

3-Hydroxy-6-tigloyloxytropane

Other names:	6-Tigloyloxytropan-3-ol
Inchi:	InChI=1S/C13H21NO3/c1-4-8(2)13(16)17-12-6-9-5-10(15)7-11(12)14(9)3/h4,9-12,15H,5
InchiKey:	FSTVJNLNEVDORU-IWMMXTRQSA-N
Formula:	C13H21NO3
SMILES:	CC=C(C)C(=O)OC1CC2CC(O)CC1N2C
Mol. weight [g/mol]:	239.31

Physical Properties

Property code	Value	Unit	Source
logp	1.092		Crippen Method
mcvol	191.300	ml/mol	McGowan Method
rinpol	1835.00		NIST Webbook
rinpol	1830.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R411159&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/70-622-3/3-Hydroxy-6-tigloyloxytropane.pdf>

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