

# 3«alpha»-Tigloyloxy-6«beta»-isobutyryloxytropan

<b>Inchi:</b>	InChI=1S/C17H27NO4/c1-6-11(4)17(20)21-13-7-12-8-15(14(9-13)18(12)5)22-16(19)10(2
<b>InchiKey:</b>	ADNCMUUXIVQCLS-QFGBMDHOSA-N
<b>Formula:</b>	C17H27NO4
<b>SMILES:</b>	CC=C(C)C(=O)OC1CC2CC(OC(=O)C(C)C)C(C1)N2C
<b>Mol. weight [g/mol]:</b>	309.40

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	2.299		Crippen Method
mcvol	249.230	ml/mol	McGowan Method
rinpol	1929.00		NIST Webbook
rinpol	1929.00		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=R421448&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R421448&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>

## 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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