

Butane, 2,3-dibromo-, threo

Inchi:	InChI=1S/C4H8Br2/c1-3(5)4(2)6/h3-4H,1-2H3/t3-,4-/m0/s1
InchiKey:	BXXWFOGWXLJPPA-IMJSIDKUSA-N
Formula:	C4H8Br2
SMILES:	CC(Br)C(C)Br
Mol. weight [g/mol]:	215.91

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	930.00		NIST Webbook
rinpol	930.00		NIST Webbook
tb	422.36	K	Joback Method
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/molxK	422.36	Joback Method
cpg	166.58	J/molxK	458.48	Joback Method
cpg	174.37	J/molxK	494.61	Joback Method
cpg	181.67	J/molxK	530.73	Joback Method
cpg	188.50	J/molxK	566.86	Joback Method
cpg	194.90	J/molxK	602.98	Joback Method
cpg	200.90	J/molxK	639.11	Joback Method
dvisc	0.0065317	Paxs	224.44	Joback Method

dvisc	0.0030527	Paxs	257.43	Joback Method
dvisc	0.0016958	Paxs	290.41	Joback Method
dvisc	0.0010621	Paxs	323.40	Joback Method
dvisc	0.0007254	Paxs	356.39	Joback Method
dvisc	0.0005285	Paxs	389.37	Joback Method
dvisc	0.0004045	Paxs	422.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R294563&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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