CAS Registry Number: 553-53-7

Molecular Formula: $C_6H_7N_3O$
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 C_6H_6)
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/Et_2O/HCl)
Melting Point: Mp 227°

>>**Derivative:** Azide

CAS Registry Number: 4013-72-3
Molecular Formula: $C_6H_4N_4O$
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, 9CI. Nicotinonitrile. 3-Cyanopyridine

CAS Registry Number: 100-54-9
Molecular Formula: $C_6H_4N_2$
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: $C_{12}H_8N_2O_3$
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