

# 3«beta»-Tigloyloxy-6«beta»-acetoxytropane

<b>Inchi:</b>	InChI=1S/C15H23NO4/c1-5-9(2)15(18)20-12-6-11-7-14(19-10(3)17)13(8-12)16(11)4/h5,1
<b>InchiKey:</b>	JZEPGIHACXZLFL-PWIXTEHPSA-N
<b>Formula:</b>	C15H23NO4
<b>SMILES:</b>	CC=C(C)C(=O)OC1CC2CC(OC(C)=O)C(C1)N2C
<b>Mol. weight [g/mol]:</b>	281.35

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	1.663		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
rinpol	1827.00		NIST Webbook

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R421537&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R421537&amp;Units=SI</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

Latest version available from:

<https://www.chemeo.com/cid/53-234-3/3-beta-Tigloyloxy-6-beta-acetoxytropane.pdf>

Generated by Cheméo on 2024-04-29 13:59:50.164798769 +0000 UTC m=+16688439.085376084.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.