



>>Entry Name: Octanedioic acid, 9CI

Synonym(s): Suberic acid, 8CI. 1,6-Hexanedicarboxylic acid

CAS Registry Number: 505-48-6

HOOC(CH₂)₆COOH

Molecular Formula: C₈H₁₄O₄

Molecular Weight: 174.196

Accurate Mass: 174.08921

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

Biological Source: Isol. from stems and leaves of *Anthyllis sericea* and roots of *Phaseolus vulgaris*. Manuf. by oxidative cleavage of cyclooctene

Use/Importance: Used in plastics industry. Monomer for polyesters and polyamides

Physical Description: Cryst. (H₂O or C₆H₆/EtOH)

Melting Point: Mp 144°

Boiling Point: Bp₁₀₀ 279°

Solubility: Insol. H₂O; sol. Et₂O, C₆H₆

pKa Value: pK_{a1} 4.53; pK_{a2} 5.52 (25°, 0.1M KNO₃)

Other Data: Subl. >300°

Aldrich: S520-0

Fluka: 60930

Sigma: S7126

>>Derivative: Mono-Me ester

Synonym(s): Methyl hydrogen suberate

CAS Registry Number: 3946-32-5

Molecular Formula: C₉H₁₆O₄

Molecular Weight: 188.223

Accurate Mass: 188.10486

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

Physical Description: Oil

Melting Point: Mp 14-15°

Boiling Point: Bp₁₈ 185-186°

Aldrich: 24244-6

>>Derivative: Me ester-chloride

Synonym(s): Methyl 7-(chloroformyl)heptanoate. Methyl suberyl chloride

CAS Registry Number: 41624-92-4

Molecular Formula: C₉H₁₅ClO₃

Molecular Weight: 206.668

Accurate Mass: 206.070972

Percentage Composition: C 52.31%; H 7.32%; Cl 17.15%; O 23.22%

Physical Description: Liq.

Refractive Index: n_D²⁰ 1.4500

Aldrich: 38556-5

Rare Chemicals Library: S13432-5

>>Derivative: Di-Me ester

Synonym(s): Dimethyl suberate

CAS Registry Number: 1732-09-8

Molecular Formula: C₁₀H₁₈O₄

Molecular Weight: 202.25

Accurate Mass: 202.12051

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

Physical Description: Oil

Melting Point: Fp -3.1°

Boiling Point: Bp 268°. Bp₉ 130-131°

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

Density: d²⁰ 1.022

Refractive Index: n_D²⁰ 1.4341

Aldrich: 14901-2

Sigma: S6007