



Physical Description: Solid (EtOAc/hexane)

Melting Point: Mp 201-203°

>>**Derivative:** Nitrile

Synonym(s): 1*H*-Indole-3-carbonitrile, 9Cl. 3-Cyanoindole

CAS Registry Number: 5457-28-3

Molecular Formula: C₉H₆N₂

Molecular Weight: 142.16

Accurate Mass: 142.053098

Percentage Composition: C 76.04%; H 4.25%; N 19.71%

Biological Source: Alkaloid from a facultatively anaerobic, halophilic bacterium

Melting Point: Mp 178°

Aldrich: 34794-9

Rare Chemicals Library: S54482-5

>>**Derivative:** Nitrile, *N*-Ac

Molecular Formula: C₁₁H₈N₂O

Molecular Weight: 184.197

Accurate Mass: 184.063663

Percentage Composition: C 71.73%; H 4.38%; N 15.21%; O 8.69%

Melting Point: Mp 202°

>>**Derivative:** *N*-Ethoxycarbonyl, Et ester

Synonym(s): Diethyl 1*H*-indole-1,3-dicarboxylate

CAS Registry Number: 13328-43-3

Molecular Formula: C₁₄H₁₅NO₄

Molecular Weight: 261.277

Accurate Mass: 261.100109

Percentage Composition: C 64.36%; H 5.79%; N 5.36%; O 24.49%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 102-104°

>>**Derivative:** *N*-Me

CAS Registry Number: 32387-21-6

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%

Physical Description: Cryst. (2-propanol) or plates (Me₂CO aq.)

Melting Point: Mp 212° (200-201° dec.)

Aldrich: 46531-3

>>**Derivative:** *N*-Me, Et ester

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 69.7-70.2°

>>**Derivative:** *N*-Me, nitrile

Synonym(s): 3-Cyano-1-methylpyridine

CAS Registry Number: 24662-37-1

Molecular Formula: C₁₀H₈N₂

Molecular Weight: 156.187

Accurate Mass: 156.068748

Percentage Composition: C 76.90%; H 5.16%; N 17.94%

Physical Description: Cryst. (Et₂O/hexane)

Melting Point: Mp 60-61°

>>**Derivative:** *N*-(1,1-Dimethyl-2-propenyl), Me ester