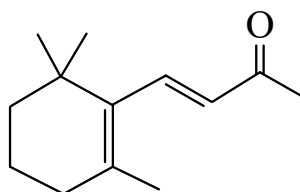




>>Entry Name: 5,7-Megastigmadien-9-one

ENTRY UNDER REVIEW

Synonym(s): 4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one, 9Cl. **β-Ionone**. Boronione. FEMA no. 2595



CAS Registry Number: 14901-07-6

Related CAS Registry Numbers(s): 79-77-6 8013-90-9

Molecular Formula: C₁₃H₂₀O

Molecular Weight: 192.3

Accurate Mass: 192.151415

Percentage Composition: C 81.20%; H 10.48%; O 8.32%

Biological Source: Found in many essential oils including oil of *Boronia megastigma*

Use/Importance: Constit. of coml. Ionone. Perfumery ingredient and flavouring agent

Physical Description: Oil

Boiling Point: Bp₂₄ 150-151°

Hazard & Toxicity: Fl. p. 112°. LD₅₀ (rat, orl) 4590 mg/kg

Aldrich: I-1260-3

>>Derivative: Semicarbazone

Physical Description: Cryst.

Melting Point: Mp 149°

>>Derivative: Thiosemicarbazone

CAS Registry Number: 2302-90-1

Molecular Formula: C₁₄H₂₃N₃S

Molecular Weight: 265.422

Accurate Mass: 265.161267

Percentage Composition: C 63.35%; H 8.73%; N 15.83%; S 12.08%

Use/Importance: Used as a 0.1% soln. in EtOH for extraction-photometric detn. of Cu (λ_{max} 380 nm, ε 17000, CHCl₃)

Physical Description: Cryst.

Melting Point: Mp 167-169°

Solubility: Sol. common org. solvs.; spar. sol. H₂O

>>Derivative: 9-Alcohol

Synonym(s): β-Ionol

CAS Registry Number: 22029-76-1

Molecular Formula: C₁₃H₂₂O

Molecular Weight: 194.316

Accurate Mass: 194.167065

Percentage Composition: C 80.36%; H 11.41%; O 8.23%

Use/Importance: Perfumery and flavouring ingredient

Boiling Point: Bp₂ 105°

>>Derivative: 7,8-Dihydro

Synonym(s): 4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-butanone, 9Cl. 5-Megastigmen-9-one. Dihydro-β-ionone

CAS Registry Number: 17283-81-7