

# 3-Hydroxy-6-isobutyryloxytropone

<b>Inchi:</b>	InChI=1S/C12H21NO3/c1-7(2)12(15)16-11-5-8-4-9(14)6-10(11)13(8)3/h7-11,14H,4-6H2,
<b>InchiKey:</b>	ZCDAAJWACVZEQQ-QPBDYMMBSA-N
<b>Formula:</b>	C12H21NO3
<b>SMILES:</b>	CC(C)C(=O)OC1CC2CC(O)CC1N2C
<b>Mol. weight [g/mol]:</b>	227.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Crippen Method
logp	0.782		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
rinpol	1591.00		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=R421577&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R421577&amp;Units=SI</a>
<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>

## 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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