



>>Entry Name: 4-Cyanobenzaldehyde

Synonym(s): 4-Formylbenzonitrile, 9CI. Terephthalaldehydonitrile, 8CI

CAS Registry Number: 105-07-7

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: Needles (H₂O)

Melting Point: Mp 101-102°

pKa Value: pK_{a1} 13.06 (25°,hydrate, 1% EtOH)

Hazard & Toxicity: LD₅₀ (mus, ipr) 100 mg/kg

Aldrich: C8960-9

Fluka: 28350

Sigma: C5265

>>Derivative: Oxime

Synonym(s): 4-Cyanobenzaldoxime

Molecular Formula: C₈H₆N₂O

Molecular Weight: 146.148

Accurate Mass: 146.048013

Percentage Composition: C 65.75%; H 4.14%; N 19.17%; O 10.95%

Physical Description: Solid

Melting Point: Mp 174-176°

>>Derivative: Phenylhydrazone

Melting Point: Mp 144-145°

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 295-298°

References:

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