



>>Entry Name: 4-Hexen-3-one

ENTRY UNDER REVIEW

Synonym(s): FEMA 3352

CAS Registry Number: 2497-21-4

$\text{H}_3\text{CCH}_2\text{COCH}=\text{CHCH}_3$

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%

Use/Importance: Flavouring ingredient

Aldrich: W33520-7

>>Variant: (*E*)-form

CAS Registry Number: 50396-87-7

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%

Boiling Point: Bp 135-137°. Bp₅₅ 58-61°

Refractive Index: n_D^{20} 1.4400

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Red cryst.

Melting Point: Mp 170°

Other Data: This deriv. presumed here to belong to the (*E*)-isomer

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 645B, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 501A, (*ir*)

Coppens, *Bull. Soc. Chim. Belg.*, 1929, **38**, 310

Stutsman, P.S. *et al.*, *J.A.C.S.*, 1939, **61**, 3303, (*synth*)

Oare, D.A. *et al.*, *J.O.C.*, 1990, **55**, 132, (*synth, ir, pmr*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 334

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1304-1305