

# Butane, 2-bromo-3-methoxy, threo

<b>Inchi:</b>	InChI=1S/C5H11BrO/c1-4(6)5(2)7-3/h4-5H,1-3H3/t4-,5-/m1/s1
<b>InchiKey:</b>	MNFFVQPIBJUTHA-RFZPGFLSSA-N
<b>Formula:</b>	C5H11BrO
<b>SMILES:</b>	COC(C)C(C)Br
<b>Mol. weight [g/mol]:</b>	167.04

## Physical Properties

Property code	Value	Unit	Source
gf	-104.34	kJ/mol	Joback Method
hf	-262.98	kJ/mol	Joback Method
hfus	8.13	kJ/mol	Joback Method
hvap	34.79	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.805		Crippen Method
mcvol	104.680	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
rinpol	823.00		NIST Webbook
tb	401.50	K	Joback Method
tc	595.30	K	Joback Method
tf	198.14	K	Joback Method
vc	0.384	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.70	J/molxK	401.50	Joback Method
cpg	227.43	J/molxK	563.00	Joback Method
cpg	219.22	J/molxK	530.70	Joback Method
cpg	210.64	J/molxK	498.40	Joback Method
cpg	201.70	J/molxK	466.10	Joback Method
cpg	192.39	J/molxK	433.80	Joback Method
cpg	235.30	J/molxK	595.30	Joback Method
dvisc	0.0002907	Paxs	401.50	Joback Method
dvisc	0.0003886	Paxs	367.61	Joback Method

dvisc	0.0005510	Paxs	333.71	Joback Method
dvisc	0.0008454	Paxs	299.82	Joback Method
dvisc	0.0014467	Paxs	265.93	Joback Method
dvisc	0.0028963	Paxs	232.03	Joback Method
dvisc	0.0073529	Paxs	198.14	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R294583&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R294583&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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