



>>Entry Name: 5-Hexen-2-one, 9CI

Synonym(s): Allylacetone. Sulcatol

CAS Registry Number: 109-49-9

$\text{H}_2\text{C}=\text{CHCH}_2\text{CH}_2\text{COCH}_3$

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}$

Molecular Weight: 98.144

Accurate Mass: 98.073165

Percentage Composition: C 73.43%; H 10.27%; O 16.30%

Biological Source: Constit. of shale tar and of *Osmanthus fragrans*

Boiling Point: Bp 129.6°. Bp₁₀₀ 69°

Aldrich: H1300-1

Fluka: 53070

>>Derivative: Oxime

CAS Registry Number: 59239-06-4

Molecular Formula: $\text{C}_6\text{H}_{11}\text{NO}$

Molecular Weight: 113.159

Accurate Mass: 113.084064

Percentage Composition: C 63.69%; H 9.80%; N 12.38%; O 14.14%

Boiling Point: Bp 190°

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 2057-91-2

Physical Description: Orange cryst. (EtOH)

Melting Point: Mp 108-109°

>>Derivative: Semicarbazone

Melting Point: Mp 100-102°

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 415B, (*ir*)
Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **1**, 645A, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 500D, (*ir*)
Merling, G., *Annalen*, 1891, **264**, 310, (*synth*)
Hoffman, W. *et al.*, *Annalen*, 1969, **729**, 52, (*synth*)
Meyer, A.I., *J.O.C.*, 1972, **37**, 4289, (*synth*)
Cornish, C.A. *et al.*, *J.C.S. Perkin 1*, 1985, 2585, (*synth*, *ir*, *pmr*)
McKenzie, T.C., *Org. Prep. Proced. Int.*, 1987, **19**, 435, (*synth*)
Ding, D. *et al.*, *J. Essent. Oil Res.*, 1989, **1**, 295, (*isol*)
Davies, S.G. *et al.*, *Tetrahedron: Asymmetry*, 1996, **7**, 1005, (*synth*)
Motorina, I.A. *et al.*, *J.O.C.*, 1997, **62**, 2098-2105, (*oxime*)