



>>Entry Name: Dicarbonic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Oxydiformic acid, 8CI. Pyrocarbonic acid. Oxybisformic acid

CAS Registry Number: 503-81-1

HOOC-O-COOH

Molecular Formula: C₂H₂O₅

Molecular Weight: 106.035

Accurate Mass: 105.990225

Percentage Composition: C 22.65%; H 1.90%; O 75.44%

>>Derivative: Di-Me ester

Synonym(s): Dimethyl dicarbonate. Dimethyl pyrocarbonate. Velcorin

CAS Registry Number: 4525-33-1

Molecular Formula: C₄H₆O₅

Molecular Weight: 134.088

Accurate Mass: 134.021525

Percentage Composition: C 35.83%; H 4.51%; O 59.66%

Use/Importance: Yeast inhibitor and preservative for alcoholic beverages esp. low alcohol wines

Melting Point: Mp 15-17°

Boiling Point: Bp₅ 44-47°

Density: d₄²⁵ 1.25

Refractive Index: n_D²⁰ 1.3948

Aldrich: 29287-7

Fluka: 40130

Sigma: D5520

>>Derivative: Di-Et ester

Synonym(s): Diethyl dicarbonate. Diethyl pyrocarbonate. Baycovin

CAS Registry Number: 1609-47-8

Molecular Formula: C₆H₁₀O₅

Molecular Weight: 162.142

Accurate Mass: 162.052825

Percentage Composition: C 44.45%; H 6.22%; O 49.34%

Use/Importance: Formerly used as a preservative for wines and soft drinks and fruit juices. No longer permitted as a food additive. Reagent for the gc sepn. of amines as urethanes

Boiling Point: Bp₃ 58.5-62°

Density: d₄²⁵ 1.12

Refractive Index: n_D²⁵ 1.3975

Hazard & Toxicity: Poss. prototocarcinogen (forms carcinogenic ethyl carbamate with dietary NH₄⁽⁺⁾). Eye, skin and mucous membrane irritant. LD₅₀ (rat, orl) 850 mg/kg

Aldrich: 15922-0

Fluka: 32490

Sigma: D5554

>>Derivative: Di-*tert*-butyl ester

Synonym(s): Di-*tert*-butyl dicarbonate. Di-*tert*-butyl pyrocarbonate

CAS Registry Number: 24424-99-5

Molecular Formula: C₁₀H₁₈O₅

Molecular Weight: 218.249

Accurate Mass: 218.115425

Percentage Composition: C 55.03%; H 8.31%; O 36.65%

Use/Importance: Coupling reagent in organic synth. Reagent for introduction of *tert*-butyloxycarbonyl protecting group. Used in protection of pyrroles and indoles and for high yield synth. of Boc-amino acids

Physical Description: Liq.

Melting Point: Mp 21-22°

Boiling Point: Bp₃ 73-75°

Refractive Index: n_D²⁵ 1.4071 n_D²⁵ 1.4085

Aldrich: 20524-9

Sigma: D0140