

# 7-Angeloyl-1-formyl-6,7-dihydro-5H-pyrrolizine

<b>Inchi:</b>	InChI=1S/C13H15NO3/c1-3-9(2)13(16)17-11-5-7-14-6-4-10(8-15)12(11)14/h3-4,6,8,11H,
<b>InchiKey:</b>	LJHFLAIWOBXLFA-OQFOIZHKSA-N
<b>Formula:</b>	C13H15NO3
<b>SMILES:</b>	CC=C(C)C(=O)OC1CCn2ccc(C=O)c21
<b>Mol. weight [g/mol]:</b>	233.26

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	2.255		Crippen Method
mcvol	178.400	ml/mol	McGowan Method
rinpola	1920.00		NIST Webbook

## 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=R299637&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R299637&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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
<b>rinpola:</b>	Non-polar retention indices

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