



>>Entry Name: 4-Amino-3-nitrophenol, 9Cl

CAS Registry Number: 610-81-1

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%

Use/Importance: Used in dyes

Physical Description: Dark-red prisms with green reflex

Melting Point: Mp 154°

Aldrich: 24931-9

Fluka: 8935

>>Derivative: Hydrochloride

Melting Point: Mp 147-148°

>>Derivative: *N*-Ac

Synonym(s): 4-Hydroxy-2-nitroacetanilide

CAS Registry Number: 7403-75-0

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: Brownish-yellow needles (H₂O)

Melting Point: Mp 218°

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

Molecular Formula: $C_{10}H_{10}N_2O_5$

Molecular Weight: 238.199

Accurate Mass: 238.058973

Percentage Composition: C 50.42%; H 4.23%; N 11.76%; O 33.58%

Physical Description: Yellow prisms (EtOH aq.)

Melting Point: Mp 146-147°

>>Derivative: Me ether

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

CAS Registry Number: 96-96-8

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: Dark-red prisms (H₂O)

Melting Point: Mp 129°

pKa Value: pK_a 0.73 (25°, HCl aq.)

Aldrich: M1740-3

Fluka: 72700

Rare Chemicals Library: S18320-2

Sigma: F1005

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

Synonym(s): 4-Methoxy-2-nitroacetanilide

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 (EtOH)

Melting Point: Mp 117°