

# 1H-3-benzazepine, 4-acetamido-3-acetyl-2,3-dihydro-

<b>Inchi:</b>	InChI=1S/C14H16N2O2/c1-10(17)15-14-9-13-6-4-3-5-12(13)7-8-16(14)11(2)18/h3-6,9H,
<b>InchiKey:</b>	YIQLBHAMNZQKBA-UHFFFAOYSA-N
<b>Formula:</b>	C14H16N2O2
<b>SMILES:</b>	CC(=O)NC1=Cc2ccccc2CCN1C(C)=O
<b>Mol. weight [g/mol]:</b>	244.29
<b>CAS:</b>	3884-08-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.97		Crippen Method
logp	1.526		Crippen Method
mcvol	192.300	ml/mol	McGowan Method

## Sources

<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=C3884080&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3884080&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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