



>>Entry Name: 2,4-Hexadienoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 1,3-Pentadiene-1-carboxylic acid. Sorbic acid, 8CI. E200

CAS Registry Number: 22500-92-1

Related CAS Registry Numbers(s): 590-00-1 821-00-1 1515-80-6 1516-01-4 2614-88-2 7492-55-9 7757-81-5 24634-61-5

$\text{H}_3\text{CCH}=\text{CHCH}=\text{CHCOOH}$

Molecular Formula: $\text{C}_6\text{H}_8\text{O}_2$

Molecular Weight: 112.128

Accurate Mass: 112.05243

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

>>Variant: (E,E)-form

Synonym(s): Panosorb

CAS Registry Number: 110-44-1

Molecular Formula: $\text{C}_6\text{H}_8\text{O}_2$

Molecular Weight: 112.128

Accurate Mass: 112.05243

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Biological Source: Isol. from berries of *Sorbus aucuparia* (rowan), prob. as artifact

Use/Importance: Preservative for many foodstuffs, cosmetics and pharmaceutical products (K and Ca salts used similarly)

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 134.5°

Boiling Point: Bp 228° dec.

Solubility: Mod. sol. hot H_2O

pKa Value: $\text{p}K_{\text{a}1}$ 4.51 (25°, 0.1M NaCl)

Other Data: Undergoes radiation-induced radical polym.

Hazard & Toxicity: Skin and eye irritant, contact sensitizer. LD₅₀ (rat, orl) 7360 mg/kg

Aldrich: H830-7

Fluka: 85510

Sigma: S6901

Supelco: R47-2630

>>Derivative: S-Benzylthiouronium salt

Melting Point: Mp 169-170°

>>Derivative: Me ester

CAS Registry Number: 689-89-4

Molecular Formula: $\text{C}_7\text{H}_{10}\text{O}_2$

Molecular Weight: 126.155

Accurate Mass: 126.06808

Percentage Composition: C 66.65%; H 7.99%; O 25.36%

Physical Description: Leaflets

Melting Point: Mp 5°

Boiling Point: Bp 180°. Bp₂₀ 70°

Aldrich: W37142-4

>>Derivative: Et ester

CAS Registry Number: 5941-48-0

Extra CAS Registry Numbers(s): 2396-84-1

Molecular Formula: $\text{C}_8\text{H}_{12}\text{O}_2$

Molecular Weight: 140.182

Accurate Mass: 140.08373

Percentage Composition: C 68.55%; H 8.63%; O 22.83%

Boiling Point: Bp₁₂ 76.5°. Bp₂₀ 85°