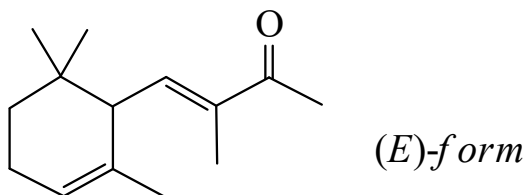




>>Entry Name: 3-Methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one, 9CI

ENTRY UNDER REVIEW

Synonym(s): 3-Methyl- α -ionone. Isomethyl- α -ionone. Cetone Alpha. FEMA 2714



CAS Registry Number: 127-51-5

Molecular Formula: C₁₄H₂₂O

Molecular Weight: 206.327

Accurate Mass: 206.167065

Percentage Composition: C 81.50%; H 10.75%; O 7.75%

Rare Chemicals Library: S40929-4

>>Variant: ($\pm$)-(*E*)-form

CAS Registry Number: 97306-52-0

Extra CAS Registry Numbers(s): 15789-90-9

Molecular Formula: C₁₄H₂₂O

Molecular Weight: 206.327

Accurate Mass: 206.167065

Percentage Composition: C 81.50%; H 10.75%; O 7.75%

Use/Importance: Important perfumery ingredient

Physical Description: Liq. with a fine violet and orris-like odour

Boiling Point: Bp₂ 103-104° (105-110°)

>>Derivative: Semicarbazone

Physical Description: Cryst. (EtOH)

Melting Point: Mp 202°

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 163.5-164°

>>Derivative: 2-Alcohol

Synonym(s): 3-Methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-ol, 9CI. 3-Methyl- α -ionol. Isomethyl- α -ionol

CAS Registry Number: 70172-00-8

Molecular Formula: C₁₄H₂₄O

Molecular Weight: 4126.481

Accurate Mass: 4126.327656

Percentage Composition: C 4.07%; H 95.93%

Use/Importance: Fragrance ingredient

>>Derivative: 2-Alcohol, Ac

CAS Registry Number: 68555-61-3

Molecular Formula: C₁₆H₂₆O₂

Molecular Weight: 250.38

Accurate Mass: 250.19328

Percentage Composition: C 76.75%; H 10.47%; O 12.78%

>>Variant: ($\pm$)-(*Z*)-form

CAS Registry Number: 13743-21-0

Molecular Formula: C₁₄H₂₂O

Molecular Weight: 206.327

Accurate Mass: 206.167065

Percentage Composition: C 81.50%; H 10.75%; O 7.75%

Boiling Point: Bp_{0.03} 69°

References: