



Formula: C31H39N5O5

MW: 561.68

CAS: 564-36-3

TNP NUMBER: TNP00323

MDL NUMBER: MFCD07189848

Smiles:

c12c3cccc1C=1[C@H](N(C[C@@H](C1)C(NC1(O[C]4(N(C1=O)[C@H](C(N1[C@H]4(CCC1))=O)C(C)C)O)C(C)C)=O)C)(Cc2c[nH]3)

THERAPEUTIC CATEGORY: Vasoconstrictor (Specific in migraine)

VET THERAP CATEGORY: Has been used as oxytocic

REFERENCE: Merck 13, 3678

SOURCE: Natural ergot alkaloid derived from lysergic acid. Isolation from Ergot.

ACCEPTORS: 5

DONORS: 3

ROTATION BONDS: 1

N+O: 10

Chiral Centers: 6

LogP: 4.5

LogS: -5.86

LIPINSKI: 3

Synonyms:

ERGOCORNINE;12'-HYDROXY-2',5'-ALPHA-BIS(1-METHYL-ETHYL)ERGOTAMAN-3',6',18-T
RIONE;18-trione,12