



>>Entry Name: 3-Cyanobenzoic acid, 9CI

Synonym(s): Isophthalic acid mononitrile

CAS Registry Number: 1877-72-1

Related CAS Registry Numbers(s): 1711-11-1

Structure by analogy with 2-Cyanobenzoic acid, [HCT24-L](#)

Molecular Formula: C₈H₅NO₂

Molecular Weight: 147.133

Accurate Mass: 147.032029

Percentage Composition: C 65.31%; H 3.43%; N 9.52%; O 21.75%

Physical Description: Needles (H₂O)

Melting Point: Mp 217°

pKa Value: pK_a 3.7 (25°)

Other Data: Sublimes with part. dec.

Aldrich: 15716-3

Fluka: 28365

>>Derivative: Me ester

CAS Registry Number: 13531-48-1

Molecular Formula: C₉H₇NO₂

Molecular Weight: 161.16

Accurate Mass: 161.047679

Percentage Composition: C 67.08%; H 4.38%; N 8.69%; O 19.86%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 65°

>>Derivative: Et ester

CAS Registry Number: 2463-16-3

Molecular Formula: C₁₀H₉NO₂

Molecular Weight: 175.187

Accurate Mass: 175.063329

Percentage Composition: C 68.56%; H 5.18%; N 8.00%; O 18.27%

Physical Description: Needles

Melting Point: Mp 56°

Boiling Point: Bp₁₀ 140-141°

>>Derivative: Chloride

Synonym(s): 3-Cyanobenzoyl chloride

CAS Registry Number: 1711-11-1

Melting Point: Mp 42-44°

Boiling Point: Bp₁₁ 125-129°

Aldrich: 30253-8

>>Derivative: Amide

Synonym(s): *m*-Cyanobenzamide. Isophthalamic nitrile

CAS Registry Number: 3441-01-8

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: Cryst. (Et₂O)

Melting Point: Mp 300°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1516C; 1517A, (*nmr*)

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

Brömme, W., *Ber.*, 1887, **20**, 524, (*synth*)

Rupe, H. *et al.*, *Helv. Chim. Acta*, 1930, **13**, 468, (*synth*)