

# Purine-6(1h)-thione, 1-cyclopentyl-

<b>Inchi:</b>	InChI=1S/C10H12N4S/c15-10-8-9(12-5-11-8)13-6-14(10)7-3-1-2-4-7/h5-7H,1-4H2,(H,11)
<b>InchiKey:</b>	KSDSMXRTLRSRPD-UHFFFAOYSA-N
<b>Formula:</b>	C10H12N4S
<b>SMILES:</b>	S=c1c2nc[nH]c2ncn1C1CCCC1
<b>Mol. weight [g/mol]:</b>	220.29
<b>CAS:</b>	37484-40-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.25		Crippen Method
logp	2.122		Crippen Method
mcvol	158.250	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=C37484405&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C37484405&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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