

# 1-Methyl-2-(methylthio)-5-mercaptoimidazole

<b>Inchi:</b>	InChI=1S/C5H8N2S2/c1-7-4(8)3-6-5(7)9-2/h3,8H,1-2H3
<b>InchiKey:</b>	PEONIPRKWXYQQD-UHFFFAOYSA-N
<b>Formula:</b>	C5H8N2S2
<b>SMILES:</b>	CSc1ncc(S)n1C
<b>Mol. weight [g/mol]:</b>	160.26

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.78		Crippen Method
logp	1.431		Crippen Method
mcvol	114.510	ml/mol	McGowan Method
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook

## 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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=R594675&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R594675&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
<b>rinpol:</b>	Non-polar retention indices

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