

# 2-Amino-6-methyl-4-oxo-1,3,3a,7-tetrazaindene

<b>Inchi:</b>	InChI=1S/C6H7N5O/c1-3-2-4(12)11-6(8-3)9-5(7)10-11/h2H,1H3,(H3,7,8,9,10)
<b>InchiKey:</b>	PQJWDADCCRTLQZ-UHFFFAOYSA-N
<b>Formula:</b>	C6H7N5O
<b>SMILES:</b>	Cc1cc(=O)n2nc(N)nc2[nH]1
<b>Mol. weight [g/mol]:</b>	165.15
<b>CAS:</b>	72436-99-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.71		Crippen Method
logp	-1.174		Crippen Method
mcvol	112.250	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=C72436998&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C72436998&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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