

Butane, 2,2,3-tribromo-

Other names:	2,2,3-Tribromobutane
Inchi:	InChI=1S/C4H7Br3/c1-3(5)4(2,6)7/h3H,1-2H3
InchiKey:	JDWNTZIECWBAO-UHFFFAOYSA-N
Formula:	C4H7Br3
SMILES:	CC(Br)C(C)(Br)Br
Mol. weight [g/mol]:	294.81
CAS:	62127-47-3

Physical Properties

Property code	Value	Unit	Source
gf	26.16	kJ/mol	Joback Method
hf	-60.93	kJ/mol	Joback Method
hfus	11.03	kJ/mol	Joback Method
hvap	42.12	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.276		Crippen Method
mcvol	119.720	ml/mol	McGowan Method
pc	5343.52	kPa	Joback Method
tb	479.20	K	NIST Webbook
tc	731.86	K	Joback Method
tf	301.66	K	Joback Method
vc	0.428	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.94	J/molxK	731.86	Joback Method
cpg	190.28	J/molxK	485.73	Joback Method
cpg	198.54	J/molxK	526.75	Joback Method
cpg	205.96	J/molxK	567.77	Joback Method
cpg	212.62	J/molxK	608.80	Joback Method
cpg	218.62	J/molxK	649.82	Joback Method
cpg	224.03	J/molxK	690.84	Joback Method
dvisc	0.0003987	Paxs	485.73	Joback Method

dvisc	0.0039222	Paxs	301.66	Joback Method
dvisc	0.0022474	Paxs	332.34	Joback Method
dvisc	0.0014149	Paxs	363.02	Joback Method
dvisc	0.0009573	Paxs	393.70	Joback Method
dvisc	0.0006854	Paxs	424.37	Joback Method
dvisc	0.0005133	Paxs	455.05	Joback Method
hvapt	51.70	kJ/mol	395.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62127473&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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