

# Acetamide, n-[9h-purin-6(1h)-thione-9-yl]-

<b>Inchi:</b>	InChI=1S/C7H7N5OS/c1-4(13)11-12-3-10-5-6(12)8-2-9-7(5)14/h2-3H,1H3,(H,11,13)(H,8
<b>InchiKey:</b>	GXGFBHCIBIAKCX-UHFFFAOYSA-N
<b>Formula:</b>	C7H7N5OS
<b>SMILES:</b>	CC(=O)Nn1cnc2c(=S)[nH]cnc21
<b>Mol. weight [g/mol]:</b>	209.23
<b>CAS:</b>	34993-27-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	0.097		Crippen Method
mcvol	138.390	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=C34993276&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C34993276&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

Latest version available from:

<https://www.chemeo.com/cid/48-350-0/Acetamide-n-9h-purin-6-1h-thione-9-yl.pdf>

Generated by Cheméo on 2024-05-04 05:55:58.096462943 +0000 UTC m=+17091407.017040259.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.