

3,6-Ditigloyloxy-7-hydroxytropane

Inchi: InChI=1S/C18H27NO5/c1-6-10(3)17(21)23-12-8-13-15(20)16(14(9-12)19(13)5)24-18(22)
InchiKey: FRQMNJFBOJQRAQ-JMQWPVDRSA-N
Formula: C18H27NO5
SMILES: CC=C(C)C(=O)OC1CC2C(O)C(OC(=O)C(C)=CC)C(C1)N2C
Mol. weight [g/mol]: 337.41
CAS: 1617-45-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.97		Crippen Method
logp	1.580		Crippen Method
mcvol	264.890	ml/mol	McGowan Method
rinpola	2429.10		NIST Webbook
rinpola	2429.10		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1617454&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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