

# 1,3-Dimethylimidazole-2(3H)-thione

<b>Other names:</b>	1,3-Dimethylimidazoline-2-thione 2H-Imidazole-2-thione, 1,3-dihydro-1,3-dimethyl- 4-Imidazoline-2-thione, 1,3-dimethyl- 1,3-Dimethyl-2-thioketoimidazole
<b>Inchi:</b>	InChI=1S/C5H8N2S/c1-6-3-4-7(2)5(6)8/h3-4H,1-2H3
<b>InchiKey:</b>	ZYPLZLQKRFFKCL-UHFFFAOYSA-N
<b>Formula:</b>	C5H8N2S
<b>SMILES:</b>	<chem>Cn1ccn(C)c1=S</chem>
<b>Mol. weight [g/mol]:</b>	128.19
<b>CAS:</b>	6596-81-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.90		Crippen Method
logp	1.093		Crippen Method
mcvol	98.160	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=C6596812&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6596812&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>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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