



>>Entry Name: Heptanedioic acid, 9CI

Synonym(s): Pimelic acid. Pentane-1,5-dicarboxylic acid

CAS Registry Number: 111-16-0

HOOC(CH₂)₅COOH

Molecular Formula: C₇H₁₂O₄

Molecular Weight: 160.169

Accurate Mass: 160.07356

Percentage Composition: C 52.49%; H 7.55%; O 39.96%

Biological Source: Isol. from stems and leaves of *Anthyllis sericea*. Manuf. by oxidation of cycloheptanone or by oxidative cleavage of Hexadecanoic acid [GXZ18-W](#)

Use/Importance: Used in manuf. of polyester and polyamide resins

Physical Description: Prisms (H₂O)

Melting Point: Mp 104-105°

Boiling Point: Bp₁₀ 212°

Solubility: Sol. H₂O, EtOH, Et₂O; BERDY SOL: Sol. MeOH, Et₂O; poorly sol. C₆H₆

pKa Value: pK_{a1} 4.46; pK_{a2} 5.58 (25°)

Other Data: Nonvolatile in steam. Dimorphic, with transition temperature at 75°

Aldrich: P4500-1

Fluka: 80500

Rare Chemicals Library: S31340-8

Sigma: P6753

>>Derivative: Mono-Me ester

Synonym(s): 6-Methoxycarbonylhexanoic acid

CAS Registry Number: 20291-40-1

Molecular Formula: C₈H₁₄O₄

Molecular Weight: 174.196

Accurate Mass: 174.08921

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

Physical Description: Liq.

Boiling Point: Bp₁₈ 181-182°. Bp_{0.15} 118°

>>Derivative: Me ester, chloride

Molecular Formula: C₈H₁₃ClO₃

Molecular Weight: 192.642

Accurate Mass: 192.055322

Percentage Composition: C 49.88%; H 6.80%; Cl 18.40%; O 24.92%

Physical Description: Liq.

Boiling Point: Bp₁₇ 135-136°. Bp_{0.02} 54°

>>Derivative: Di-Me ester

CAS Registry Number: 1732-08-7

Molecular Formula: C₉H₁₆O₄

Molecular Weight: 188.223

Accurate Mass: 188.10486

Percentage Composition: C 57.43%; H 8.57%; O 34.00%

Physical Description: Liq.

Melting Point: Mp -21°

Boiling Point: Bp 257°. Bp₁₁ 121-122°

Solubility: Sl. sol. H₂O; sol. EtOH, Et₂O, C₆H₆

Density: d²⁰ 1.062

Refractive Index: n_D²⁰ 1.4309

Aldrich: 18006-8

Fluka: 80623