

# Adenine, n-[2-[[2-(p-tolylthio)ethyl]thio]ethyl]-

<b>Inchi:</b>	InChI=1S/C16H19N5S2/c1-12-2-4-13(5-3-12)23-9-8-22-7-6-17-15-14-16(19-10-18-14)21
<b>InchiKey:</b>	NGMPHTILBPAGMZ-UHFFFAOYSA-N
<b>Formula:</b>	C16H19N5S2
<b>SMILES:</b>	Cc1ccc(SCCSCCNc2nc[nH]c3ncnc2-3)cc1
<b>Mol. weight [g/mol]:</b>	345.49

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.60		Crippen Method
logp	3.068		Crippen Method
mcvol	256.220	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=B6008321&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008321&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

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