

# 4-Pyrimidinol, 5-acetamido-6-amino-

<b>Inchi:</b>	InChI=1S/C6H8N4O2/c1-3(11)10-4-5(7)8-2-9-6(4)12/h2H,1H3,(H,10,11)(H3,7,8,9,12)
<b>InchiKey:</b>	LWBWVRFFKJXJQY-UHFFFAOYSA-N
<b>Formula:</b>	C6H8N4O2
<b>SMILES:</b>	CC(=O)Nc1c(N)ncnc1O
<b>Mol. weight [g/mol]:</b>	168.15
<b>CAS:</b>	50609-15-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.39		Crippen Method
logp	-0.277		Crippen Method
mcvol	119.000	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=C50609159&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C50609159&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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