



Formula: C37H41N5O11

MW: 731.76

CAS: 379-79-3

MDL: MFCD01104976

TNP: TNP00163



LogP: 1.78

LogS: -5.24

Acceptors: 11

Donors: 7

Rotation Bonds: 5

Chiral Centers: 8

N+O: 16

LIPINSKY: 1

Info: Vasoconstrictor found in ergot of Central Europe

IUPAC:

Smiles:

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N12C(OC(N[C@](C3C=C4c5c6c([nH]cc6CC4N(C3)C)ccc5)=O)(C)C1=O)(C1N(C(=O)C2Cc2ccc  
cc2)CCC1)O.C(C(C(C(=O)O)O)O)(=O)O
```

THERAPEUTIC CATEGORY: Antimigraine. In Veterinary tartrate used as oxytocic

