>>**Entry Name: 5-Amino-3-nitrobenzoic acid,** 8CI

CAS Registry Number: 618-84-8

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: Golden-yellow prisms (H_2O)
Melting Point: Mp 211-213°
pKa Value: pK_{a1} 1.55; pK_{a2} 3.55 (25°)

Rare Chemicals Library: S72235-9

>>**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%
Melting Point: Mp 291-295°

>>**Derivative:** Me ester

CAS Registry Number: 23218-93-1
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 (H_2O), prisms (EtOH)
Melting Point: Mp 160°

>>**Derivative:** Et ester

CAS Registry Number: 10394-67-9
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 155°

References:

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Curtius, T. *et al.*, *J. Prakt. Chem.*, 1907, **76**, 288, *(synth)*
Larsen, A.A. *et al.*, *J.A.C.S.*, 1956, **78**, 3210, *(synth)*
Pitre, D. *et al.*, *Chimia*, 1965, **19**, 462, *(synth)*
Abraham, D.J. *et al.*, *J. Med. Chem.*, 1984, **27**, 1549, *(synth, pmr, ir)*