



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

Synonym(s): 3-Amino-*p*-toluic acid, 8Cl

CAS Registry Number: 2458-12-0

Related CAS Registry Numbers(s): 56773-04-7

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

Melting Point: Mp 165°

pKa Value: pK_{a1} 4.49 (25°, H₂O)

Aldrich: A6280-9

Fluka: 8407

>>Derivative: Me ester

CAS Registry Number: 18595-18-1

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 116°

Fluka: 8415

Rare Chemicals Library: S65286-5

>>Derivative: Amide

CAS Registry Number: 19406-86-1

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%

Melting Point: Mp 124-126°

Other: PB A24255

>>Derivative: Nitrile

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

CAS Registry Number: 60710-80-7

Molecular Formula: C₈H₈N₂

Molecular Weight: 132.165

Accurate Mass: 132.068748

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

Physical Description: Prisms (EtOH)

Melting Point: Mp 81-82°

Other Data: Intense sweet taste

>>Derivative: *N*-Ac

CAS Registry Number: 6946-14-1

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 (AcOH), cryst. (Et₂O)

Melting Point: Mp 279-281°

Rare Chemicals Library: S45489-3

References: