



>>Entry Name: 5-Amino-2-methylbenzoic acid, 9Cl

Synonym(s): 5-Amino-*o*-toluic acid, 8Cl

CAS Registry Number: 2840-04-2

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: Prisms (H₂O)

Melting Point: Mp 196°

pKa Value: pK_{a1} 4.14 (25°, H₂O)

>>Derivative: Me ester

CAS Registry Number: 18595-12-5

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 39-40°

>>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: Needles (EtOH)

Melting Point: Mp 177°

pKa Value: pK_a 3.82 (20°, 1% EtOH)

>>Derivative: Nitrile

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

CAS Registry Number: 50670-64-9

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 (petrol)

Melting Point: Mp 88°

References:

Landsberger, W., *Ber.*, 1898, **31**, 2880-2889, (*synth*)

Yasue, M., *Yakugaku Zasshi*, 1955, **75**, 615-620; *CA*, **50**, 3317c, (*synth*)

Peltier, D. *et al.*, *Bull. Soc. Chim. Fr.*, 1960, 1141-1147, (*ir*, *pK*)

Hooper, J.F. *et al.*, *Aust. J. Chem.*, 1964, **17**, 946-948, (*synth*)

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

Bird, T.G.C. *et al.*, *J. Med. Chem.*, 1991, **34**, 2167-2176, (*Me ester*, *synth*, *pmr*)