

3«alpha»-Seneciolyoxy-6«beta»-hydroxytropone

Inchi: InChI=1S/C13H21NO3/c1-8(2)4-13(16)17-10-5-9-6-12(15)11(7-10)14(9)3/h4,9-12,15H,5
InchiKey: UUQGYKIAWSKORN-WISYIIOYSA-N
Formula: C13H21NO3
SMILES: CC(C)=CC(=O)OC1CC2CC(O)C(C1)N2C
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 | 1865.00 | | NIST Webbook |
| rinpol | 1865.00 | | NIST Webbook |
| rinpol | 1865.00 | | 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=R570095&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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