



>>Entry Name: 4-Amino-2-methylbenzoic acid, 9CI

Synonym(s): 4-Amino-*o*-toluic acid, 8CI

CAS Registry Number: 2486-75-1

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 165°

pKa Value: pK_{a1} 5.15 (25°, H₂O)

Other Data: Sublimes

>>Derivative: Me ester

CAS Registry Number: 6933-47-7

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%

Melting Point: Mp 68°

>>Derivative: *N*-Ac

Molecular Formula: C₁₀H₁₁NO₃

Molecular Weight: 193.202

Accurate Mass: 193.073894

Percentage Composition: C 62.17%; H 5.74%; N 7.25%; O 24.84%

Physical Description: Reddish-yellow cryst. (H₂O)

Melting Point: Mp 243°

pKa Value: pK_{a1} 4.12 (20°, 1% EtOH)

>>Derivative: Nitrile

Synonym(s): 4-Cyano-3-methylaniline

CAS Registry Number: 72115-06-1

Molecular Formula: C₈H₈N₂

Molecular Weight: 132.165

Accurate Mass: 132.068748

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

Physical Description: Pale yellow needles

Melting Point: Mp 76-77° (90°)

References:

Gabriel, S. *et al.*, *Ber.*, 1919, **52**, 1079-1092, (*synth*)

Pettier, D., *Bull. Soc. Chim. Fr.*, 1960, **241**, 1141-1147, (*ir, pK*)

Gallum, A.B. *et al.*, *J.O.C.*, 1962, **27**, 1426-1430, (*nitrile*)

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

Collins, M.J. *et al.*, *Aust. J. Chem.*, 1992, **45**, 1119-1134, (*pmr, nitrile*)