>>**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

$H_3CCH=CHCH=CHCOOH$

Molecular Formula: $C_6H_8O_2$
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: $C_6H_8O_2$
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: pK_{a1} 4.51 (25°, 0.1*M* NaCl)
Other Data: Undergoes radiation-induced radical polym.
Hazard & Toxicity: Skin and eye irritant, contact sensitizer. LD_{50} (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: $C_7H_{10}O_2$
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°. Bp_{20} 70°
Aldrich: W37142-4

>>**Derivative:** Et ester

CAS Registry Number: 5941-48-0
Extra CAS Registry Numbers(s): 2396-84-1
Molecular Formula: $C_8H_{12}O_2$
Molecular Weight: 140.182
Accurate Mass: 140.08373
Percentage Composition: C 68.55%; H 8.63%; O 22.83%
Boiling Point: Bp_{12} 76.5°. Bp_{20} 85°