



Formula: C₃₂H₄₁N₅O₅

MW: 575.71

CAS: 511-09-1

TNP NUMBER: TNP00320

MDL NUMBER: MFCD02185004

Smiles:

```
O[C@@]12N([C@@H](CC(C)C)C(N3[C@H]1(CCC3))=O)C([C](O2)(NC(=O)[C@@H]1C=C2c3c4c(C[C@H]2(N(C1)C))c[nH]c4ccc3)C(C)C)=O
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THERAPEUTIC CATEGORY: Vasoconstrictor

VET THERAP CATEGORY: Has been used as an oxytoxic

REFERENCE: Larson, B.T., Alkaloid binding and activation D2 dopamine receptors in cell culture. J. Anim. Sci. 77, 942, (1999) abstract Merck Index, 12th Ed. 3689

SOURCE: from Ergot

ACCEPTORS: 5

DONORS: 3

ROTATION BONDS: 2

N+O: 10

Chiral Centers: 6

LogP: 5

LogS: -6.09

LIPINSKI: 3

Synonyms: 12