

# 2(1H)-Pyrimidinethione, 4-amino-

<b>Other names:</b>	Cytosine, thio- Cytosine, 2-thio- Thiocyosine 2(1H)-Pyrimidinone, 4-aminothio- 2-Thiocyosine 4-Amino-2-mercaptopyrimidine 4-aminopyrimidine-2-thiol
<b>Inchi:</b>	InChI=1S/C4H5N3S/c5-3-1-2-6-4(8)7-3/h1-2H,(H3,5,6,7,8)
<b>InchiKey:</b>	DCPSTSVLRXOYGS-UHFFFAOYSA-N
<b>Formula:</b>	C4H5N3S
<b>SMILES:</b>	<chem>N=c1ccnc(S)[nH]1</chem>
<b>Mol. weight [g/mol]:</b>	127.17
<b>CAS:</b>	333-49-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Crippen Method
logp	-0.304		Crippen Method
mcpvol	89.750	ml/mol	McGowan Method

## 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.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=C333493&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C333493&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

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