

# 6-Hydroxy-2-mercaptopurine

<b>Other names:</b>	6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo-Xanthine, 2-thio- 2-Mercapto-6-hydroxypurine 2-Thioxanthine 6-Hydroxypurine-2-thiol 1,2,3,7-Tetrahydro-2-thioxo-6H-purin-6-one 2-Thio-6-oxypurine Hypoxanthine, 2-mercapto- 2-Mercaptohypoxanthine 6H-Purin-6-one, 1,2,3,9-tetrahydro-2-thioxo- NSC 36822 NSC 680828
<b>Inchi:</b>	InChI=1S/C5H4N4OS/c10-4-2-3(7-1-6-2)8-5(11)9-4/h1H,(H3,6,7,8,9,10,11)
<b>InchiKey:</b>	XNHFAGRBSMMFKL-UHFFFAOYSA-N
<b>Formula:</b>	C5H4N4OS
<b>SMILES:</b>	Oc1nc(S)nc2[nH]cnc12
<b>Mol. weight [g/mol]:</b>	168.18
<b>CAS:</b>	2487-40-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Crippen Method
logp	-0.135		Crippen Method
mcvol	104.530	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2487403&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2487403&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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