



>>Entry Name: 3-Iodobenzylamine

Synonym(s): 3-Iodobenzenemethanamine, 9CI. α -Amino-3-iodotoluene

CAS Registry Number: 696-40-2

Molecular Formula: C_7H_8IN

Molecular Weight: 233.051

Accurate Mass: 232.970147

Percentage Composition: C 36.08%; H 3.46%; I 54.45%; N 6.01%

Boiling Point: Bp₈ 132°

Aldrich: 10006-4

>>Derivative: Hydrochloride

CAS Registry Number: 3718-88-5

Physical Description: Needles (EtOH)

Melting Point: Mp 193°

Aldrich: 13499-6

>>Derivative: N-Ac

Molecular Formula: $C_9H_{10}INO$

Molecular Weight: 275.089

Accurate Mass: 274.980712

Percentage Composition: C 39.30%; H 3.66%; I 46.13%; N 5.09%; O 5.82%

Physical Description: Needles (petrol)

Melting Point: Mp 114.5°

References:

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **2**, 601C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1284D, (*ir*)

Shoppee, C.J., *J.C.S.*, 1932, 702

Zeller, V. *et al.*, *J. Med. Chem.*, 1965, **8**, 440, (*synth*)

Fuller, R.W. *et al.*, *J. Med. Chem.*, 1973, **16**, 101