

# Benzothiazole, 2-methyl-6-nitro-

<b>Other names:</b>	2-Methyl-6-nitrobenzothiazole
<b>Inchi:</b>	InChI=1S/C8H6N2O2S/c1-5-9-7-3-2-6(10(11)12)4-8(7)13-5/h2-4H,1H3
<b>InchiKey:</b>	YAQKYKGFPPQE-UHFFFAOYSA-N
<b>Formula:</b>	C8H6N2O2S
<b>SMILES:</b>	<chem>Cc1nc2ccc([N+](=O)[O-])cc2s1</chem>
<b>Mol. weight [g/mol]:</b>	194.21
<b>CAS:</b>	2941-63-1

## Physical Properties

Property code	Value	Unit	Source
ie	9.15	eV	NIST Webbook
log10ws	-3.93		Crippen Method
logp	2.513		Crippen Method
mcvol	128.410	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=C2941631&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2941631&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>ie:</b>	Ionization energy
<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/27-095-7/Benzothiazole-2-methyl-6-nitro.pdf>

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