



>>Entry Name: 3-Amino-2-methylbenzoic acid, 9Cl

Synonym(s): 3-Amino-*o*-toluic acid, 8Cl

CAS Registry Number: 52130-17-3

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%

Melting Point: Mp 191°

pKa Value: p*K*_{a1} 3.92 (25°, H₂O)

Aldrich: 33418-9

Fluka: 8405

Rare Chemicals Library: S31421-8

>>Derivative: Me ester

CAS Registry Number: 18583-89-6

Molecular Formula: C₉H₁₁NO₂

Molecular Weight: 165.191

Accurate Mass: 165.078979

Percentage Composition: C 65.44%; H 6.71%; N 8.48%; O 19.37%

Physical Description: Oil

>>Derivative: Nitrile

Synonym(s): 3-Cyano-2-methylaniline

CAS Registry Number: 69022-35-1

Molecular Formula: C₈H₈N₂

Molecular Weight: 132.165

Accurate Mass: 132.068748

Percentage Composition: C 72.70%; H 6.10%; N 21.20%

Physical Description: Needles (H₂O)

Melting Point: Mp 95.5°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1098A, (*nmr*)

Nölting, E., *Ber.*, 1904, **37**, 1015-1032, (*synth*)

Niculescu-Duvăz, I. *et al.*, *J. Med. Chem.*, 1968, **11**, 500-503, (*Me ester, synth, ir*)