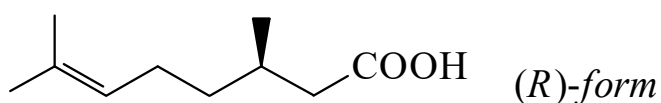




>>Entry Name: 3,7-Dimethyl-6-octenoic acid

ENTRY UNDER REVIEW

Synonym(s): Citronellic acid. Rhodinic acid. Callitrol. FEMA 3142



CAS Registry Number: 502-47-6

Related CAS Registry Numbers(s): 51566-62-2

Type of Compound Code(s): WE2000

Molecular Formula: C₁₀H₁₈O₂

Molecular Weight: 170.251

Accurate Mass: 170.13068

Percentage Composition: C 70.55%; H 10.66%; O 18.80%

Source/Synthesis: Readily obt. from naturally occurring 3,7-Dimethyl-6-octenal [JSX87-E](#), as partially racemic (*R*)-enantiomer

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 2610 mg/kg. LD₅₀ (rbt, skn) 450 mg/kg

Aldrich: 30342-9

>>Variant: (*R*)-form

CAS Registry Number: 18951-85-4

Molecular Formula: C₁₀H₁₈O₂

Molecular Weight: 170.251

Accurate Mass: 170.13068

Percentage Composition: C 70.55%; H 10.66%; O 18.80%

Physical Description: Oil

Boiling Point: Bp 257°. Bp₁₀ 143°

Optical Rotation: [α]_D +10.3 (c, 5.0 in CHCl₃) (98% ee)

Refractive Index: n_D²⁵ 1.4520

Aldrich: 34049-9

Sigma: C7080

>>Derivative: Nitrile

Synonym(s): Citronellonitrile

CAS Registry Number: 35931-93-2

Molecular Formula: C₁₀H₁₇N

Molecular Weight: 151.251

Accurate Mass: 151.136099

Percentage Composition: C 79.41%; H 11.33%; N 9.26%

Use/Importance: Used in perfumery

>>Variant: (*S*)-form

CAS Registry Number: 2111-53-7

Type of Compound Code(s): VS0100

Molecular Formula: C₁₀H₁₈O₂

Molecular Weight: 170.251

Accurate Mass: 170.13068

Percentage Composition: C 70.55%; H 10.66%; O 18.80%

Biological Source: Constit. of *Callitris glauca*, *Callitris intratropica*, *Chamaecyparis obtusa*, *Thujopsis dolabrata*, *Juniperus* spp. and other plants

Boiling Point: Bp_{0.6} 118°

Optical Rotation: [α]_D²⁴ -6.6

Aldrich: 36442-8

Sigma: C6955