



>>Entry Name: Cyanoformic acid

Synonym(s): Carbonocyanidic acid, 9Cl. Oxalic mononitrile

CAS Registry Number: 19270-07-6

NCCOOH

Molecular Formula: C₂HNO₂

Molecular Weight: 71.035

Accurate Mass: 71.000729

Percentage Composition: C 33.82%; H 1.42%; N 19.72%; O 45.05%

General Statement: Parent compd. unknown

Other Data: Trimerises to 1,3,5-Triazine-2,4,6-tricarboxylic acid [BMP13-R](#)

>>Derivative: Me ester

Synonym(s): Methyl cyanoformate. Mander's reagent

CAS Registry Number: 17640-15-2

Molecular Formula: C₃H₃NO₂

Molecular Weight: 85.062

Accurate Mass: 85.016379

Percentage Composition: C 42.36%; H 3.55%; N 16.47%; O 37.62%

Use/Importance: Reagent for condensations

Physical Description: Fuming liq.

Boiling Point: Bp 101°

Aldrich: 31981-3

Fluka: 28325

>>Derivative: Et ester

CAS Registry Number: 623-49-4

Molecular Formula: C₄H₅NO₂

Molecular Weight: 99.089

Accurate Mass: 99.032029

Percentage Composition: C 48.49%; H 5.09%; N 14.14%; O 32.29%

Boiling Point: Bp 115-116°. Bp₃₀ 30-32°

Refractive Index: n_D²⁵ 1.3800

Aldrich: E1885-9

Fluka: 28317

>>Derivative: *tert*-Butyl ester

Synonym(s): *tert*-Butyl cyanoformate

CAS Registry Number: 57022-34-1

Molecular Formula: C₆H₉NO₂

Molecular Weight: 127.143

Accurate Mass: 127.063329

Percentage Composition: C 56.68%; H 7.13%; N 11.02%; O 25.17%

Use/Importance: *N*-Protecting reagent used in peptide synth.

Boiling Point: Bp₅₅ 64-65°

>>Derivative: Benzyl ester

Synonym(s): Benzyl cyanoformate

CAS Registry Number: 5532-86-5

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%

Boiling Point: Bp_{0.6} 66-67°

Refractive Index: n_D²⁰ 1.5046

Aldrich: 32058-7

Fluka: 28320