



CAS Registry Number: 553-53-7

Molecular Formula: C₆H₇N₃O

Molecular Weight: 137.141

Accurate Mass: 137.058912

Percentage Composition: C 52.55%; H 5.14%; N 30.64%; O 11.67%

Biological Use/Importance: Bactericide

Physical Description: Needles (EtOH or C₆H₆)

Melting Point: Mp 161-162°

Calculated Log P Data: Log P -0.71 (calc)

Aldrich: 10742-5

Fluka: 72400

Sigma: N3508

>>Derivative: Hydrazide; hydrochloride (1:2)

Physical Description: Cryst. (EtOH/Et₂O/HCl)

Melting Point: Mp 227°

>>Derivative: Azide

CAS Registry Number: 4013-72-3

Molecular Formula: C₆H₄N₄O

Molecular Weight: 148.124

Accurate Mass: 148.038511

Percentage Composition: C 48.65%; H 2.72%; N 37.82%; O 10.80%

Melting Point: Mp 47-48°

>>Derivative: Nitrile

Synonym(s): 3-Pyridinecarbonitrile, 9Cl. Nicotinonitrile. 3-Cyanopyridine

CAS Registry Number: 100-54-9

Molecular Formula: C₆H₄N₂

Molecular Weight: 104.111

Accurate Mass: 104.037448

Percentage Composition: C 69.22%; H 3.87%; N 26.91%

Physical Description: Cryst. (petrol)

Melting Point: Mp 50°

Boiling Point: Bp 240-245°

pKa Value: pK_a 1.35 (25°)

Aldrich: C9480-7

Fluka: 28580

Sigma: C5880

>>Derivative: Anhydride

CAS Registry Number: 16837-38-0

Molecular Formula: C₁₂H₈N₂O₃

Molecular Weight: 228.207

Accurate Mass: 228.053493

Percentage Composition: C 63.16%; H 3.53%; N 12.28%; O 21.03%

Physical Description: Needles

Melting Point: Mp 123-124°

>>Derivative: *N*-Me, betaine