



Formula: C₁₂H₁₀N₂

MW: 182.22

CAS: 486-84-0

MDL: MFCD00004957

TNP: TNP00419



LogP: 3.81

LogS: -4.42

Acceptors: 0

Donors: 1

Rotation Bonds: 0

Chiral Centers: 0

N+O: 2

LIPINSKY: 4

Info: Harmane 98%, From Bark of Sickingia rubra

IUPAC: methylbeta-carboline

Smiles: c1ccc2c([nH]c3c2ccnc3C)c1

Merck 13 Reference: 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); Sp