

# C9H8N2O2S

<b>Inchi:</b>	InChI=1S/C9H8N2O2S/c12-8(13)5-14-9-10-6-3-1-2-4-7(6)11-9/h1-4H,5H2,(H,10,11)(H,1
<b>InchiKey:</b>	UYNVBLJQBCTRKV-UHFFFAOYSA-N
<b>Formula:</b>	C9H8N2O2S
<b>SMILES:</b>	O=C(O)CSc1nc2ccccc2[nH]1
<b>Mol. weight [g/mol]:</b>	208.24
<b>CAS:</b>	3042-00-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	1.258		Crippen Method
mcvol	142.500	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3042000&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3042000&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>
<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>

## 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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