



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

Synonym(s): 6-Amino-*m*-toluic acid, 8CI. 5-Methylantranilic acid

CAS Registry Number: 2941-78-8

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: Leaflets (EtOH)

Melting Point: Mp 175°

pKa Value: pK_{a1} 2.48; pK_{a2} 5.13 (25°, 0.1M KCl)

Aldrich: 41944-3

Fluka: 8403

>>Derivative: Me ester

CAS Registry Number: 18595-16-9

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: Cryst. (H₂O)

Melting Point: Mp 62°

>>Derivative: Amide

CAS Registry Number: 40545-33-3

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: Prisms (CHCl₃)

Melting Point: Mp 179°

>>Derivative: Nitrile

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

CAS Registry Number: 5925-93-9

Molecular Formula: C₈H₈N₂

Molecular Weight: 132.165

Accurate Mass: 132.068748

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

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 63°

>>Derivative: *N*-Me

Synonym(s): 5-Methyl-2-(methlamino)benzoic acid

CAS Registry Number: 54675-16-0

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%

Physical Description: Cryst.

Melting Point: Mp 149°

References:

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Werbel, I.M. *et al.*, *J. Het. Chem.*, 1987, **24**, 345, (nitrile)