

3«alpha»-Hydroxy-6«beta»-tigloyloxytropane

Inchi: InChI=1S/C12H19NO3/c1-3-8(2)12(15)16-7-13-9-4-10(13)6-11(14)5-9/h3,9-11,14H,4-7H
InchiKey: SNECHSBCFLJKND-VSXIURAQSA-N
Formula: C12H19NO3
SMILES: CC=C(C)C(=O)OCN1C2CC(O)CC1C2
Mol. weight [g/mol]: 225.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	1.051		Crippen Method
mcvol	177.210	ml/mol	McGowan Method
rinpol	1891.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1891.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R421413&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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