



>>Entry Name: 3-Pyridinemethanol, 9Cl, 8Cl

Synonym(s): 3-Hydroxymethylpyridine. NicotinyI alcohol, BAN. NSC 526046

CAS Registry Number: 100-55-0

Molecular Formula: C₆H₇NO

Molecular Weight: 109.127

Accurate Mass: 109.052764

Percentage Composition: C 66.04%; H 6.47%; N 12.84%; O 14.66%

Use/Importance: Vasodilator

Boiling Point: Bp₁₅ 142-143°. Bp_{0.1} 110°

pKa Value: pK_a 4.93 (25°)

Calculated Log P Data: Log P -0.39 (calc)

Aldrich: P6680-7

Fluka: 55780

Sigma: H5512

>>Derivative: Hydrochloride

CAS Registry Number: 52761-08-7

Melting Point: Mp 118-121°

>>Derivative: Methochloride

Melting Point: Mp 49°

>>Derivative: Methiodide

CAS Registry Number: 6457-55-2

Melting Point: Mp 159°

>>Derivative: Tartrate (salt)

Synonym(s): Ronicol. Roniacol

CAS Registry Number: 6164-87-0

Melting Point: Mp 147-148°

>>Derivative: Picrate

Physical Description: Yellow needles (H₂O)

Melting Point: Mp 162-163°

>>Derivative: Ac

CAS Registry Number: 10072-09-0

Molecular Formula: C₈H₉NO₂

Molecular Weight: 151.165

Accurate Mass: 151.063329

Percentage Composition: C 63.57%; H 6.00%; N 9.27%; O 21.17%

Boiling Point: Bp₃₀ 150-151°

>>Derivative: O-Benzoyl

CAS Registry Number: 58550-50-8

Molecular Formula: C₁₃H₁₁NO₂

Molecular Weight: 213.235

Accurate Mass: 213.078979

Percentage Composition: C 73.23%; H 5.20%; N 6.57%; O 15.01%

Boiling Point: Bp₁₇ 196-198°

>>Derivative: O-Benzoyl; hydrochloride

Melting Point: Mp 116°