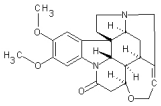

Formula: C23H26N2O4

MW: 394.47

CAS: 357-57-3

MDL: MFCD00065029

TNP: TNP00116

LogP: 1.35

LogS: -3.09

Acceptors: 4

Donors: 0

Rotation Bonds: 2

Chiral Centers: 6

N+O: 6

LIPINSKY: 4

IUPAC: (11S,18S,22S,1R,20R,21R)-4,5-dimethoxy-12-oxa-8,17-diazaheptacyclo[15.5.2.0<1,18>.0<2,7>.0<8,22>.0<11,21>.0<15,20>]tetracosa-2,4,6,14-tetraen-9-one

Smiles: N12C3C4(c5c2cc(c(c5)OC)OC)C2N(CC=5C(C2)C3C(CC1=O)OCC5)CC4

Merck 13 Reference: Monograph Number: 0001440

Title: Brucine

CAS Registry Number: 357-57-3

CAS Name: 2,3-Dimethoxystrychnidin-10-one

Additional Names: 10,11-dimethoxystrychnine

Molecular Formula: C23H26N2O4

Molecular Weight: 394.46.

Percent Composition: C 70.03%, H 6.64%, N 7.10%, O 16.22%

Literature References: Toxic alkaloid resembling strychnine. Isoln from Strychnos seeds (Strychnos nux-vomica L. and S. ignatii Berg., Loganiaceae): C. Hartwick, P. Geiger, Arch. Pharm. 239, 491 (1901). Prepn from strychnine, q.v.: E. Tedeschi et al., Tetrahedron 24, 4573 (1968). 13C-NMR study: E. Wenkert et al., J. Org. Chem. 43, 1099 (1978). Electrophoretic determn in seeds: Y.-Y. Zong, C. Che, Planta Med. 61, 456 (1995). Toxicity data: M. H. Malone et al., J. Ethnopharmacol. 35, 295 (1992). Use as reagent for sulfur compounds: M. K. Tummuru et al., Analyst 109, 1105 (1984); for nitrates: J. Masini et al., Anal. Chem. 69, 1077 (1997). Review of structural elucidation: H. L. Holmes, Elucidation of the Structure of Strychnine and Brucine in The Alkaloids vol. I, R. H. F. Manske, Ed. (Academic Press, New York, 1950) pp 377-420.

Properties: Needles from acetone + water, mp 178. [a]D -127 (chloroform), -85 (in abs alcohol). uv max (ethanol): 263, 301 nm (log e 4.09, 3.93).

Melting point: mp 178

Optical Rotation: [a]D -127 (chloroform), -85 (in abs alcohol)

Absorption maximum: uv max (ethanol): 263, 301 nm (log e 4.09, 3.93)

Derivative Type: Tetrahydrate

Properties: Monoclinic prisms. Also forms a dihydrate. Very bitter taste. Bitterness threshold 1:220,000. Very poisonous! Handle dry powder in hood only. Becomes anhydr at 100. One gram dissolves in 0.8 ml methanol, 1.3 ml alcohol, 5 ml chloroform, 25 ml ethyl acetate, 36 ml glycerol, about 100 ml benzene, 187 ml ether, 1320 ml water, 750 ml boiling water. pH of satd water soln 9.5. pK1 6.04, pK2 11.7. LD50 in mice (mg/kg): 12.0 i.v.; 62.0 i.p.; 150.0 orally (Malone).

pKa: pK1 6.04, pK2 11.7

Toxicity data: LD50 in mice (mg/kg): 12.0 i.v.; 62.0 i.p.; 150.0 orally (Malone)

Use: Denaturing alcohol and oils; in analytical chemistry; for separating racemic mixtures. Addition agent to lubricants.

Therap-Cat: CNS stimulant.