

# 5-Carbethoxy-4-oxo-1,3,3a,7-tetrazaindene

<b>Inchi:</b>	InChI=1S/C8H8N4O3/c1-2-15-7(14)5-3-9-8-10-4-11-12(8)6(5)13/h3-4H,2H2,1H3,(H,9,10
<b>InchiKey:</b>	JPAVBMQNWIVDPU-UHFFFAOYSA-N
<b>Formula:</b>	C8H8N4O3
<b>SMILES:</b>	CCOC(=O)c1c[nH]c2ncnn2c1=O
<b>Mol. weight [g/mol]:</b>	208.17
<b>CAS:</b>	89977-78-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.27		Crippen Method
logp	-0.888		Crippen Method
mcvol	137.890	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=C89977786&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C89977786&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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