

3«alpha»-Tigloyloxy-6«beta»-acetoxytropane

Inchi: InChI=1S/C15H23NO4/c1-5-9(2)15(18)20-12-6-11-7-14(19-10(3)17)13(8-12)16(11)4/h5,11-14,16-18,20
InchiKey: JZEPGIHACXZLFL-ABEMTERESA-N
Formula: C15H23NO4
SMILES: CC=C(C)C(=O)OC1CC2CC(OC(C)=O)C(C1)N2C
Mol. weight [g/mol]: 281.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	1.663		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
rinpol	1815.00		NIST Webbook
rinpol	1815.00		NIST Webbook

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=R421433&Units=SI>

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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