



>>Entry Name: 2-Amino-4-nitrobenzoic acid, 9CI

Synonym(s): 4-Nitroanthranilic acid

CAS Registry Number: 619-17-0

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: Orange prisms (EtOH aq.)

Melting Point: Mp 269°

Solubility: Spar. sol. hot  $H_2O$

pKa Value:  $pK_{a1}$  0.65;  $pK_{a2}$  3.7 (25°, 0.1M KCl)

Other Data: Sweet taste

Hazard & Toxicity: LD<sub>50</sub> (rat, orl) 640 mg/kg

Aldrich: 38546-8

>>Derivative: Me ester

CAS Registry Number: 3558-19-8

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 needles

Melting Point: Mp 157°

Rare Chemicals Library: S65548-1

>>Derivative: Et ester

CAS Registry Number: 55204-24-5

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: Orange prisms (EtOH)

Melting Point: Mp 100°

>>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: Needles (EtOH aq.)

Melting Point: Mp 220-222°

>>Derivative: N-Et

CAS Registry Number: 49565-61-9

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: Golden-yellow needles or plates

Melting Point: Mp 223°

#### References:

Aldrich Library of  $^{13}C$  and  $^1H$  FT NMR Spectra, 1992, **2**, 1130B, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 224A, (ir)

Spring, F.S. *et al.*, *J.C.S.*, 1945, 627, (synth)

Mori, M. *et al.*, *Chem. Pharm. Bull.*, 1986, **34**, 4859, (synth, pmr, deriv)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, NES500