

# 13-Acetoxyanagryne

<b>Inchi:</b>	InChI=1S/C17H22N2O3/c1-11(20)22-14-5-6-18-9-12-7-13(16(18)8-14)10-19-15(12)3-2-4
<b>InchiKey:</b>	WOXXKFZZPFAEHI-UHFFFAOYSA-N
<b>Formula:</b>	C17H22N2O3
<b>SMILES:</b>	CC(=O)OC1CCN2CC3CC(Cn4c3cccc4=O)C2C1
<b>Mol. weight [g/mol]:</b>	302.37

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	1.361		Crippen Method
mcvol	227.320	ml/mol	McGowan Method
rinpole	2690.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R308444&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R308444&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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
<b>rinpole:</b>	Non-polar retention indices

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