

3-Tigloyloxy-6,7-dihydroxytropane

Inchi: InChI=1S/C13H21NO4/c1-4-7(2)13(17)18-8-5-9-11(15)12(16)10(6-8)14(9)3/h4,8-12,15-17
InchiKey: YZFJTFVPCWEPND-QPJJXVBHSA-N
Formula: C13H21NO4
SMILES: CC=C(C)C(=O)OC1CC2C(O)C(O)C(C1)N2C
Mol. weight [g/mol]: 255.31
CAS: 526-13-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.43		Crippen Method
logp	0.063		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
rinpol	2086.40		NIST Webbook
rinpol	2074.00		NIST Webbook
rinpol	2086.40		NIST Webbook
rinpol	2074.00		NIST Webbook

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=C526136&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/120-026-9/3-Tigloyloxy-6-7-dihydroxytropane.pdf>

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