



CAS Registry Number: 78686-01-8

Molecular Formula: C₁₁H₁₄N₂O₆

Molecular Weight: 270.241

Accurate Mass: 270.085188

Percentage Composition: C 48.89%; H 5.22%; N 10.37%; O 35.52%

Biological Source: Isol. from human urine. Constit. of *Rothmannia longiflora*

Physical Description: Cryst. (EtOH)

Melting Point: Mp 211-212°

Optical Rotation: [α]_D²⁵ -97.1 (c, 0.25 in MeOH)

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

Synonym(s): 1,4-Dihydro-1-methyl-4-oxo-3-pyridinecarbonitrile. 3-Cyano-1-methyl-4(1*H*)-pyridinone

CAS Registry Number: 767-98-6

Molecular Formula: C₇H₆N₂O

Molecular Weight: 134.137

Accurate Mass: 134.048013

Percentage Composition: C 62.68%; H 4.51%; N 20.88%; O 11.93%

Biological Source: Alkaloid from *Mallotus repandus*

Physical Description: Prisms (MeOH)

Melting Point: Mp 185-186° (179-181°)

UV: [neutral] $\lambda_{\max}$ 258 (log ϵ 4.21); 263 (log ϵ 4.2); 289 (log ϵ 3.76) (MeOH)

>> **Variant:** *OH*-form

Molecular Formula: C₆H₅NO₃

Molecular Weight: 139.11

Accurate Mass: 139.026944

Percentage Composition: C 51.80%; H 3.62%; N 10.07%; O 34.50%

>> **Derivative:** Me ether

Synonym(s): 4-Methoxy-3-pyridinecarboxylic acid

CAS Registry Number: 10177-31-8

Molecular Formula: C₇H₇NO₃

Molecular Weight: 153.137

Accurate Mass: 153.042594

Percentage Composition: C 54.90%; H 4.61%; N 9.15%; O 31.34%

Physical Description: Plates (EtOH)

Melting Point: Mp 178-179 dec.°

>> **Derivative:** Me ether, Me ester

CAS Registry Number: 10177-32-9

Molecular Formula: C₈H₉NO₃

Molecular Weight: 167.164

Accurate Mass: 167.058244

Percentage Composition: C 57.48%; H 5.43%; N 8.38%; O 28.71%

Physical Description: Cryst. (cyclohexane)

Melting Point: Mp 82-84°

>> **Derivative:** Me ether, nitrile

Synonym(s): 3-Cyano-4-methoxypyridine

CAS Registry Number: 74133-20-3

Molecular Formula: C₇H₆N₂O

Molecular Weight: 134.137

Accurate Mass: 134.048013

Percentage Composition: C 62.68%; H 4.51%; N 20.88%; O 11.93%

Biological Source: Alkaloid from *Hernandia nymphaefolia* (Hernadiaceae)

Physical Description: Needles (Et₂O)

Melting Point: Mp 124°