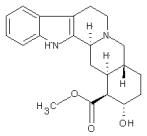

Formula: C21H26N2O3

MW: 354.45

CAS: 483-10-3

MDL: MFCD02114025

TNP: TNP00252

RAUHIMBINE; 17ALPHA-HYDROXYYOHIMBAN-16BETA-CARBOXYLIC ACID METHYL ESTER; CORYNANTHINE; CORYNANTHINE DIHYDRATE; corynanthine free base; methyl (16beta,17alpha)-17-hydroxyyohimban-16-carboxylate; CORYNANTHINE HCL(RG); Corynanthin

LogP: 2.14

LogS: -4.12

Acceptors: 3

Donors: 2

Rotation Bonds: 1

Chiral Centers: 5

N+O: 5

LIPINSKY: 4

IUPAC: methyl (3S,4S,4aS,5aS,14aR)-3-hydroxy-1,2,3,4,5,11,14,14a,4a,5a-decahydrobenzo[3,2-g]indolo[2,3-a]quinolizine-4-carboxylate

Smiles:
c12c(c3ccccc3[nH]1)CCN1[C@H]2(C[C@@H]2([C@H](C(=O)OC)[C@@H](O)CC[C@@H]2(C

1)))

SOURCE: from bark Pseudocichona africana Chev., Corynanthe johimbe K. Schum., Rubiaceae and Rauwolfia serpentina (L.) Benth., Apocynaceae

Specification: Alkaloids CORYNANTHINE Chemical Properties:

 mp 225-230C storage temp. 2-8C Safety Information Risk Statements 25 Safety Statements 1-20-45 RIDADR 1544 WGK Germany 3 CORYNANTHINE Usage And Synthesis CORYNANTHINE

Merck 13 Reference: Monograph Number: 0002573

Title: Corynanthine

CAS Registry Number: 483-10-3

CAS Name: (16b,17a)-17-Hydroxyyohimban-16-carboxylic acid methyl ester

Additional Names: rauhimbine

Molecular Formula: C21H26N2O3

Molecular Weight: 354.44.

Percent Composition: C 71.16%, H 7.39%, N 7.90%, O 13.54%

Literature References: From bark of Pseudocinchona africana Chev., Corynanthe johimbe K. Schum., Rubiaceae and Rauwolfia serpentina (L.) Benth., Apocynaceae: Raymond-Hamet, Compt. Rend. 212, 305 (1941); Jorio, Ann. Chim. Farm. 1939, 50, C.A. 33, 93069 (1939); Le Hir et al., Ann. Pharm. Fr. 11, 546 (1953); Hofmann, Helv. Chim. Acta 37, 314 (1954). Identity with rauhimbine: idem, ibid. 849. Structure and stereochemistry: Janot et al., Bull. Soc. Chim. Fr. 1952, 1085; 1961, 637.

Properties: Stout prisms from acetone, dec 225-226. [a]D19 -85 (c = 0.5 in pyridine). uv max (methanol): 226, 283, 290 nm (log e 4.56, 3.87, 3.79). Practically insol in water or petr ether. Sol in 40 parts of boiling chloroform, in 60 parts of boiling benzene, in 20 parts of boiling ethyl acetate, in 5 parts of boiling alcohol.

Optical Rotation: [a]D19 -85 (c = 0.5 in pyridine)

Absorption maximum: uv max (methanol): 226, 283, 290 nm (log e 4.56, 3.87, 3.79)

Derivative Type: O,N-Dibutyrylcorynanthine hydrochloride

Literature References: Prepn: Reiser et al., US 2975183 (1961 to Chemische Werke Albert).

Properties: Crystals from benzene, mp 208-210.

Melting point: mp 208-210

Derivative Type: O,N-Dipropionylcorynanthine hydrochloride

Literature References: Prepn: Reiser et al., loc. cit.

Properties: Crystals from isopropanol, mp 236-237.

Melting point: mp 236-237