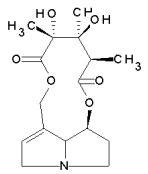

Formula: C16H23NO6

MW: 325.36

CAS: 315-22-0

MDL: MFCD03225492

TNP: TNP00298

MONOCROTALIN; MONOCROTALINE; CROTALIN; CROTALINE; (13-alpha,14-alpha)-14,19-dihydro-12,13-dihydroxy-20-norcrotalanan-11,15-dio; (13-alpha,14-alpha)-14,19-Dihydro-12,13-dihydroxy-20-norcrotalanan-11,15-dione; (2,3,4-gh)pyrrolizine-2,6(3h)-dione,(4,5,8,10,12,13,1

LogP: 0.34

LogS: -3.3

Acceptors: 6

Donors: 2

Rotation Bonds: 0

Chiral Centers: 5

N+O: 7

LIPINSKY: 4

IUPAC: (1S,5S,4R,6R)-5,6-dihydroxy-4,5,6-trimethyl-2,8-dioxa-13-azatricyclo[8.5.1.0]hexadec-10-ene-3,7-dione

Smiles: O=C1O[C@@H]2C3N(CC2)CC=C3COC([C@]([C@@]([C@H]1C)(C)O)(C)O)=O

SOURCE: Toxic pyrrolizidine alkaloid isolated from Crotallaria spp.

Specification: Miscellaneous Natural Products MONOCROTALINE Chemical Properties:

 mp 204 C (dec.)(lit.) alpha -54.8o (C=5 IN CHLOROFORM) storage temp. 2-8C Merck 13,6274 Safety Information Hazard Codes T Risk Statements 25-40-35 Safety Statements 36/37/39-45 RIDADR UN 1544 6.1/PG 3 WGK Germany 3 RTECS QB3140000 HazardClass 6.1(b) PackingGroup IIIMONOCROTALINE Usage And Synthesis Chemical Properties:

White to light tan powder MONOCROTALINE

Merck 13 Reference: Monograph Number: 0006274

Title: Monocrotaline

CAS Registry Number: 315-22-0

CAS Name: (13a,14a)-14,19-Dihydro-12,13-dihydroxy-20-norcrotolanan-11,15-dione

Additional Names: crotaline; MCT

Manufacturers' Codes: NSC-28693; NCI-C56462

Molecular Formula: C16H23NO6

Molecular Weight: 325.36.

Percent Composition: C 59.06%, H 7.13%, N 4.30%, O 29.50%

Literature References: Toxic pyrrolizidine alkaloid isolated from Crotalaria spp. Isoln: R. Adams, E. F. Rogers, J. Am. Chem. Soc. 61, 2815 (1939); R. B. Tinker, W. M. Lauter, Econ. Bot. 10, 254 (1956); C. C. J. Culvenor, L. W. Smith, Aust. J. Chem. 16, 239 (1963). Structure: R. Adams et al., J. Am. Chem. Soc. 74, 5612 (1952). Stereochemistry: D. J. Robins, D. H. G. Crout, J. Chem. Soc. C 1969, 1386. Crystal structure: H. Stoeckli-Evans, Acta Crystallogr. B35, 231 (1979). Stereoselective synthesis: H. Niwa et al., Tetrahedron 48, 10531 (1992). ELISA measurment: M. A. Bober et al., Toxicon 27, 1059 (1989). Toxicology: P. M. Newberne et al., Toxicol. Appl. Pharmacol. 18, 387 (1971); R. A. Roth et al., ibid. 60, 193 (1981). Review of carcinogenicity studies: IARC Monographs 10, 291-302, 333-342 (1976). Comprehensive reviews: L. Bull et al., The Pyrrolizidine Alkaloids (North-Holland, Amsterdam, 1968) 293 pp; D. J. Robins, Fortschr. Chem. Org. Naturst. 41, 115-203 (1982). Review of pulmonary toxicity: D. W. Wilson et al., Crit. Rev. Toxicol. 22, 307-325 (1992).

Properties: White prisms from abs ethanol, mp 197-198 (dec). [a]D26 -54.7 (c = 5.054 in chloroform). Also reported as colorless crystals from ethanol, mp 187-190 (dec). [a]D12 -55.0 (c = 0.16 in CHCl3). uv max (96% ethanol): 217 nm (log e 3.32), Sim