

# Barbituric acid, 5-(4-pyridylmethylene)-

<b>Inchi:</b>	InChI=1S/C10H7N3O3/c14-8-7(9(15)13-10(16)12-8)5-6-1-3-11-4-2-6/h1-5H,(H2,12,13,14)
<b>InchiKey:</b>	HUPODFHCNLKIGW-UHFFFAOYSA-N
<b>Formula:</b>	C10H7N3O3
<b>SMILES:</b>	O=C1N=C(O)C(=Cc2ccncc2)C(O)=N1
<b>Mol. weight [g/mol]:</b>	217.18
<b>CAS:</b>	68160-62-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.93		Crippen Method
logp	1.512		Crippen Method
mcvol	147.490	ml/mol	McGowan Method

## 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=C68160623&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C68160623&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

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