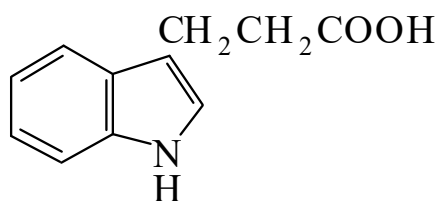




>>Entry Name: **1*H*-Indole-3-propanoic acid**

Synonym(s): 3-(3-Indolyl)propionic acid. KG 431B. Antibiotic KG 431B



CAS Registry Number: 830-96-6

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%

Biological Source: Isol. from *Claviceps* (ergot) cultures

Melting Point: Mp 134° (111-112°)

Aldrich: 22002-7

Fluka: 57410

Rare Chemicals Library: S31656-3

Sigma: I3125

>>Derivative: Me ester

CAS Registry Number: 5548-09-4

Molecular Formula: C₁₂H₁₃NO₂

Molecular Weight: 203.24

Accurate Mass: 203.094629

Percentage Composition: C 70.92%; H 6.45%; N 6.89%; O 15.74%

Melting Point: Mp 79-80°

Rare Chemicals Library: S36976-4

>>Derivative: Cyclohexyl ester

Synonym(s): Indobinine

CAS Registry Number: 109897-76-9

Molecular Formula: C₁₇H₂₁NO₂

Molecular Weight: 271.358

Accurate Mass: 271.157229

Percentage Composition: C 75.25%; H 7.80%; N 5.16%; O 11.79%

Biological Source: Alkaloid from roots of *Rauwolfia serpentina* (Apocynaceae)

Physical Description: Elongated rods (MeOH)

Melting Point: Mp 180-181°

>>Derivative: Benzyl ester

Synonym(s): Indobine

CAS Registry Number: 85612-35-7

Molecular Formula: C₁₈H₁₇NO₂

Molecular Weight: 279.338

Accurate Mass: 279.125929

Percentage Composition: C 77.40%; H 6.13%; N 5.01%; O 11.46%

Biological Source: Alkaloid from the roots of *Rauwolfia serpentina* (Apocynaceae)

Physical Description: Needles (MeOH)

Melting Point: Mp 163-164°

>>Derivative: Amide

Synonym(s): 1*H*-Indole-3-propanamide