

# Isothiazole, 3-methyl-

<b>Other names:</b>	3-Methylisothiazole
<b>Inchi:</b>	InChI=1S/C4H5NS/c1-4-2-3-6-5-4/h2-3H,1H3
<b>InchiKey:</b>	WOTIUKDGBXFLG-UHFFFAOYSA-N
<b>Formula:</b>	C4H5NS
<b>SMILES:</b>	Cc1ccsn1
<b>Mol. weight [g/mol]:</b>	99.15
<b>CAS:</b>	693-92-5

## Physical Properties

Property code	Value	Unit	Source
ie	9.60	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.452		Crippen Method
mcvol	74.090	ml/mol	McGowan Method
rinpol	842.00		NIST Webbook
rinpol	796.00		NIST Webbook

## Sources

<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>
<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=C693925&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C693925&amp;Units=SI</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
<b>rinpol:</b>	Non-polar retention indices

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