



>>Entry Name: 4-Amino-2-nitrophenol, 9CI

CAS Registry Number: 119-34-6

Molecular Formula: $C_6H_6N_2O_3$

Molecular Weight: 154.125

Accurate Mass: 154.037843

Percentage Composition: C 46.76%; H 3.92%; N 18.18%; O 31.14%

Physical Description: Dark-red plates or needles

Melting Point: Mp 131°

pKa Value: pK_{a1} 7.81 (25°)

Hazard & Toxicity: LD₅₀ (rat, orl) 1470 mg/kg. Exp. carcinogenic data

Aldrich: 14721-4

>>Derivative: *N*-Ac

Synonym(s): 4-Hydroxy-3-nitroacetanilide

CAS Registry Number: 51288-37-0

Molecular Formula: $C_8H_8N_2O_4$

Molecular Weight: 196.162

Accurate Mass: 196.048408

Percentage Composition: C 48.98%; H 4.11%; N 14.28%; O 32.62%

Physical Description: Yellow needles (H₂O)

Melting Point: Mp 159°

pKa Value: pK_{a1} 6.78 (25°)

>>Derivative: *N*-Me

Molecular Formula: $C_7H_8N_2O_3$

Molecular Weight: 168.152

Accurate Mass: 168.053493

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

Physical Description: Purple-black leaflets or reddish-brown cryst.

Melting Point: Mp 115-116°

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

Molecular Formula: $C_8H_{10}N_2O_3$

Molecular Weight: 182.179

Accurate Mass: 182.069143

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

Physical Description: Black lustrous prisms

Melting Point: Mp 54°

>>Derivative: Me ether

Synonym(s): 4-Methoxy-3-nitroaniline. 4-Methoxy-3-nitrobenzenamine, 9CI. 3-Nitro-*p*-anisidine, 8CI. 4-Amino-2-nitroanisole

Molecular Formula: $C_7H_8N_2O_3$

Molecular Weight: 168.152

Accurate Mass: 168.053493

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

Physical Description: Red prisms (Et₂O/petrol)

Melting Point: Mp 57-57.5°

pKa Value: pK_a 3.36 (25°)

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

Synonym(s): 4-Methoxy-3-nitroacetanilide

CAS Registry Number: 50651-39-3

Molecular Formula: $C_9H_{10}N_2O_4$

Molecular Weight: 210.189

Accurate Mass: 210.064058

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

Physical Description: Yellow needles (H₂O)

Melting Point: Mp 153°