



Formula: C<sub>20</sub>H<sub>26</sub>N<sub>2</sub>O<sub>4</sub>

MW: 358.44

CAS: 207801-27-2

MDL: MFCD03225485

TNP: TNP00087



LogP: 2.63

LogS: -4.02

Acceptors: 4

Donors: 5

Rotation Bonds: 1

Chiral Centers: 5

N+O: 6

LIPINSKY: 4

IUPAC: (3S,4aS,5aS,4R,14aR)-3-hydroxy-1,2,3,4,5,11,14,14a,4a,5a-decahydrobenzo[1,2-g] indolo[2,3-a]quinolizine-4-carboxylic acid, oxamethane

Smiles:

c12c(c3cccc3[nH]1)CCN1[C@H]2(C[C@@H]2(C([C@](=O)O)[C@H](CC[C@@H]2C1)O)).O