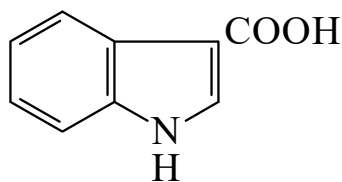




>>Entry Name: **1*H*-Indole-3-carboxylic acid**

Synonym(s): Indole- β -carboxylic acid



CAS Registry Number: 771-50-6

Molecular Formula: C₉H₇NO₂

Molecular Weight: 161.16

Accurate Mass: 161.047679

Percentage Composition: C 67.08%; H 4.38%; N 8.69%; O 19.86%

Biological Source: Present in plants, e.g. *Pyrus malus*, *Pisum sativum*, *Brassica* spp, and the marine algae *Undaria pinnatifida* and *Botryocladia leptopoda*

Melting Point: Mp 210-218° (198-200°)

pKa Value: pK_{a1} 3.87; pK_{a2} 15.59 (25°,NH)

Aldrich: 28473-4

Fluka: 57225

Rare Chemicals Library: S60373-2

Sigma: I2006

>>Derivative: α -L-Rhamnopyranosyl ester

Molecular Formula: C₁₅H₁₇NO₆

Molecular Weight: 307.302

Accurate Mass: 307.105589

Percentage Composition: C 58.63%; H 5.58%; N 4.56%; O 31.24%

Biological Source: Prod. by *Streptomyces* sp. GT 61150

Physical Description: Light yellow powder (CHCl₃/MeOH)

Melting Point: Mp 132-133°

Optical Rotation: [α]_D²⁵ -36.8 (c, 0.1 in MeOH)

UV: [neutral] $\lambda_{\max}$ 211 (log ϵ 3.45); 227 (sh) (log ϵ 1.56); 284 (log ϵ 0.97) (MeOH)

>>Derivative: Me ester

CAS Registry Number: 942-24-5

Molecular Formula: C₁₀H₉NO₂

Molecular Weight: 175.187

Accurate Mass: 175.063329

Percentage Composition: C 68.56%; H 5.18%; N 8.00%; O 18.27%

Biological Source: Isol. from the red alga *Botryocladia leptopoda*

Melting Point: Mp 147-148° (140°)

Other Data: Probably an artifact

Aldrich: 39530-7

>>Derivative: Et ester

CAS Registry Number: 776-41-0

Molecular Formula: C₁₁H₁₁NO₂

Molecular Weight: 189.213

Accurate Mass: 189.078979

Percentage Composition: C 69.83%; H 5.86%; N 7.40%; O 16.91%

Melting Point: Mp 122-124°

Rare Chemicals Library: S28796-2

>>Derivative: Amide

Synonym(s): **1*H*-Indole-3-carboxamide**, 9CI

CAS Registry Number: 1670-85-5