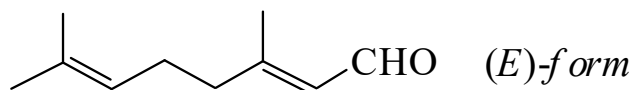




>>Entry Name: 3,7-Dimethyl-2,6-octadienal

ENTRY UNDER REVIEW

Synonym(s): Citral. FEMA 2303



CAS Registry Number: 5392-40-5

Related CAS Registry Numbers(s): 7549-37-3

Molecular Formula: C₁₀H₁₆O

Molecular Weight: 152.236

Accurate Mass: 152.120115

Percentage Composition: C 78.90%; H 10.59%; O 10.51%

Source/Synthesis: Citral as (E,Z)-mixt. is isol. from essential oils (*Litsea cubeba*, lemongrass) and synth. from 3,7-Dimethyl-2,6-octadien-1-ol [JVC33-F](#) or stepwise from 2-Methylpropene [DDL05-H](#) and formaldehyde

Hazard & Toxicity: Fl. p. 91°. Human and exp. skin irritant. LD₅₀ (rat, orl) 4960 mg/kg. Exp. reprod. effects (large dose)

Aldrich: C8300-7

Fluka: 27450

Sigma: C1645

>>Variant: (E)-form

Synonym(s): Geranial. Citral a

CAS Registry Number: 141-27-5

Type of Compound Code(s): WE2000 VS0100 WI2000

Molecular Formula: C₁₀H₁₆O

Molecular Weight: 152.236

Accurate Mass: 152.120115

Percentage Composition: C 78.90%; H 10.59%; O 10.51%

Biological Source: Occurs in lemon grass oil (*Cymbopogon citratus*), lemon, orange and many other essential oils. Sex pheromone of the parasitic wasp *Itoplectis conquisitor*; recruiting pheromone for honey bees, alarm pheromone for various formicine ants, the myrmicine ant *Atta sexdens* and the bee *Lestrimelitta limao*

Use/Importance: Important in the food and perfume industry

Boiling Point: Bp 229°. Bp₂₀ 119°

Refractive Index: n_D²⁰ 1.4898

>>Derivative: Semicarbazone

Physical Description: Cryst.

Melting Point: Mp 164°

>>Derivative: Di-Et acetal

Synonym(s): 1,1-Diethoxy-3,7-dimethyl-2,6-octadiene

CAS Registry Number: 7492-66-2

Molecular Formula: C₁₄H₂₆O₂

Molecular Weight: 226.358

Accurate Mass: 226.19328

Percentage Composition: C 74.29%; H 11.58%; O 14.14%

Use/Importance: Used in soap perfumes

Physical Description: Liq. with woody-citrus odour

Boiling Point: Bp₁₅ 140-142°

Refractive Index: n_D²⁰ 1.4503

Other Data: Props. prob. refer to a mixt. with the Z-isomer

Aldrich: W23040-5