

7-Senecioldretronecine

Inchi: InChI=1S/C13H19NO3/c1-9(2)7-12(16)17-11-4-6-14-5-3-10(8-15)13(11)14/h3,7,11,13,15
InchiKey: JWVMHVYNWULPCC-AAEUAGOBBSA-N
Formula: C13H19NO3
SMILES: CC(C)=CC(=O)OC1CCN2CC=C(CO)C12
Mol. weight [g/mol]: 237.29

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.68 | | Crippen Method |
| logp | 0.871 | | Crippen Method |
| mcvol | 187.000 | ml/mol | McGowan Method |
| rinpol | 1816.00 | | NIST Webbook |
| rinpol | 1816.00 | | NIST Webbook |
| rinpol | 1816.00 | | NIST Webbook |
| rinpol | 1863.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R495231&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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