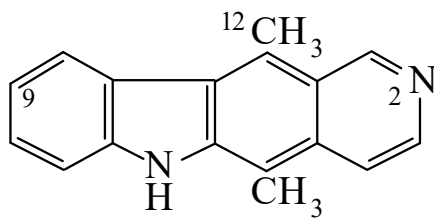




>>Entry Name: Ellipticine

Synonym(s): 5,11-Dimethyl-6*H*-pyrido[4,3-*b*]carbazole, 9Cl. NSC 71795



CAS Registry Number: 519-23-3

Type of Compound Code(s): VX5840 XA1950

Molecular Formula: C₁₇H₁₄N₂

Molecular Weight: 246.311

Accurate Mass: 246.115698

Percentage Composition: C 82.90%; H 5.73%; N 11.37%

Biological Source: Alkaloid from *Ochrosia elliptica* and several other *Ochrosia* spp. and from *Aspidosperma subincanum* and *Bleekeria vitiensis* (Apocynaceae)

Use/Importance: Shows broad-spectrum antineoplastic activity. An intercalating agent. Cytochrome P-450 (CYPIA) inhibitor

Physical Description: Yellow needles (MeOH), orange rods or rosettes (AcOH or CHCl₃)

Melting Point: Mp 311-315 dec.°

Calculated Log P Data: Log P 4.37 (calc)

UV: [neutral] λ_{max} 224 (ε 30200); 237 (sh) (ε 26900); 245 (sh) (ε 21900); 275 (ε 57500); 285 (ε 75900); 293 (ε 70800); 331 (ε 7080); 346 (ε 5010); 380 (ε 3800); 400 (ε 3800) (EtOH) (Derep) [neutral] λ_{max} 239 (ε 17000); 277 (ε 40700); 286 (ε 57500); 294 (ε 55000); 332 (ε 4460); 382 (ε 4080); 400 (ε 3400) (EtOH) (Berdy)

Hazard & Toxicity: LD₅₀ (mus, orl) 178 mg/kg. Exp. adverse cardiovascular effects. Mutagen ; BERDY HAZD : LD₅₀ (mus, ivn) 20 mg/kg , LD₅₀ (mus, orl) 190 mg/kg

Aldrich: 28573-0

Fluka: 45145

Sigma: E3380

>>Derivative: N²-Me

Synonym(s): N-Methylellipticine

Type of Compound Code(s): VX5840

Molecular Formula: C₁₈H₁₇N₂⁽⁺⁾

Molecular Weight: 261.346

Accurate Mass: 261.139173

Percentage Composition: C 82.72%; H 6.56%; N 10.72%

Biological Source: Minor quaternary alkaloid from the bark of *Aspidosperma subincanum* (Apocynaceae)

>>Derivative: N²-Me, iodide

Molecular Formula: C₁₈H₁₇IN₂

Molecular Weight: 388.25

Accurate Mass: 388.043646

Percentage Composition: C 55.69%; H 4.41%; I 32.69%; N 7.22%

Melting Point: Mp 360 dec.°

>>Derivative: N²-Me, nitrate

Molecular Formula: C₁₈H₁₇N₃O₃

Molecular Weight: 323.351

Accurate Mass: 323.126992

Percentage Composition: C 66.86%; H 5.30%; N 13.00%; O 14.84%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 293-304 dec.°

>>Derivative: N²-Oxide

Synonym(s): Ellipticine N²-oxide

CAS Registry Number: 37687-33-5

Type of Compound Code(s): VX5840

Molecular Formula: C₁₇H₁₄N₂O

Molecular Weight: 262.31

Accurate Mass: 262.110613

Percentage Composition: C 77.84%; H 5.38%; N 10.68%; O 6.10%

Biological Source: Alkaloid from *Ochrosia vieillardii*, *Ochrosia moorei* and *Strychnos dinklagei* (Apocynaceae, Strychnaceae)

Physical Description: Noncryst.