



>>Entry Name: 2-Amino-6-nitrobenzoic acid, 9CI

Synonym(s): 6-Nitroanthranilic acid

CAS Registry Number: 50573-74-5

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 184°

>>Derivative: Me ester

CAS Registry Number: 57113-89-0

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: Orange cryst. (MeOH aq.)

Melting Point: Mp 108-110°. Mp 105-108°

>>Derivative: *N*-Ac

CAS Registry Number: 73721-78-5

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: Cryst. (H_2O)

Melting Point: Mp 212-214 dec.°

>>Derivative: Anilide

Molecular Formula: $C_{13}H_{11}N_3O_3$

Molecular Weight: 257.248

Accurate Mass: 257.080042

Percentage Composition: C 60.70%; H 4.31%; N 16.33%; O 18.66%

Physical Description: Yellow needles ($CHCl_3$)

Melting Point: Mp 137°

>>Derivative: Nitrile

CAS Registry Number: 63365-23-1

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: Cryst. (EtOH/EtOAc)

Melting Point: Mp 190-191°

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

Synonym(s): 2-(Dimethylamino)-6-nitrobenzonitrile

CAS Registry Number: 63140-76-1

Molecular Formula: $C_9H_9N_3O_2$

Molecular Weight: 191.189

Accurate Mass: 191.069477

Percentage Composition: C 56.54%; H 4.74%; N 21.98%; O 16.74%

Physical Description: Bright orange needles (cyclohexane)

Melting Point: Mp 111-113°

References: