

# 3«alpha»-Propionyloxytropene

<b>Inchi:</b>	InChI=1S/C11H19NO2/c1-3-11(13)14-10-6-8-4-5-9(7-10)12(8)2/h8-10H,3-7H2,1-2H3/t8-
<b>InchiKey:</b>	NUFSBXOAMBFLRJ-MYJAWHEDSA-N
<b>Formula:</b>	C11H19NO2
<b>SMILES:</b>	CCC(=O)OC1CC2CCC(C1)N2C
<b>Mol. weight [g/mol]:</b>	197.27

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.98		Crippen Method
logp	1.565		Crippen Method
mcvol	161.550	ml/mol	McGowan Method
rinpol	1405.00		NIST Webbook

## 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=R509598&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R509598&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
<b>rinpol:</b>	Non-polar retention indices

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