



>>Entry Name: Decanedioic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Sebacic acid. Octane-1,8-dicarboxylic acid. Ipomic acid

CAS Registry Number: 111-20-6

Related CAS Registry Numbers(s): 51877-43-1

HOOC(CH₂)₈COOH

Molecular Formula: C₁₀H₁₈O₄

Molecular Weight: 202.25

Accurate Mass: 202.12051

Percentage Composition: C 59.39%; H 8.97%; O 31.64%

Biological Source: Isol. from yeasts. Manuf. by alkaline cleavage of ricinoleic acid from castor oil or by electrolytic dimerisation of monomethyl adipate

Use/Importance: Used as a cross-linking agent for epoxy resins and for pptn. separation of Th from lanthanides (pH 2.5). Used for manuf. of nylon-6,10. Esters used as plasticisers

Physical Description: Leaflets

Melting Point: Mp 134.5°

Boiling Point: Bp₁₀₀ 294.5°. Bp₁₅ 243.5°

Solubility: Spar. sol. H₂O; sol. EtOH, Et₂O

pKa Value: pK_{a1} 4.58; pK_{a2} 5.54 (25°, 0.1M KNO₃)

Hazard & Toxicity: LD₅₀ (rat, orl) 3400 mg/kg

Aldrich: 28325-8

Fluka: 84809

Sigma: S2625

>>Derivative: Mono-Me ester

CAS Registry Number: 818-88-2

Molecular Formula: C₁₁H₂₀O₄

Molecular Weight: 216.277

Accurate Mass: 216.13616

Percentage Composition: C 61.09%; H 9.32%; O 29.59%

Physical Description: Viscous liq.

Melting Point: Mp 40-41°

Boiling Point: Bp₂₀ 208°. Bp₁ 157°

Aldrich: 24245-4

Fluka: 84872

Rare Chemicals Library: S66976-8

>>Derivative: Di-Me ester

CAS Registry Number: 106-79-6

Molecular Formula: C₁₂H₂₂O₄

Molecular Weight: 230.303

Accurate Mass: 230.15181

Percentage Composition: C 62.58%; H 9.63%; O 27.79%

Use/Importance: Monomer for manuf. of polyesters

Melting Point: Mp 26.4° (38°)

Boiling Point: Bp₇₅₄ 293°. Bp₂₀ 175°

Solubility: Insol. H₂O; sol. EtOH, Et₂O, Me₂CO

Hazard & Toxicity: Fl. p. 145° (oc)

Aldrich: 22311-5

Fluka: 84860

Sigma: S3000

>>Derivative: Mono-Et ester

CAS Registry Number: 693-55-0

Molecular Formula: C₁₂H₂₂O₄

Molecular Weight: 230.303

Accurate Mass: 230.15181

Percentage Composition: C 62.58%; H 9.63%; O 27.79%

Melting Point: Mp 35-36°

Boiling Point: Bp₁ 158-160°