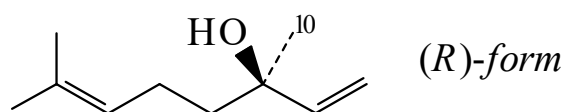




>>Entry Name: 3,7-Dimethyl-1,6-octadien-3-ol

ENTRY UNDER REVIEW

Synonym(s): Linalool. Linalol. Linalyl alcohol. Licareol. Coriandrol. β -Linalool. FEMA 2635



CAS Registry Number: 78-70-6

Related CAS Registry Numbers(s): 82928-12-9

Type of Compound Code(s): WE2000 XA1150 WE4500 XA2250 XA1400

Molecular Formula: $C_{10}H_{18}O$

Molecular Weight: 154.252

Accurate Mass: 154.135765

Percentage Composition: C 77.87%; H 11.76%; O 10.37%

Source/Synthesis: Prod. synthetically by several routes

Use/Importance: Spasmolytic agent. Used extensively in perfumery industry. Flavouring agent. Important intermed. in manuf. of α -Tocopherol [BDR14-R](#). Possesses antimicrobial, anticonvulsant props.

Calculated Log P Data: Log P 2.55 (calc)

Other Data: Natural enantiomeric composition of the various esters of Linalool is mostly not well documented. The phys. props. are given here under the racemates but some props. may refer to opt. active samples

Hazard & Toxicity: Fl. p. 71/76°. Skin irritant. LD₅₀ (rat, orl) 2790 mg/kg

Aldrich: W26351-6

Fluka: 62140

Sigma: L5255

Supelco: 48-2635

>>Variant: (R)-form

CAS Registry Number: 126-91-0

Type of Compound Code(s): WE2000 WE4500 VS0100 XA6300

Molecular Formula: $C_{10}H_{18}O$

Molecular Weight: 154.252

Accurate Mass: 154.135765

Percentage Composition: C 77.87%; H 11.76%; O 10.37%

Biological Source: Constit. of many essential oils including *Melissa officinalis* (lemon balm), rose, neroli and lavender. Major component of oil of *Mentha arvensis*

Biological Use/Importance: Shows sedative and antibacterial props.; active ingredient of herbal medicines containing lemon balm extracts

Physical Description: Oil

Boiling Point: Bp₇₅₆ 197-200°

Optical Rotation: $[\alpha]_D^{20} -17$

Calculated Log P Data: Log P 2.55 (calc)

Hazard & Toxicity: LD₅₀ (mus, ivn) 180 mg/kg

Fluka: 62139

>>Derivative: 3-O-[α -L-Rhamnopyranosyl-(1→2)-glucopyranoside]

Synonym(s): Anatolioside

CAS Registry Number: 147612-75-7

Type of Compound Code(s): VS0100

Molecular Formula: $C_{22}H_{38}O_{10}$

Molecular Weight: 462.536

Accurate Mass: 462.2465

Percentage Composition: C 57.13%; H 8.28%; O 34.59%

Biological Source: Constit. of *Viburnum orientale*

Physical Description: Amorph. powder

Optical Rotation: $[\alpha]_D^{20} -31.4$ (c, 0.29 in MeOH)