

3-Tigloyloxy-6,7-epoxytropane

Inchi: InChI=1S/C13H19NO3/c1-4-7(2)13(15)16-8-5-9-11-12(17-11)10(6-8)14(9)3/h4,8-12H,5-6
InchiKey: MAHIMWLGPYDSP-QPJJXVBHSA-N
Formula: C13H19NO3
SMILES: CC=C(C)C(=O)OC1CC2C3OC3C(C1)N2C
Mol. weight [g/mol]: 237.29
CAS: 1341219-18-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	1.108		Crippen Method
mcvol	180.440	ml/mol	McGowan Method
rinpol	1808.90		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=C1341219188&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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<https://www.chemeo.com/cid/113-625-2/3-Tigloyloxy-6-7-epoxytropane.pdf>

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