



>>Entry Name: 4-Fluoro-2-nitrobenzoic acid

CAS Registry Number: 394-01-4

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

Molecular Formula: $C_7H_4FNO_4$

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: Cryst. (MeOH aq. or EtOH)

Melting Point: Mp 147-148°

>>Derivative: Amide

Molecular Formula: $C_7H_5FN_2O_3$

Molecular Weight: 184.127

Accurate Mass: 184.028421

Percentage Composition: C 45.66%; H 2.74%; F 10.32%; N 15.21%; O 26.07%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 154-155°

>>Derivative: Nitrile

Molecular Formula: $C_7H_3FN_2O_2$

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%

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 69-71°

Boiling Point: Bp₁₁ 145-150°

References:

v. Hove, T., *Bull. Soc. Chim. Belg.*, 1923, **32**, 52

Adlerová, E. *et al.*, *Coll. Czech. Chem. Comm.*, 1960, **25**, 784

Valkanias, G. *et al.*, *J.C.S.*, 1963, 1925

Protiva, M. *et al.*, *Coll. Czech. Chem. Comm.*, 1986, **51**, 698