



>>Entry Name: Propanedioic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Malonic acid, 8CI. Methanedicarboxylic acid

CAS Registry Number: 141-82-2

Related CAS Registry Numbers(s): 141-95-7 156-80-9 813-56-9 6148-64-7 18424-76-5 36148-03-5 38330-80-2

HOOCCH₂COOH

Molecular Formula: C₃H₄O₄

Molecular Weight: 104.062

Accurate Mass: 104.01096

Percentage Composition: C 34.63%; H 3.87%; O 61.50%

Biological Source: Widespread in plants in small amts.

Use/Importance: Used as aq. soln. for extraction-separation of U; as an eluant in ion-exchange sepn. of Sn(IV); alkalimetric standard; complexing agent. Monomer for polyamides and polyesters

Physical Description: Cryst.

Melting Point: Mp 135.6°

Solubility: Sol. H₂O, EtOH, Et₂O; mod. sol. Py.; BERDY SOL: Sol. H₂O

pKa Value: pK_{a1} 2.77; pK_{a2} 5.7 (25°,H₂O)

Other Data: Sublimes *in vacuo*

Hazard & Toxicity: Skin and eye irritant. LD₅₀ (rat, orl) 1310 mg/kg

Aldrich: M129-6

Fluka: 63301

Sigma: M1750

Supelco: 4-6938

>>Derivative: Mono-Me ester

Synonym(s): Monomethyl malonate. Methyl malonate‡

CAS Registry Number: 16695-14-0

Molecular Formula: C₄H₆O₄

Molecular Weight: 118.089

Accurate Mass: 118.02661

Percentage Composition: C 40.68%; H 5.12%; O 54.19%

Boiling Point: Bp₆ 130°. Bp_{0.5} 90°

>>Derivative: Di-Me ester

Synonym(s): Dimethyl malonate

CAS Registry Number: 108-59-8

Molecular Formula: C₅H₈O₄

Molecular Weight: 132.116

Accurate Mass: 132.04226

Percentage Composition: C 45.46%; H 6.10%; O 48.44%

Melting Point: Mp -62°

Boiling Point: Bp 181°

Solubility: Sl. sol. H₂O; sol. oxygenated solvs.

Hazard & Toxicity: Reacts violently with methyl azide in presence of base, low oral tox.

Aldrich: 13644-1

Fluka: 63380

Sigma: M7253

>>Derivative: Me-tert-butyl ester

CAS Registry Number: 42726-73-8

Molecular Formula: C₈H₁₄O₄

Molecular Weight: 174.196

Accurate Mass: 174.08921

Percentage Composition: C 55.16%; H 8.10%; O 36.74%

Boiling Point: Bp₁₁ 80°

Refractive Index: n_D²⁰ 1.4160

Aldrich: 36001-5

Fluka: 63310