



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

Synonym(s): 2-Amino-*p*-toluic acid, 8Cl

CAS Registry Number: 2305-36-4

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 (EtOH)

Melting Point: Mp 177 dec.°

pKa Value: pK_{a1} 2.35; pK_{a2} 5.07 (25°, 0.1M KCl)

>>Derivative: Me ester

CAS Registry Number: 18595-17-0

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 35°

>>Derivative: *N*-Ac

CAS Registry Number: 81115-52-8

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

Melting Point: Mp 183°

pKa Value: pK_{a1} 3.73 (20°, 1% EtOH)

>>Derivative: Amide

CAS Registry Number: 39549-79-6

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: Leaflets

Melting Point: Mp 146-147°

>>Derivative: Nitrile

Synonym(s): 2-Cyano-5-methylaniline

CAS Registry Number: 26830-96-6

Molecular Formula: C₈H₈N₂

Molecular Weight: 132.165

Accurate Mass: 132.068748

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

Physical Description: Leaflets (EtOH aq.)

Melting Point: Mp 94°

Other Data: Steam-volatile

Aldrich: 21428-0

References:

Niementowski, S., *J. Prakt. Chem.*, 1889, **40**, 1

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

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

Joshi, B. *et al.*, *Indian J. Chem., Sect. B*, 1987, **26**, 602-604, (*amide*)