

# Methanesulfonic acid, butyl ester

<b>Other names:</b>	n-Butyl methanesulfonate Butyl mesylate Butyl methanesulfonate butyl methanesulphonate
<b>Inchi:</b>	InChI=1S/C5H12O3S/c1-3-4-5-8-9(2,6)7/h3-5H2,1-2H3
<b>InchiKey:</b>	LFLBHTZRLVHUQC-UHFFFAOYSA-N
<b>Formula:</b>	C5H12O3S
<b>SMILES:</b>	CCCCOS(C)(=O)=O
<b>Mol. weight [g/mol]:</b>	152.21
<b>CAS:</b>	1912-32-9

## Physical Properties

Property code	Value	Unit	Source
gf	-582.32	kJ/mol	Joback Method
hf	-732.10	kJ/mol	Joback Method
hfus	21.27	kJ/mol	Joback Method
hvap	47.77	kJ/mol	Joback Method
log10ws	-0.83		Crippen Method
logp	0.763		Crippen Method
mcvol	115.270	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
tb	384.00	K	Joback Method
tc	547.79	K	Joback Method
tf	206.90	K	Joback Method
vc	0.460	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.08	J/molxK	384.00	Joback Method
cpg	224.89	J/molxK	411.30	Joback Method
cpg	234.46	J/molxK	438.60	Joback Method
cpg	243.79	J/molxK	465.89	Joback Method
cpg	252.86	J/molxK	493.19	Joback Method

cpg	261.68	J/mol×K	520.49	Joback Method
cpg	270.22	J/mol×K	547.79	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1912329&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1912329&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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>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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