

3«alpha»-(Tigloyloxy)tropane

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: UVHGSMZRSVGWDJ-RUDMXATFSA-N
Formula: C13H21NO2
SMILES: CC=C(C)C(=O)OC1CC2CCC(C1)N2C
Mol. weight [g/mol]: 223.31
CAS: 533-08-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Crippen Method
logp	2.121		Crippen Method
mcvol	185.430	ml/mol	McGowan Method
rinpola	1917.30		NIST Webbook
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Sources

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=C533084&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/76-758-7/3-alpha-Tigloyloxy-tropane.pdf>

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