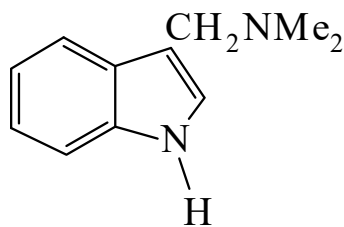




>>Entry Name: 3-(Dimethylaminomethyl)indole

ENTRY UNDER REVIEW

Synonym(s): *N,N*-Dimethyl-1*H*-indole-3-methanamine, 9Cl. **Gramine**. Donaxine. Doranine



CAS Registry Number: 87-52-5

Related CAS Registry Numbers(s): 6170-37-2

Type of Compound Code(s): WA4500 WI2500 VX4000

Molecular Formula: C₁₁H₁₄N₂

Molecular Weight: 174.245

Accurate Mass: 174.115698

Percentage Composition: C 75.82%; H 8.10%; N 16.08%

Biological Source: Alkaloid from *Arundo donax*, *Phalaris arundinacea*, some *Lupinus* spp. and barley shoots (Gramineae, Leguminosae). Also from *Acer saccharinum*, *Acer rubrum*, *Brassica oleracea* and *Desmodium pulchellum*

Melting Point: Mp 138-139°

pKa Value: pK_a 16 (25°,NH, aq. KOH)

Hazard & Toxicity: LD₅₀ (mus, ipr) 122 mg/kg ; BERDY HAZD : LD₅₀ (mus, ipr) 122 mg/kg

Aldrich: G1080-6

Fluka: 50860

Rare Chemicals Library: S12024-3

Sigma: G1647

>>Derivative: Picrate

Melting Point: Mp 144-145°

>>Derivative: *N*-Oxide

Synonym(s): Gramine *N*-oxide

CAS Registry Number: 17206-03-0

Type of Compound Code(s): VX4000

Molecular Formula: C₁₁H₁₄N₂O

Molecular Weight: 190.244

Accurate Mass: 190.110613

Percentage Composition: C 69.45%; H 7.42%; N 14.72%; O 8.41%

Biological Source: Alkaloid from *Acer donax* (Gramineae)

Physical Description: Noncryst.

Melting Point: Mp 122° (H₂O₂ solvate)

>>Derivative: *N*-Me

Synonym(s): Gramine methosalt

CAS Registry Number: 5457-31-8

Type of Compound Code(s): VX4000

Molecular Formula: C₁₂H₁₇N₂⁽⁺⁾

Molecular Weight: 189.28

Accurate Mass: 189.139173

Percentage Composition: C 76.15%; H 9.05%; N 14.80%

Biological Source: Alkaloid from flowers of *Arundo donax* (Gramineae)

Melting Point: Mp 168-169° (iodide)

Other Data: CAS no. refers to iodide