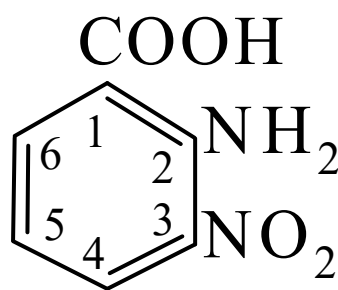




>>Entry Name: 2-Amino-3-nitrobenzoic acid, 9CI

Synonym(s): 3-Nitroanthranilic acid



CAS Registry Number: 606-18-8

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: Yellow needles (H_2O)

Melting Point: Mp 208-209°

Other Data: Spar. steam-volatile

>>Derivative: *N*-Ac

Molecular Formula: $C_9H_8N_2O_5$

Molecular Weight: 224.173

Accurate Mass: 224.043323

Percentage Composition: C 48.22%; H 3.60%; N 12.50%; O 35.69%

Physical Description: Yellow needles (H_2O or AcOH)

Melting Point: Mp 180-181°

>>Derivative: Et ester

CAS Registry Number: 61063-11-4

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 plates

Melting Point: Mp 109°

Other Data: V. steam-volatile

>>Derivative: Chloride

Molecular Formula: $C_7H_5ClN_2O_3$

Molecular Weight: 200.581

Accurate Mass: 199.99887

Percentage Composition: C 41.92%; H 2.51%; Cl 17.68%; N 13.97%; O 23.93%

Physical Description: Yellow solid

>>Derivative: Amide

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: Orange needles (EtOH or Me_2CO)

Melting Point: Mp 234°

>>Derivative: *N*-Me

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: Reddish-brown needles (EtOH aq.)

Melting Point: Mp 146°