



>>Entry Name: 3-Hepten-2-one, 9CI

ENTRY UNDER REVIEW

Synonym(s): FEMA 3400

CAS Registry Number: 1119-44-4

$\text{H}_3\text{C}(\text{CH}_2)_2\text{CH}=\text{CHCOCH}_3$

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}$

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Use/Importance: Flavouring ingredient

Boiling Point: Bp_{23} 66°

>>Variant: (E)-form

CAS Registry Number: 5609-09-6

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}$

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Boiling Point: Bp_{11} 51-52°

Density: d^{20} 0.85

Refractive Index: n_D^{20} 1.4436

>>Derivative: Semicarbazone

Melting Point: Mp 128°

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Cryst. (EtOH)

Melting Point: Mp 124.5-125°

>>Variant: (Z)-form

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}$

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Boiling Point: Bp_{11} 34-39°

Density: d^{20} 0.88

Refractive Index: n_D^{20} 1.4325

>>Derivative: Semicarbazone

Melting Point: Mp 107.5-108.5°

References:

Sturtz, G., *Bull. Soc. Chim. Fr.*, 1967, 2477, (synth)

Sharpless, K.B. *et al.*, *J.A.C.S.*, 1973, **95**, 6137, (synth)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 319

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1275