



>>Entry Name: 4-Amino-3-nitrobenzoic acid, 9CI

CAS Registry Number: 1588-83-6

Molecular Formula: $C_7H_6N_2O_4$

Molecular Weight: 182.135

Accurate Mass: 182.032758

Percentage Composition: C 46.16%; H 3.32%; N 15.38%; O 35.14%

Physical Description: Reddish-yellow needles (EtOH)

Melting Point: Mp 284°

Rare Chemicals Library: S56428-1

>>Derivative: Me ester

CAS Registry Number: 3987-92-6

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 cryst. (Me₂CO aq.)

Melting Point: Mp 199.5-200°

>>Derivative: Et ester

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 145°

>>Derivative: Amide

CAS Registry Number: 41263-65-4

Molecular Formula: $C_7H_7N_3O_3$

Molecular Weight: 181.151

Accurate Mass: 181.048742

Percentage Composition: C 46.41%; H 3.89%; N 23.20%; O 26.50%

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 227°

>>Derivative: Nitrile

Synonym(s): 2-Nitro-4-cyanoaniline

CAS Registry Number: 6393-40-4

Molecular Formula: $C_7H_5N_3O_2$

Molecular Weight: 163.135

Accurate Mass: 163.038177

Percentage Composition: C 51.54%; H 3.09%; N 25.76%; O 19.61%

Physical Description: Yellow needles

Melting Point: Mp 159-160°

Aldrich: 32469-8

Fluka: 8857

>>Derivative: *N*-Formyl

Molecular Formula: $C_8H_6N_2O_5$

Molecular Weight: 210.146

Accurate Mass: 210.027673

Percentage Composition: C 45.72%; H 2.88%; N 13.33%; O 38.07%

Physical Description: Needles (EtOH)

Melting Point: Mp 221 dec.°