

# 2-Pyridinethiol, 3-amino-

<b>Inchi:</b>	InChI=1S/C5H6N2S/c6-4-2-1-3-7-5(4)8/h1-3H,6H2,(H,7,8)
<b>InchiKey:</b>	ADMMJKIQWOJMSK-UHFFFAOYSA-N
<b>Formula:</b>	C5H6N2S
<b>SMILES:</b>	Nc1cccnc1S
<b>Mol. weight [g/mol]:</b>	126.18
<b>CAS:</b>	38240-21-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.38		Crippen Method
logp	0.953		Crippen Method
mcvol	93.860	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=C38240210&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C38240210&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>

## 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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<https://www.chemeo.com/cid/96-750-3/2-Pyridinethiol-3-amino.pdf>

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