



>>Entry Name: 3-Cyanobenzaldehyde

Synonym(s): 3-Formylbenzonitrile, 9CI. Isophthalaldehydonitrile

CAS Registry Number: 24964-64-5

Structure by analogy with 2-Cyanobenzaldehyde, [HJN49-P](#)

Molecular Formula: C₈H₅NO

Molecular Weight: 131.134

Accurate Mass: 131.037114

Percentage Composition: C 73.27%; H 3.84%; N 10.68%; O 12.20%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 77-79°

pKa Value: pK_{a1} 13.26 (25°,hydrate, 1% EtOH)

Aldrich: 14625-0

Fluka: 28345

>>Derivative: Thiosemicarbazone

Physical Description: Cryst.

Melting Point: Mp 246°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1516A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 448A, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1411C, (*ir*)

Dyer, F.J. *et al.*, *J.C.S.*, 1952, 4778, (*synth*)

Davis, A.L. *et al.*, *Arch. Biochem. Biophys.*, 1960, **87**, 88, (*synth*)

Friedman, L. *et al.*, *J.O.C.*, 1961, **26**, 2522, (*synth*)