



>>Entry Name: Nonanedioic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 1,7-Heptanedicarboxylic acid. **Azelaic acid**, INN, USAN. Anchoic acid. Lepargylic acid. Emerox 1144. Skinoren. ZK 62498

CAS Registry Number: 123-99-9

HOOC(CH₂)₇COOH

Molecular Formula: C₉H₁₆O₄

Molecular Weight: 188.223

Accurate Mass: 188.10486

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

Biological Source: Occurs in rancid fats. Isol. from *Lycopodium* spp. and a few higher plants. Manuf. by ozonolysis of oleic acid

Use/Importance: Used to treat acne. Antiproliferative and cytotoxic effect on human malignant melanocyte. Used for manuf. of polyester and alkyd resins and for nylon 6,9

Physical Description: Needles or leaflets

Development Status: Launched 1989

Melting Point: Mp 106.5°

Boiling Point: Bp 360° part. dec.. Bp₁₀ 226°

Solubility: Spar. sol. H₂O, Et₂O, C₆H₆; sol. EtOH; BERDY SOL: Sol. H₂O, Me₂CO

pKa Value: pK_{a1} 4.56; pK_{a2} 5.53 (25°, 0.1M KNO₃)

Calculated Log P Data: Log P 1.48 (calc)

UV: [neutral] λ_{max} (H₂O) (Berdy)

Other Data: Not steam-volatile

Hazard & Toxicity: Skin and eye irritant

Aldrich: 24637-9

Fluka: 11480

Sigma: A2257

>>Derivative: Mono-Me ester

Synonym(s): Methyl hydrogen azelate

CAS Registry Number: 2104-19-0

Molecular Formula: C₁₀H₁₈O₄

Molecular Weight: 202.25

Accurate Mass: 202.12051

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

Physical Description: Liq.

Melting Point: Mp 22-24°

Boiling Point: Bp₃ 159-160°

Refractive Index: n_D²⁰ 1.4470

Aldrich: A9620-7

Fluka: 11535

>>Derivative: Di-Me ester

Synonym(s): Dimethyl azelate

CAS Registry Number: 1732-10-1

Molecular Formula: C₁₁H₂₀O₄

Molecular Weight: 216.277

Accurate Mass: 216.13616

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

Physical Description: Liq.

Melting Point: Mp -3.9°

Boiling Point: Bp₈ 140°

Solubility: Insol. H₂O; sol. EtOH, Me₂CO, C₆H₆

Density: d²⁰ 1.008

Refractive Index: n_D²⁰ 1.4367

Aldrich: 17102-6

Fluka: 11530

Rare Chemicals Library: S55799-4

>>Derivative: Mono-Et ester

Synonym(s): Ethyl hydrogen azelate