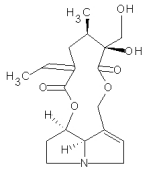

Formula: C18H25NO6

MW: 351.4

CAS: 480-54-6

MDL: MFCD05675778

TNP: TNP00104

LogP: 12.02

LogS: -9.25

Acceptors: 6

Donors: 2

Rotation Bonds: 2

Chiral Centers: 4

N+O: 7

LIPINSKY: 3

IUPAC: (7S,1R,6R,17R)-4-ethylidene-7-hydroxy-7-(hydroxymethyl)-6-methyl-2,9-dioxa-14-azatricyclo[9.5.1.0<14,17>]heptadec-11-ene-3,8-dione

Smiles:
C1(/C(C[C@H]([C@](C(OCC=2[C@@H]3([C@H](CCN3CC2)O1))=O)(O)CO)C)=C/C)=O

REFERENCE: Retrorsine

SOURCE: Hepatoxic pyrrolizidine alkaloid; common constituent of Senecio species.

Merck 13 Reference: Monograph Number: 0008253

Title: Retrorsine

CAS Registry Number: 480-54-6

CAS Name: 12,18-Dihydroxysenecionan-11,16-dione

Additional Names: b-longilobine

Molecular Formula: C18H25NO6

Molecular Weight: 351.39.

Percent Composition: C 61.52%, H 7.17%, N 3.99%, O 27.32%

Literature References: Hepatotoxic pyrrolizidine alkaloid; common constituent of Senecio species. Isoln from Senecio retrorsus DC, Compositae: R. H. F. Manske, Can. J. Chem. 5, 651 (1931); G. Barger et al., J. Chem. Soc. 1935, 11; from Crotalaria usaramoensis E. G. Baker, Leguminosae: C. C. J. Culvenor, L. W. Smith, Aust. J. Chem. 19, 2127 (1966). Structure: S. M. H. Christie et al., J. Chem. Soc. 1949, 1700; E. C. Leisegang, F. L. Warren, ibid. 1950, 702. Identity with b-longilobine: F. L. Warren et al., J. Am. Chem. Soc. 72, 1421 (1950). Review and evaluation of toxicity and carcinogenicity studies: IARC Monographs 10, 303-312, 333-342 (1976). Comprehensive reviews of pyrrolizidine alkaloids: L. B. Bull et al., The Pyrrolizidine Alkaloids (North Holland, Amsterdam, 1968) 293 pp; F. L. Warren in The Alkaloids vol. 12, R. H. F. Manske, Ed. (Academic Press, New York, 1970) pp 245-331.

Properties: Crystals from ethyl acetate, mp 212 (Barger et al.); 216-216.5 (Bull et al.). [a]D18 -17.6 (c = 1.99 in ethanol). uv max (water): 217 nm (log e 3.85). Readily sol in alcohol, chloroform; slightly sol in water, acetone, ethyl acetate; practically insol in ether.

Melting point: mp 212 (Barger et al.); 216-216.5 (Bull et al.)

Optical Rotation: [a]D18 -17.6 (c = 1.99 in ethanol)

Absorption maximum: uv max (water): 217 nm (log e 3.85)

Derivative Type: N-Oxide

Additional Names: Isatidine; 12,18-dihydroxysenecionan-11,16-dione-4-oxide; retrorsine N-oxide

Molecular Formula: C18H25NO7

Molecular Weight: 367.39.

Percent Composition: C 58.85%, H 6.86%, N 3.81%, O 30.48%

Literature References: Isolated from Senecio species. Review and evaluation of carcinogenicity and toxicity studies: IARC Monographs 10, 269-273 (1976).

Properties: Crystals from ethanol, mp 140.5-141.5 (Christie et al.).

Melting point: mp 140.5-141.5 (Christie et al.)