

# 2-Propanone, 6-purinylthio)-

<b>Inchi:</b>	InChI=1S/C8H8N4OS/c1-5(13)2-14-8-6-7(10-3-9-6)11-4-12-8/h3-4H,2H2,1H3,(H,9,10,11
<b>InchiKey:</b>	RSMPCQAGEDQKEV-UHFFFAOYSA-N
<b>Formula:</b>	C8H8N4OS
<b>SMILES:</b>	CC(=O)CSc1ncnc2nc[nH]c12
<b>Mol. weight [g/mol]:</b>	208.24
<b>CAS:</b>	5441-78-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	0.552		Crippen Method
mcvol	142.500	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5441781&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5441781&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

Latest version available from:

<https://www.chemeo.com/cid/59-740-5/2-Propanone-6-purinylthio.pdf>

Generated by Cheméo on 2024-04-19 22:39:15.777959481 +0000 UTC m=+15855604.698536792.

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