



>>Entry Name: 2,4-Hexadien-1-ol, 9Cl

Synonym(s): Sorbic alcohol. Sorbyl alcohol

CAS Registry Number: 111-28-4

Related CAS Registry Numbers(s): 17102-64-6 53384-66-0 80639-28-7 108965-88-4 114988-57-7

$\text{H}_3\text{CCH}=\text{CHCH}=\text{CHCH}_2\text{OH}$

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}$

Molecular Weight: 98.144

Accurate Mass: 98.073165

Percentage Composition: C 73.43%; H 10.27%; O 16.30%

Biological Source: Sex pheromone component of many insect species

Hazard & Toxicity: Skin and eye irritant. LD₅₀ (rat, orl) 2140 mg/kg. LD₅₀ (rat, skn) 1010 mg/kg

Rare Chemicals Library: S65944-4

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

CAS Registry Number: 17102-64-6

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}$

Molecular Weight: 98.144

Accurate Mass: 98.073165

Percentage Composition: C 73.43%; H 10.27%; O 16.30%

Biological Source: *Tagetes* sp. leaf oil and other plant spp.

Physical Description: Needles

Melting Point: Mp 30.5-31.5°

Boiling Point: Bp₁₂ 76-77°

Other Data: Steam-volatile

Aldrich: 18305-9

Fluka: 52482

>>Derivative: Ac

CAS Registry Number: 57006-69-6

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%

Biological Source: Isol. from the scent glands of various Heteroptera and from the defence secretions of *Thaumastella* spp.

Use/Importance: Sex pheromone and defence secretion. Used in regioselective cycloadditions with a variety of dienophiles

Boiling Point: Bp₃₀ 95°. Bp₁₉ 83-84°

>>Derivative: Propanoyl

CAS Registry Number: 95994-92-6

Molecular Formula: $\text{C}_9\text{H}_{14}\text{O}_2$

Molecular Weight: 154.208

Accurate Mass: 154.09938

Percentage Composition: C 70.10%; H 9.15%; O 20.75%

Biological Source: Isol. from the scent glands of various Heteroptera

Use/Importance: Sex pheromone

>>Derivative: 3,5-Dinitrobenzoyl

Physical Description: Yellow needles (petrol)

Melting Point: Mp 85°