

narwedine

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| Other names: | 6H-Benzofuro[3a,3,2-ef][2]benzazepin-6-one, 4a,5,9,10,11,12-hexahydro-3-methoxy-11-methyl-(4aR,8aR)-rel |
| Inchi: | InChI=1S/C17H19NO3/c1-18-8-7-17-6-5-12(19)9-14(17)21-16-13(20-2)4-3-11(10-18)15(|
| InchiKey: | QENVUHCAYYXAROT-UHFFFAOYSA-N |
| Formula: | C17H19NO3 |
| SMILES: | COc1ccc2c3c1OC1CC(=O)C=CC31CCN(C)C2 |
| Mol. weight [g/mol]: | 285.34 |
| CAS: | 1668-86-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.08 | | Crippen Method |
| logp | 2.058 | | Crippen Method |
| mcvol | 213.040 | ml/mol | McGowan Method |
| rinpol | 2414.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| 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=C1668866&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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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