

# 6H-Purin-6-one, 1,7-dihydro-1-methyl-

<b>Other names:</b>	Hypoxanthine, 1-methyl- 1-Methylhypoxanthine Purin-6(1H)-one, 1-methyl
<b>Inchi:</b>	InChI=1S/C6H6N4O/c1-10-3-9-5-4(6(10)11)7-2-8-5/h2-3H,1H3,(H,7,8)
<b>InchiKey:</b>	KIQMCGMHGVXDFW-UHFFFAOYSA-N
<b>Formula:</b>	C6H6N4O
<b>SMILES:</b>	Cn1cnc2[nH]cnc2c1=O
<b>Mol. weight [g/mol]:</b>	150.14
<b>CAS:</b>	1125-39-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	-0.825		Crippen Method
mcvol	102.270	ml/mol	McGowan Method
rinsol	1969.00		NIST Webbook

## 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=C1125399&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1125399&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
<b>rinsol:</b>	Non-polar retention indices

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