

# Purine, 6-(methylthiomethylthio)-

<b>Inchi:</b>	InChI=1S/C7H8N4S2/c1-12-4-13-7-5-6(9-2-8-5)10-3-11-7/h2-3H,4H2,1H3,(H,8,9,10,11)
<b>InchiKey:</b>	UDVRVMSQVYHWIF-UHFFFAOYSA-N
<b>Formula:</b>	C7H8N4S2
<b>SMILES:</b>	CSCSc1ncnc2nc[nH]c12
<b>Mol. weight [g/mol]:</b>	212.29
<b>CAS:</b>	98277-50-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	1.284		Crippen Method
mcvol	143.190	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C98277500&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C98277500&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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