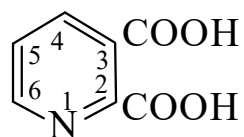




>>Entry Name: **2,3-Pyridinedicarboxylic acid**, 9Cl, 8Cl

Synonym(s): Quinolinic acid



CAS Registry Number: 89-00-9

Molecular Formula: C₇H₅NO₄

Molecular Weight: 167.121

Accurate Mass: 167.021859

Percentage Composition: C 50.31%; H 3.02%; N 8.38%; O 38.29%

Biological Source: Intermed. in the biosynth. of nicotinic acid dinucleotide in microorganisms

Physical Description: Prisms (H₂O)

Melting Point: Mp 188°. Mp 190-195 dec.°

Solubility: Spar. sol. H₂O; prac. insol. EtOH, Et₂O

pKa Value: pK_{a1} 2.43; pK_{a2} 4.78 (25°, 0.1M NaClO₄)

Aldrich: P6320-4

Fluka: 22690

>>Derivative: *N*-Oxide

CAS Registry Number: 38557-80-1

Molecular Formula: C₇H₅NO₅

Molecular Weight: 183.12

Accurate Mass: 183.016774

Percentage Composition: C 45.91%; H 2.75%; N 7.65%; O 43.69%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 261°

>>Derivative: 2-Me ester

CAS Registry Number: 24195-07-1

Molecular Formula: C₈H₇NO₄

Molecular Weight: 181.148

Accurate Mass: 181.037509

Percentage Composition: C 53.04%; H 3.89%; N 7.73%; O 35.33%

Physical Description: Cryst. + 1H₂O (H₂O), anhyd. cryst.(EtOAc)

Melting Point: Mp 123° (anhyd.)

>>Derivative: 3-Me ester

CAS Registry Number: 24195-02-6

Molecular Formula: C₈H₇NO₄

Molecular Weight: 181.148

Accurate Mass: 181.037509

Percentage Composition: C 53.04%; H 3.89%; N 7.73%; O 35.33%

Physical Description: Cryst. (C₆H₆ or EtOAc)

Melting Point: Mp 106°

>>Derivative: Di-Me ester

CAS Registry Number: 605-38-9

Molecular Formula: C₉H₉NO₄

Molecular Weight: 195.174

Accurate Mass: 195.053159

Percentage Composition: C 55.39%; H 4.65%; N 7.18%; O 32.79%

Physical Description: Plates (CS₂/petrol)

Melting Point: Mp 53-54°

Rare Chemicals Library: S28803-9