



Formula: C₁₂H₁₀N₂

MW: 182.22

CAS: 486-84-0

TNP NUMBER: TNP00419

MDL NUMBER: MFCD00004957

IUPAC: methylbeta-carboline

Smiles: c1ccc2c([nH]c3c2ccnc3C)c1

Harmane 98%, From Bark of Sickingia rubra

ACCEPTORS: 0

DONORS: 1

ROTATION BONDS: 0

N+O: 2

Chiral Centers: 0

LogP: 3.18

LogS: -3.84

LIPINSKI: 4

Monograph Number: 0004630

Title: Harman

CAS Registry Number: 486-84-0

CAS Name: 1-Methyl-9H-pyrido[3,4-b]indole

Additional Names: 3-methyl-4-carboline; 2-methyl-b-carboline; aribine; loturine; passiflorin

Molecular Formula: C₁₂H₁₀N₂

Molecular Weight: 182.22.

Percent Composition: C 79.10%, H 5.53%, N 15.37%

Literature References: From bark of *Sickingia rubra* (Mart.) K. Schum. (*Arariba rubra* Mart.), Rubiaceae; *Symplocus racemosa* Roxb., Symplocaceae; and *Passiflora incarnata* L., Passifloraceae: Rieth, Wohler, Ann. 120, 247 (1861); Spath, Monatsh. Chem. 40, 351; 41, 401 (1920); Neu, *Arzneim.-Forsch.* 4, 601 (1954). Structure: Neu, *ibid.* 6, 94 (1956). Synthesis: Harvey, Robson, *J. Chem. Soc.* 1938, 97; Snyder et al., *J. Am. Chem. Soc.* 70, 222 (1948); Clemo, Holt, *J. Chem. Soc.* 1953, 1313; Kametani et al., *ibid.* (C) 1968, 1006. Isoln from cigarette smoke: Poindexter, Carpenter, *Chem. Ind. (London)* 1962, 176. Toxicity study: E. B. Sigg et al., *Arch. Int. Pharmacodyn.* 149, 164 (1964).

Properties: Bitter orthorhombic crystals from heptane + cyclohexane, mp 237-238. Exhibits bright blue fluorescence in uv light. pKa: 7.37, 14.6. uv max (methanol): 234, 287, 347 nm (log e 4.57, 4.21, 3.66). Absorption and fluorescence spectra: O. S. Wolfbeis et al., *Monatsh. Chem.* 113, 509 (1982). Practically insol in water. Sol in dil acids. LD50 i.p. in mice: 50 mg/kg (Sigg).

Melting point: mp 237-238

pKa: pKa: 7.37, 14.6

Absorption maximum: uv max (methanol): 234, 287, 347 nm (log e 4.57, 4.21, 3.66)

Toxicity data: LD50 i.p. in mice: 50 mg/kg (Sigg)

Derivative Type: Hydrochloride

Molecular Formula: C₁₂H₁₀N₂.HCl

Molecular Weight: 218.68.

Percent Composition: C 65.91%, H 5.07%, N 12.81%, Cl 16.21%

Properties: Rosettes of needles from ethanol + 20% HCl in water, sublimes at 120-130.

