

Butane, 1-bromo-2-methyl-, (S)-

Other names:	(S)-1-Bromo-2-methylbutane (S)-(+)-1-Bromo-2-methylbutane (+)-(S)-1-Bromo-2-methylbutane (+)-1-Bromo-2-methylbutane Butane, 1-bromo-2-methyl-, (S)-(+)- (S)-2-Methyl-1-bromobutane (S)-(+)-2-Methyl-1-bromobutane (+)-2-Methyl-1-bromobutane (+)-2-Methylbutyl bromide 1-Bromo-2-methylbutane, (S)- Butane, 1-bromo-2-methyl-, (2S)-
Inchi:	InChI=1S/C5H11Br/c1-3-5(2)4-6/h5H,3-4H2,1-2H3/t5-/m1/s1
InchiKey:	XKVLZBNEPALHIO-RXMQYKEDSA-N
Formula:	C5H11Br
SMILES:	CCC(C)CBr
Mol. weight [g/mol]:	151.04
CAS:	534-00-9

Physical Properties

Property code	Value	Unit	Source
gf	3.10	kJ/mol	Joback Method
hf	-125.48	kJ/mol	Joback Method
hfus	10.47	kJ/mol	Joback Method
hvap	32.77	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.427		Crippen Method
mcvol	98.810	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
tb	394.80	K	NIST Webbook
tc	568.83	K	Joback Method
tf	190.91	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.30	J/molxK	379.52	Joback Method
cpg	170.96	J/molxK	411.07	Joback Method
cpg	180.18	J/molxK	442.62	Joback Method
cpg	188.97	J/molxK	474.18	Joback Method
cpg	197.35	J/molxK	505.73	Joback Method
cpg	205.34	J/molxK	537.28	Joback Method
cpg	212.94	J/molxK	568.83	Joback Method
dvisc	0.0061616	Paxs	190.91	Joback Method
dvisc	0.0027207	Paxs	222.34	Joback Method
dvisc	0.0014710	Paxs	253.78	Joback Method
dvisc	0.0009108	Paxs	285.21	Joback Method
dvisc	0.0006202	Paxs	316.65	Joback Method
dvisc	0.0004527	Paxs	348.08	Joback Method
dvisc	0.0003481	Paxs	379.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C534009&Units=SI
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
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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