



>>Entry Name: 4-Fluoro-3-nitrobenzoic acid

CAS Registry Number: 453-71-4

Structure by analogy with 2-Fluoro-3-nitrobenzoic acid, [DTN33-G](#)

Molecular Formula: C₇H₄FNO₄

Molecular Weight: 185.111

Accurate Mass: 185.012437

Percentage Composition: C 45.42%; H 2.18%; F 10.26%; N 7.57%; O 34.57%

Physical Description: Needles (H₂O)

Melting Point: Mp 122°

pKa Value: pK_a 3.36 (25°)

Aldrich: 32904-5

Sigma: N1637

>>Derivative: Et ester

Molecular Formula: C₉H₈FNO₄

Molecular Weight: 213.165

Accurate Mass: 213.043737

Percentage Composition: C 50.71%; H 3.78%; F 8.91%; N 6.57%; O 30.02%

Physical Description: Yellow cryst.

Melting Point: Mp 45°

>>Derivative: Nitrile

Synonym(s): 4-Fluoro-3-nitrobenzonitrile

CAS Registry Number: 1009-35-4

Molecular Formula: C₇H₃FN₂O₂

Molecular Weight: 166.111

Accurate Mass: 166.017856

Percentage Composition: C 50.61%; H 1.82%; F 11.44%; N 16.86%; O 19.26%

Use/Importance: Reacts with amines, amino acids and NH-heteroaromatic compds. Also an antiauxin.

Physical Description: Needles (hexane/CH₂Cl₂)

Melting Point: Mp 94-95°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1127B, (*nmr*)

Govaert, F., *CA*, 1930, **24**, 2448

Das, N., *Indian. J. Plant Physiol.*, 1958, **1**, 44

Wilshire, J.F.K., *Aust. J. Chem.*, 1967, **20**, 2269, (*pmr*)