



>>Entry Name: 4-Cyanobenzoic acid, 9CI

Synonym(s): Terephthalic acid mononitrile

CAS Registry Number: 619-65-8

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

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: Leaflets (H_2O)

Melting Point: Mp 219°

pKa Value: pK_a 3.51 (25°)

Aldrich: C8980-3

Fluka: 28370

>>Derivative: Me ester

CAS Registry Number: 1129-35-7

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: Leaflets (EtOH)

Melting Point: Mp 62°

Other Data: Steam-volatile

Aldrich: 23063-4

Fluka: 28375

>>Derivative: Et ester

CAS Registry Number: 7153-22-2

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

Melting Point: Mp 54°

Boiling Point: Bp_{11} 139-140°

Aldrich: E1860-3

>>Derivative: Chloride

CAS Registry Number: 6068-72-0

Molecular Formula: C_8H_4ClNO

Molecular Weight: 165.578

Accurate Mass: 164.998141

Percentage Composition: C 58.03%; H 2.43%; Cl 21.41%; N 8.46%; O 9.66%

Melting Point: Mp 68-70°

Aldrich: 12482-6

Fluka: 28376

>>Derivative: Amide

Synonym(s): *p*-Cyanobenzamide. Terephthalamic nitrile

CAS Registry Number: 3034-34-2

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

Melting Point: Mp 223°

References: