



Synonym(s): 2-Methoxy-5-nitroaniline. 2-Methoxy-5-nitrobenzenamine, 9Cl. 5-Nitro-*o*-anisidine, 8Cl. 2-Amino-4-nitroanisole

CAS Registry Number: 99-59-2

Molecular Formula: C₇H₈N₂O₃

Molecular Weight: 168.152

Accurate Mass: 168.053493

Percentage Composition: C 50.00%; H 4.80%; N 16.66%; O 28.54%

Physical Description: Orange-red needles (EtOH)

Melting Point: Mp 118°

pKa Value: pK_a 2.49 (25°)

Hazard & Toxicity: LD₅₀ (rat, orl) 704 mg/kg. Exp. carcinogen

Aldrich: 16119-5

>>Derivative: Me ether, *N*-Ac

Synonym(s): 2-Methoxy-5-nitroacetanilide

CAS Registry Number: 33721-54-9

Molecular Formula: C₉H₁₀N₂O₄

Molecular Weight: 210.189

Accurate Mass: 210.064058

Percentage Composition: C 51.43%; H 4.80%; N 13.33%; O 30.45%

Physical Description: Needles (H₂O)

Melting Point: Mp 178°

>>Derivative: *O,N*-Di-Me

Molecular Formula: C₈H₁₀N₂O₃

Molecular Weight: 182.179

Accurate Mass: 182.069143

Percentage Composition: C 52.74%; H 5.53%; N 15.38%; O 26.35%

Physical Description: Orange cryst. (petrol)

Melting Point: Mp 87°

>>Derivative: Me ether, *N*-benzoyl

CAS Registry Number: 34326-53-9

Molecular Formula: C₁₄H₁₂N₂O₄

Molecular Weight: 272.26

Accurate Mass: 272.079708

Percentage Composition: C 61.76%; H 4.44%; N 10.29%; O 23.51%

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 160-161°

>>Derivative: *O,N,N*-Tri-Me

CAS Registry Number: 7501-46-4

Molecular Formula: C₉H₁₂N₂O₃

Molecular Weight: 196.205

Accurate Mass: 196.084793

Percentage Composition: C 55.09%; H 6.16%; N 14.28%; O 24.46%

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 68-69°

>>Derivative: Et ether

Synonym(s): 2-Ethoxy-5-nitroaniline. 5-Nitro-*o*-phenetidine

CAS Registry Number: 136-79-8

Molecular Formula: C₈H₁₀N₂O₃

Molecular Weight: 182.179

Accurate Mass: 182.069143

Percentage Composition: C 52.74%; H 5.53%; N 15.38%; O 26.35%

Physical Description: Yellow needles (EtOH aq.)

Melting Point: Mp 96°

Boiling Point: Bp₁₄ 205-206°