

# Adenine, n-[o-(methylthio)phenyl]-

<b>Inchi:</b>	InChI=1S/C12H11N5S/c1-18-9-5-3-2-4-8(9)17-12-10-11(14-6-13-10)15-7-16-12/h2-7H,1
<b>InchiKey:</b>	KMFJDXWOXHUCSJ-UHFFFAOYSA-N
<b>Formula:</b>	C12H11N5S
<b>SMILES:</b>	CSc1ccccc1Nc1ncnc2[nH]cnc12
<b>Mol. weight [g/mol]:</b>	257.31

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	2.337		Crippen Method
mcvol	183.510	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008710&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008710&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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