

Integerrimine

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| Other names: | Inegerrimine Intergerrimine Pyrrolizine-2,7-dione, 3-ethylidene-3,4,5,6,9,11,13,14,14a,14b,decahydro-6-hydroxy-5,6-dimethyl(1,6)dioxacycl Senecionan-11,16-dione, 12-hydroxy-, (15E)- Squalidin Squalidine |
| Inchi: | InChI=1S/C18H25NO5/c1-4-12-9-11(2)18(3,22)17(21)23-10-13-5-7-19-8-6-14(15(13)19) |
| InchiKey: | HKODIGSRFALUTA-IKZAEVNJSA-N |
| Formula: | C18H25NO5 |
| SMILES: | <chem>CC=C1CC(C)C(C)(O)C(=O)OCC2=CCN3CCC(OC1=O)C23</chem> |
| Mol. weight [g/mol]: | 335.39 |
| CAS: | 480-79-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.40 | | Crippen Method |
| logp | 1.193 | | Crippen Method |
| mcvol | 254.030 | ml/mol | McGowan Method |
| rinpol | 2362.00 | | NIST Webbook |
| rinpol | 2350.00 | | NIST Webbook |
| rinpol | 2355.00 | | NIST Webbook |
| rinpol | 2367.00 | | NIST Webbook |
| rinpol | 2402.00 | | NIST Webbook |
| rinpol | 2370.00 | | NIST Webbook |
| rinpol | 2402.00 | | NIST Webbook |
| rinpol | 2352.00 | | NIST Webbook |
| rinpol | 2402.00 | | NIST Webbook |
| rinpol | 2367.00 | | 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 |

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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