



>>Entry Name: 4-Benzylpyridine, 8Cl

Synonym(s): 4-(Phenylmethyl)pyridine, 9Cl. Phenyl-4-pyridylmethane

CAS Registry Number: 2116-65-6

Molecular Formula: C₁₂H₁₁N

Molecular Weight: 169.226

Accurate Mass: 169.089149

Percentage Composition: C 85.17%; H 6.55%; N 8.28%

Physical Description: Liq.

Boiling Point: Bp₇₄₂ 287°. Bp₃₁ 180-181°

Density: d₀⁰ 1.076

pKa Value: pK_a 5.59 (25°)

Aldrich: B3040-5

Fluka: 13860

>>Derivative: Picrate

Physical Description: Needles (EtOH)

Melting Point: Mp 140-141°

>>Derivative: N-Oxide

CAS Registry Number: 7259-53-2

Molecular Formula: C₁₂H₁₁NO

Molecular Weight: 185.225

Accurate Mass: 185.084064

Percentage Composition: C 77.81%; H 5.99%; N 7.56%; O 8.64%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 107-108°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 252B, (nmr)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1520A, (ir)

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 1311D, (ir)

Laforge, F.B., *J.A.C.S.*, 1928, **50**, 2484

Veer, W.L. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1946, **65**, 793

Benkeser, R.A. *et al.*, *J.A.C.S.*, 1951, **73**, 5861

Jerchel, D. *et al.*, *Chem. Ber.*, 1960, **93**, 2966

Proctor, G.R. *et al.*, *J.C.S. Perkin I*, 1981, 1754, (oxide)

Shiao, M. *et al.*, *Synth. Commun.*, 1991, **21**, 401, (synth)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, BFG750