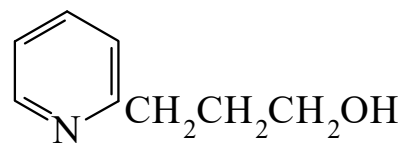




>>Entry Name: 2-Pyridinepropanol, 9Cl, 8Cl

Synonym(s): 3-(2-Pyridyl)-1-propanol. 2-(3-Hydroxypropyl)pyridine



CAS Registry Number: 2859-68-9

Molecular Formula: C₈H₁₁NO

Molecular Weight: 137.181

Accurate Mass: 137.084064

Percentage Composition: C 70.04%; H 8.08%; N 10.21%; O 11.66%

Physical Description: Liq.

Boiling Point: Bp₂₀ 190-195°

pKa Value: pK_{a1} 5.61 pK_{a2} 18

Refractive Index: n_D²⁵ 1.5280

Aldrich: P7100-2

>>Derivative: Picrate

Physical Description: Cryst. (EtOH)

Melting Point: Mp 72-74°

>>Derivative: Ac

CAS Registry Number: 38456-23-4

Molecular Formula: C₁₀H₁₃NO₂

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

Physical Description: Liq.

Boiling Point: Bp_{0.08} 59-62°

>>Derivative: N-Oxide

Molecular Formula: C₈H₁₁NO₂

Molecular Weight: 153.18

Accurate Mass: 153.078979

Percentage Composition: C 62.73%; H 7.24%; N 9.14%; O 20.89%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 52-54°

References:

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 1319B, (ir)

Sadtler Standard Infrared Spectra, No 20461

Sadtler Standard NMR Spectra, No 18147, 2373, (pmr, cmr)

Sadtler Standard Ultraviolet Spectra, No 6910

Chichibabine, A.E., *Bull. Soc. Chim. Fr.*, 1938, **5**, 436, (Et ether)

Boekelheide, V. *et al.*, *J.O.C.*, 1957, **22**, 589, (oxide)

Lowe, O.G. *et al.*, *J.O.C.*, 1959, **24**, 1200, (synth)

Tissier, M. *et al.*, *Bull. Soc. Chim. Fr.*, 1967, 3155, (props)

Cooks, R.G. *et al.*, *J.O.C.*, 1973, **38**, 1114, (synth, ms)

Tilley, J.W. *et al.*, *J.O.C.*, 1988, **53**, 386, (synth, pmr)