

# N-Methanesulfonylimidazole

<b>Other names:</b>	1-Methanesulfonylimidazole 1H-Imidazole, 1-(methylsulfonyl)- 1-(methylsulphonyl)-1H-imidazole
<b>Inchi:</b>	InChI=1S/C4H6N2O2S/c1-9(7,8)6-3-2-5-4-6/h2-4H,1H3
<b>InchiKey:</b>	ZBHRCOWHFFHJZFP-UHFFFAOYSA-N
<b>Formula:</b>	C4H6N2O2S
<b>SMILES:</b>	CS(=O)(=O)n1ccnc1
<b>Mol. weight [g/mol]:</b>	146.17
<b>CAS:</b>	40736-26-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.51		Crippen Method
logp	-0.309		Crippen Method
mcvol	95.810	ml/mol	McGowan Method

## Sources

<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=C40736263&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C40736263&amp;Units=SI</a>
<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>

## 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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