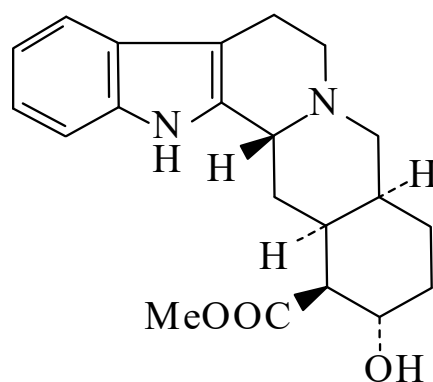




>>Entry Name: Isorauhimbine

Synonym(s): Methyl (3 β ,16 β ,17 α ,20 α)-17-hydroxy-yohimban-16-carboxylate, 9Cl. 3-*epi*- α -Yohimbine. 3-Epirauwolscline. Isorauwolscline. Alkaloid Su 3078. Epi- α -yohimbine



Absolute
configuration

CAS Registry Number: 483-09-0

Molecular Formula: C₂₁H₂₆N₂O₃

Molecular Weight: 354.448

Accurate Mass: 354.194343

Percentage Composition: C 71.16%; H 7.39%; N 7.90%; O 13.54%

Biological Source: Alkaloid from *Rauwolfia serpentina* and *Voacanga africana* (Apocynaceae)

Physical Description: Prisms (MeOH aq.)

Melting Point: Mp 225°

Optical Rotation: [α]_D²⁰ -104 (c, 0.5 in Py)

Other Data: Polymorphs having lower Mps are formed from other solvs.

>>Derivative: Hydrochloride

Physical Description: Prisms (MeOH/Et₂O)

Melting Point: Mp 235-240 dec.°

Optical Rotation: [α]_D²⁶ -75 (c, 1.0 in H₂O)

>>Derivative: Methiodide

Melting Point: Mp 234-238 dec.°

Optical Rotation: [α]_D²⁵ -28 (c, 1.0 in EtOH)

References:

Hofmann, A., *Helv. Chim. Acta*, 1954, **37**, 314, (*isol*)

Bader, F.E. *et al.*, *J.A.C.S.*, 1955, **77**, 3547, (*isol, struct*)

Goutarel, R. *et al.*, *Helv. Chim. Acta*, 1957, **40**, 156, (*ir, struct, stereochem*)

Töke, L. *et al.*, *J.O.C.*, 1973, **38**, 2496, (*synth, pmr, ir, ms*)

Honty, K. *et al.*, *J.O.C.*, 1982, **47**, 5111, (*synth*)