



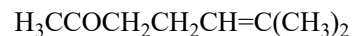
>>Entry Name: 6-Methyl-5-hepten-2-one, 9CI

ENTRY UNDER REVIEW

Synonym(s): Sulcatone

CAS Registry Number: 110-93-0

Related CAS Registry Numbers(s): 409-02-9



Molecular Formula: C₈H₁₄O

Molecular Weight: 126.198

Accurate Mass: 126.104465

Percentage Composition: C 76.14%; H 11.18%; O 12.68%

Biological Source: Present in Ceylon citronella oil, lemon-grass oil and palmarosa oil. Produced by *Endoconidiophora coerulescens* and other spp. Isol. from the Australian meat ant, *Iridomyrmex purpureus*. Chemical scent constit. of urine of red fox *Vulpes vulpes*. Sex pheromone of the aphid *Alloxysta victrix*. Product of α-farnesene 1,3,6,10-Farnesatetraene JXF60-O oxidation in stored apples affected by superficial scald

Use/Importance: Intermed. in the manuf. of terpene alcohols. Insecticidal agent

Boiling Point: Bp 172-174° (161-162°). Bp₁₀ 58.5°

Hazard & Toxicity: Fl. p. 57°

Aldrich: W27073-3

Fluka: 67320

Sigma: M8137

>>Derivative: Oxime

CAS Registry Number: 22418-73-1

Molecular Formula: C₈H₁₅NO

Molecular Weight: 141.213

Accurate Mass: 141.115364

Percentage Composition: C 68.04%; H 10.71%; N 9.92%; O 11.33%

Boiling Point: Bp₁₂ 99°

>>Derivative: Semicarbazone

CAS Registry Number: 16769-68-9

Melting Point: Mp 135 approx.°

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 6147-43-9

Melting Point: Mp 78°

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 415D, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 646B, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 501B, (*ir*)
Birkinshaw, J.H. *et al.*, *Biochem. J.*, 1950, **47**, 55, (*isol*)
Mousseron, M. *et al.*, *Bull. Soc. Chim. Fr.*, 1963, 376, (*synth*)
Saucy, G. *et al.*, *Helv. Chim. Acta*, 1967, **50**, 2091, (*synth*)
Sato, K. *et al.*, *J.O.C.*, 1970, **35**, 565, (*synth*)
Boccaro, N. *et al.*, *Bull. Soc. Chim. Fr.*, 1972, 1448, (*synth*)
Ishihara, T. *et al.*, *Agric. Biol. Chem.*, 1974, **38**, 439, (*synth, bibl*)
Dennison, N.R. *et al.*, *Aust. J. Chem.*, 1975, **28**, 1339, (*synth*)
Savoia, D. *et al.*, *J.O.C.*, 1978, **43**, 2907, (*synth*)
Whitten, W.K. *et al.*, *J. Chem. Ecol.*, 1980, **6**, 49
McKenzie, T.C., *Org. Prep. Proced. Int.*, 1987, **19**, 435, (*synth*)
Kim, J.H. *et al.*, *J. Nat. Prod.*, 1989, **52**, 63, (*biosynth*)
Micha, S.H. *et al.*, *Eur. J. Entomol.*, 1993, **90**, 439
Mir, N.A. *et al.*, *J. Agric. Food Chem.*, 1999, **47**, 7-11, (*occur*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, MKK000