

3«beta»-Tigloyloxytropene

Inchi:	InChI=1S/C13H21NO2/c1-4-9(2)13(15)16-12-7-10-5-6-11(8-12)14(10)3/h4,10-12H,5-8H2
InchiKey:	UVHGSMZRSVGDJ-WJKWCMVSA-N
Formula:	C13H21NO2
SMILES:	CC=C(C)C(=O)OC1CC2CCC(C1)N2C
Mol. weight [g/mol]:	223.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Crippen Method
logp	2.121		Crippen Method
mcvol	185.430	ml/mol	McGowan Method
rinpole	1579.00		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R421557&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpole:	Non-polar retention indices

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<https://www.chemeo.com/cid/49-255-5/3-beta-Tigloyloxytropene.pdf>

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