



>>Entry Name: 6-Methyl-3,5-heptadien-2-one, 9CI

ENTRY UNDER REVIEW

Synonym(s): FEMA 3363

CAS Registry Number: 1604-28-0



Molecular Formula: $\text{C}_8\text{H}_{12}\text{O}$

Molecular Weight: 124.182

Accurate Mass: 124.088815

Percentage Composition: C 77.38%; H 9.74%; O 12.88%

Biological Source: Isol. from lavender oil (*Lavendula officinalis* hybrid)

>>Variant: (*E*)-(?) -form

CAS Registry Number: 16647-04-4

Molecular Formula: $\text{C}_8\text{H}_{12}\text{O}$

Molecular Weight: 124.182

Accurate Mass: 124.088815

Percentage Composition: C 77.38%; H 9.74%; O 12.88%

Boiling Point: Bp_{12} 89°

Refractive Index: n_{D}^{20} 1.5265

>>Derivative: Oxime

Molecular Formula: $\text{C}_8\text{H}_{13}\text{NO}$

Molecular Weight: 139.197

Accurate Mass: 139.099714

Percentage Composition: C 69.03%; H 9.41%; N 10.06%; O 11.49%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 114-115°

>>Derivative: Semicarbazone

Physical Description: Needles (MeOH)

Melting Point: Mp 192 dec.°

References:

Lacey, R.N., *J.C.S.*, 1954, 827, (*synth, uv*)

U.K. Pat., 1955, 741 047; *CA*, **50**, 16839, (*synth*)

Stadler, P.A. *et al.*, *Helv. Chim. Acta*, 1960, **43**, 1601, (*isol*)

Heck, R.F., *J.A.C.S.*, 1963, **85**, 3383, (*synth*)

Schirmann, J.-P. *et al.*, *Bull. Soc. Chim. Fr.*, 1967, 3896, (*synth*)

Saucy, G. *et al.*, *Helv. Chim. Acta*, 1967, **50**, 1158, (*synth*)

Julia, M. *et al.*, *Bull. Soc. Chim. Fr.*, 1976, 1941, (*synth*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 506

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1768-1769