89	J/mol×K	723.92	Joback Method
cpg	186.87	J/mol×K	488.52	Joback Method
cpg	194.55	J/mol×K	527.75	Joback Method
cpg	201.63	J/mol×K	566.99	Joback Method
cpg	208.15	J/mol×K	606.22	Joback Method
cpg	214.17	J/mol×K	645.45	Joback Method
cpg	219.73	J/mol×K	684.68	Joback Method
dvisc	0.0003845	Pa×s	488.52	Joback Method

dvisc	0.0041502	Pa×s	284.24	Joback Method
dvisc	0.0022583	Pa×s	318.29	Joback Method
dvisc	0.0013822	Pa×s	352.33	Joback Method
dvisc	0.0009224	Pa×s	386.38	Joback Method
dvisc	0.0006573	Pa×s	420.43	Joback Method
dvisc	0.0004927	Pa×s	454.47	Joback Method
hvapt	49.40	kJ/mol	425.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51122e+01
Coeff. B	-4.32567e+03
Coeff. C	-7.71890e+01
Temperature range (K), min.	368.98
Temperature range (K), max.	518.55

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=C3675681&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume