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>>Entry Name: 3-Iodobenzylamine

Synonym(s): 3-Iodobenzenemethanamine, 9CI.  $\alpha$ -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: Bp<sub>8</sub> 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*)

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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