



Formula: C37H41N5O11

MW: 731.76

CAS: 379-79-3

TNP NUMBER: TNP00163

MDL NUMBER: MFCD01104976

Smiles:

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(=O)O)O)O)(=O)O

Vasoconstrictor found in ergot of Central Europe

THERAPEUTIC CATEGORY: Antimigraine. In Veterinary tartrate used as oxytocic

ACCEPTORS: 11

DONORS: 7

ROTATION BONDS: 5

N+O: 16

Chiral Centers: 8

LogP: 1.78

LogS: -5.24

LIPINSKI: 1

