



**CAS Registry Number:** 78686-01-8

**Molecular Formula:** C<sub>11</sub>H<sub>14</sub>N<sub>2</sub>O<sub>6</sub>

**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:** [ $\alpha$ ]<sub>D</sub><sup>25</sup> -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:** C<sub>7</sub>H<sub>6</sub>N<sub>2</sub>O

**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  $\epsilon$  4.21); 263 (log  $\epsilon$  4.2); 289 (log  $\epsilon$  3.76) (MeOH)

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

**Molecular Formula:** C<sub>6</sub>H<sub>5</sub>NO<sub>3</sub>

**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:** C<sub>7</sub>H<sub>7</sub>NO<sub>3</sub>

**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:** C<sub>8</sub>H<sub>9</sub>NO<sub>3</sub>

**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:** C<sub>7</sub>H<sub>6</sub>N<sub>2</sub>O

**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 (Et<sub>2</sub>O)

**Melting Point:** Mp 124°