



Accurate Mass: 154.09938
Percentage Composition: C 70.10%; H 9.15%; O 20.75%
Use/Importance: Preservative used in cosmetics

>>**Derivative:** Chloride

CAS Registry Number: 2614-88-2
Molecular Formula: C₆H₇ClO
Molecular Weight: 130.573
Accurate Mass: 130.018542
Percentage Composition: C 55.19%; H 5.40%; Cl 27.15%; O 12.25%
Boiling Point: Bp₁₂ 69-71°. Bp₁₆ 78°

>>**Derivative:** Amide

CAS Registry Number: 16468-94-3
Molecular Formula: C₆H₉NO
Molecular Weight: 111.143
Accurate Mass: 111.068414
Percentage Composition: C 64.84%; H 8.16%; N 12.60%; O 14.40%
Physical Description: Needles (H₂O)
Melting Point: Mp 172°

>>**Derivative:** Nitrile

Synonym(s): 1-Cyano-1,3-pentadiene

CAS Registry Number: 35684-10-7
Molecular Formula: C₆H₇N
Molecular Weight: 93.128
Accurate Mass: 93.057849
Percentage Composition: C 77.38%; H 7.58%; N 15.04%
Boiling Point: Bp₁₅ 64-68°. Bp₂₀ 72°

>>**Derivative:** 2-Propenyl ester

Synonym(s): 2-Propenyl 2,4-hexadienoate. Allyl sorbate. FEMA 2041

CAS Registry Number: 7493-75-6

Molecular Formula: C₉H₁₂O₂
Molecular Weight: 152.193
Accurate Mass: 152.08373
Percentage Composition: C 71.03%; H 7.95%; O 21.03%
Use/Importance: Flavouring ingredient

>>**Variant:** (2Z,4E)-form

CAS Registry Number: 5309-57-9
Molecular Formula: C₆H₈O₂
Molecular Weight: 112.128
Accurate Mass: 112.05243
Percentage Composition: C 64.27%; H 7.19%; O 28.54%
Physical Description: Needles (pentane)
Melting Point: Mp 33-36°
Boiling Point: Bp₁₆ 121-125°

>>**Derivative:** S-Benzylthiuronium salt

Melting Point: Mp 137°

>>**Derivative:** Me ester

CAS Registry Number: 6932-46-3
Boiling Point: Bp₁₁ 60°. Bp₂₁ 80°