

# Purine-6(1h)-one, 1-[2-(p-tolythio)ethyl]-

<b>Inchi:</b>	InChI=1S/C14H14N4OS/c1-10-2-4-11(5-3-10)20-7-6-18-9-17-13-12(14(18)19)15-8-16-13
<b>InchiKey:</b>	VAYFKKRRGNTGQQ-UHFFFAOYSA-N
<b>Formula:</b>	C14H14N4OS
<b>SMILES:</b>	Cc1ccc(SCCn2cnc3nc[nH]c3c2=O)cc1
<b>Mol. weight [g/mol]:</b>	286.35
<b>CAS:</b>	7702-67-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.16		Crippen Method
logp	1.738		Crippen Method
mcvol	207.580	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=C7702672&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7702672&amp;Units=SI</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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