



>>Entry Name: 2-Fluoro-5-nitrobenzoic acid

CAS Registry Number: 7304-32-7

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. (H₂O)

Melting Point: Mp 139-140°

pKa Value: pK_a 2.73 (25°)

Aldrich: 36265-4

>>Derivative: Et ester

Molecular Formula: $C_9H_8FNO_4$

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%

Melting Point: Mp 49.5°

>>Derivative: Nitrile

Synonym(s): 2-Cyano-1-fluoro-4-nitrobenzene

CAS Registry Number: 17417-09-3

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%

Use/Importance: Reacts with amines, NH-heteroaromatic compds. and amino acids and used for characterisation

Physical Description: Cryst. (hexane/CH₂Cl₂)

Melting Point: Mp 73-75°

Boiling Point: Bp_{0.5} 94°

Hazard & Toxicity: Irritant

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1126B, (*nmr*)

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

Wilshire, J.F.K., *Aust. J. Chem.*, 1967, **20**, 1663, (*pmr*)

Bil, M., *Chem. Ind. (London)*, 1970, 892

Bridges, A.J. *et al.*, *J. Het. Chem.*, 1997, **34**, 1163-1172, (*nitrile*)