

5,6-Dihydro-7,9-dimethoxy-7H-pyrrolizine

Inchi: InChI=1S/C10H17NO2/c1-12-7-8-3-5-11-6-4-9(13-2)10(8)11/h3,9-10H,4-7H2,1-2H3/t9-,1
InchiKey: NTHXXXBCILAZIH-RGURZIINSA-N
Formula: C10H17NO2
SMILES: COCC1=CCN2CCC(OC)C12
Mol. weight [g/mol]: 183.25

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -0.62 | | Crippen Method |
| logp | 0.662 | | Crippen Method |
| mcvol | 147.460 | ml/mol | McGowan Method |
| rinpol | 1413.00 | | NIST Webbook |
| rinpol | 1415.00 | | NIST Webbook |
| rinpol | 1415.00 | | NIST Webbook |
| rinpol | 1413.00 | | 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=R240492&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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