

3-Hydroxy-6-Tigloyloxytropane isomer

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|-----------------------------|--|
| Inchi: | InChI=1S/C13H21NO3/c1-4-8(2)13(16)17-12-6-9-5-10(15)7-11(12)14(9)3/h4,9-12,15H,5 |
| InchiKey: | FSTVJNLNEVDORU-XBXARRHUSA-N |
| Formula: | C13H21NO3 |
| SMILES: | CC=C(C)C(=O)OC1CC2CC(O)CC1N2C |
| Mol. weight [g/mol]: | 239.31 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.05 | | Crippen Method |
| logp | 1.092 | | Crippen Method |
| mcvol | 191.300 | ml/mol | McGowan Method |
| rinpol | 1894.20 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U414821&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 |
| rinpol: | Non-polar retention indices |

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