

# Thiazole, 2-bromo-5-nitro-

<b>Other names:</b>	2-Bromo-5-nitrothiazole 5-Nitro-2-bromothiazole 2-bromo-5-nitro-1,3-thiazole
<b>Inchi:</b>	InChI=1S/C3HBrN2O2S/c4-3-5-1-2(9-3)6(7)8/h1H
<b>InchiKey:</b>	ANIJFZVZXZQFDH-UHFFFAOYSA-N
<b>Formula:</b>	C3HBrN2O2S
<b>SMILES:</b>	O=[N+]([O-])c1cnc(Br)s1
<b>Mol. weight [g/mol]:</b>	209.02
<b>CAS:</b>	3034-48-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Crippen Method
logp	1.814		Crippen Method
mcvol	94.920	ml/mol	McGowan Method

## Sources

<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=C3034488&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3034488&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>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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<https://www.chemeo.com/cid/73-196-4/Thiazole-2-bromo-5-nitro.pdf>

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