

3«alpha»,6«beta»-Ditigloyloxy-7«beta»-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-MNSVWEGHSA-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

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.97 | | Crippen Method |
| logp | 1.580 | | Crippen Method |
| mcvol | 264.890 | ml/mol | McGowan Method |
| rinpol | 2315.00 | | 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=R421384&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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