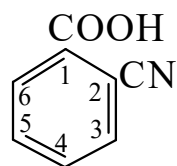




>>Entry Name: 2-Cyanobenzoic acid, 9CI

Synonym(s): Phthalic acid mononitrile



CAS Registry Number: 3839-22-3

Molecular Formula: $C_8H_5NO_2$

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 (EtOH)

Melting Point: Mp 180-190°

pKa Value: pK_a 3.14 (25°)

Other Data: Mp depends on rate of heating. Tautomerises to 3-Imino-1(3*H*)-isobenzofuranone [HGG52-H](#) at Mp

>>Derivative: Me ester

CAS Registry Number: 6587-24-2

Molecular Formula: $C_9H_7NO_2$

Molecular Weight: 161.16

Accurate Mass: 161.047679

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

Physical Description: Needles (MeOH aq.)

Melting Point: Mp 51°

Rare Chemicals Library: S44539-8

>>Derivative: Et ester

CAS Registry Number: 6525-45-7

Molecular Formula: $C_{10}H_9NO_2$

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 (EtOH aq.)

Melting Point: Mp 65-66°. Mp 70°

>>Derivative: Amide

Synonym(s): *o*-Cyanobenzamide. Phthalamic nitrile

CAS Registry Number: 17174-98-0

Molecular Formula: $C_8H_6N_2O$

Molecular Weight: 146.148

Accurate Mass: 146.048013

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

Physical Description: Needles (AcOH)

Melting Point: Mp 173°

Rare Chemicals Library: S94920-5

References:

Hoogewerff, S. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1892, **11**, 84, (*synth*)

v. Braun, A. *et al.*, *Ber.*, 1907, **40**, 2710, (*synth*)

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

Sakamoto, T. *et al.*, *J.C.S. Perkin 1*, 1999, 2323-2326, (*Me ester, synth, ir, pmr, ms*)