

# Imidazole, 5(4)-(methylthio)-4(5)-nitro-

<b>Inchi:</b>	InChI=1S/C4H5N3O2S/c1-10-4-3(7(8)9)5-2-6-4/h2H,1H3,(H,5,6)
<b>InchiKey:</b>	LIRFYGRDQORNCR-UHFFFAOYSA-N
<b>Formula:</b>	C4H5N3O2S
<b>SMILES:</b>	CSc1[nH]cnc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	159.17
<b>CAS:</b>	113121-55-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Crippen Method
logp	0.558		Crippen Method
mcvol	101.490	ml/mol	McGowan Method

## Sources

<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>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=C113121554&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C113121554&amp;Units=SI</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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