



>>Entry Name: 4-Amino-3-methylbenzoic acid, 9CI

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

CAS Registry Number: 2486-70-6

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%

Physical Description: Needles (H₂O)

Melting Point: Mp 169°

pKa Value: pK_{a1} 4.81 (25°, 1% EtOH aq.)

Aldrich: A6300-7

>>Derivative: Me ester

CAS Registry Number: 18595-14-7

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%

Physical Description: Prisms (EtOH)

Melting Point: Mp 120-121°

>>Derivative: Amide

Molecular Formula: C₈H₁₀N₂O

Molecular Weight: 150.18

Accurate Mass: 150.079313

Percentage Composition: C 63.98%; H 6.71%; N 18.65%; O 10.65%

Physical Description: Cryst. + 1H₂O (H₂O)

Melting Point: Mp 115° (anhyd.)

>>Derivative: Nitrile

Synonym(s): 4-Cyano-2-methylaniline

CAS Registry Number: 78881-21-7

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°

>>Derivative: *N*-Me

Synonym(s): 3-Methyl-4-(methylanino)benzoic acid

CAS Registry Number: 153304-74-6

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: Needles (H₂O)

Melting Point: Mp 201°

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **2**, 217C, (*ir*)
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Müller, E., *Ber.*, 1909, **42**, 423-434, (*synth*)
Houben, J. *et al.*, *Ber.*, 1909, **42**, 4488-4496
Gabriel, S. *et al.*, *Ber.*, 1919, **52**, 1079-1092, (*synth*)
Peltier, D., *Bull. Soc. Chim. Fr.*, 1960, 1141-1147, (*ir, pK*)
Bartoli, G. *et al.*, *Tetrahedron*, 1987, **43**, 4221-4226, (*Me ester, nitrile*)