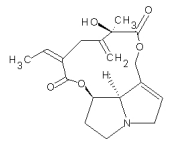

Formula: C18H23NO5

MW: 333.38

CAS: 480-81-9

TNP NUMBER: TNP00334

MDL NUMBER: MFCD07189862

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

Smiles: C[C@]1(C(CC(/C(O[C@@H]2CCN3[C@@H]2(C(=CC3)COC1=O))=O)=C/C)=C)O

ACCEPTORS: 5

DONORS: 1

ROTATION BONDS: 0

N+O: 6

Chiral Centers: 3

LogP: 2.49

LogS: -4.17

LIPINSKI: 4

Monograph Number: 0008526

Title: Seneciphylline

CAS Registry Number: 480-81-9

CAS Name: 13,19-Didehydro-12-hydroxysenecionan-11,16-dione

Additional Names: jacodine; a-longilobine

Molecular Formula: C18H23NO5

Molecular Weight: 333.38.

Percent Composition: C 64.85%, H 6.95%, N 4.20%, O 24.00%

Literature References: Hepatotoxic pyrrolizidine alkaloid, common constituent of Senecio species. Isoln from Senecio platyphllus DC. Compositae: A. Orechoff, W. Tiedebel, Ber. 68, 650 (1935); from S. jacobaea L.: G. Barger, J. J. Blackie, J. Chem. Soc. 1937, 584; from Crotalaria juncea L. Leguminosae: R. Adams, M. Gianturco, J. Am. Chem. Soc. 78, 1919 (1956). Identity with a-longilobine: R. Adams, J. H. Looker, ibid. 73, 134 (1951). Identity with jacodine: R. B. Bradbury, C. C. J. Culvenor, Chem. Ind. (London) 1954, 1021. Structural study: R. Adams et al., J. Am. Chem. Soc. 74, 700 (1952). Revised structure: S. Masume, Chem. Ind. (London) 1959, 21. Review and evaluation of toxicity and carcinogenicity studies: IARC Monographs 10, 319-325, 333-342 (1976). Comprehensive reviews of seneciphylline and other pyrrolizidine alkaloids: L. 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: Small rhombic platelets from hot alcohol or acetone, mp 217-218. [a]D -128 (chloroform). Easily sol in chloroform, ethylene chloride; less sol in alc, acetone. Difficultly sol in ether, ligroin.

Melting point: mp 217-218

Optical Rotation: [a]D -128 (chloroform)

Synonyms:
JACODINE;ALPHA-LONGILOBINE;SENECIPHYLLIN;(15cis)-12-Hydroxy-13,19-didehydrosenecionan-11,16-dione;13,19-didehydro-12-hydroxysenecionan-11,16-dione;16-dione,13,19-didehy

dro-12-hydroxy-senecionan-1;16-dione,13,19-didehydro-12-hydroxy-senecionin-1;NSC 30622

CAS:480-81-9

MF:C18H23NO5

MW:333.38

EINECS:

Product Categories: SENECIPHYLLIN

Chemical Properties: mp 217C Stability:Stable, but reacts with oxygen in the air. Incompatible with alkali, oxidizing agents. Store under inert gas.

Safety Information: Risk Statements 23/24/25 Safety Statements 1-20-24/25-45 RIDADR 1544 HazardClass 6.1(b) PackingGroup III SENECIPHYLLIN

Usage And Synthesis:

Chemical Properties: white powder General DescriptionWhite powder. Air & Water ReactionsReacts slowly with atmospheric oxygen. . Insoluble in water. Reactivity ProfileSENECIPHYLLIN is readily hydrolyzed with alkali; SENECIPHYLLIN reacts readily with oxidizing agents . Fire HazardFlash point data are not available for SENECIPHYLLIN, but SENECIPHYLLIN is probably combustible. SENECIPHYLLIN