

9(10H)-Acridinone, 1-hydroxy-2,3,4-trimethoxy-10-methyl-

Other names: 9-Acridanone, 1-hydroxy-2,3,4-trimethoxy-10-methyl-

Normelicopicine

O-Normelicopicine

Inchi: InChI=1S/C17H17NO5/c1-18-10-8-6-5-7-9(10)13(19)11-12(18)15(21-2)17(23-4)16(22-3)

InchiKey: UGEKWKMLXLFVIY-UHFFFAOYSA-N

Formula: C17H17NO5

SMILES: COc1c(OC)c(OC)c2c(c1O)c(=O)c1cccc1n2C

Mol. weight [g/mol]: 315.32

CAS: 7008-68-6

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.70 | | Crippen Method |
| logp | 2.423 | | Crippen Method |
| mcvol | 227.040 | ml/mol | McGowan Method |
| rinpol | 2854.00 | | NIST Webbook |
| rinpol | 2854.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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=C7008686&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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