

3,7-Dihydroxy-6-tigloyloxytropane

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|-----------------------------|--|
| Inchi: | InChI=1S/C12H19NO4/c1-3-7(2)12(16)17-8-4-9-11(15)10(5-8)13(9)6-14/h3,8-11,14-15H |
| InchiKey: | WTNSOAMJOANJTH-XVNBXDOJSA-N |
| Formula: | C12H19NO4 |
| SMILES: | CC=C(C)C(=O)OC1CC2C(O)C(C1)N2CO |
| Mol. weight [g/mol]: | 241.28 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.39 | | Crippen Method |
| logp | 0.022 | | Crippen Method |
| mcvol | 183.080 | ml/mol | McGowan Method |
| rinpola | 1955.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R421379&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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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