



>>Entry Name: 5-Hydroxy-4-octanone, 9CI

ENTRY UNDER REVIEW

Synonym(s): Butyrolin. FEMA 1380

CAS Registry Number: 496-77-5

Related CAS Registry Numbers(s): 86838-18-8 116214-05-2

$\text{H}_3\text{CCH}_2\text{CH}_2\text{CH}(\text{OH})\text{COCH}_2\text{CH}_2\text{CH}_3$

Molecular Formula: $\text{C}_8\text{H}_{16}\text{O}_2$

Molecular Weight: 144.213

Accurate Mass: 144.11503

Percentage Composition: C 66.63%; H 11.18%; O 22.19%

Use/Importance: Flavouring ingredient

Physical Description: Oil with a sweet, slightly pungent, buttery/nut-like odour and a sweet, oily taste

Density: d^{20}_4 0.92

Refractive Index: n^{20}_D 1.4290

Aldrich: W25870-9

>>Variant: ($\pm$)-form

CAS Registry Number: 116296-89-0

Molecular Formula: $\text{C}_8\text{H}_{16}\text{O}_2$

Molecular Weight: 144.213

Accurate Mass: 144.11503

Percentage Composition: C 66.63%; H 11.18%; O 22.19%

Physical Description: Oil

Boiling Point: Bp 180-190°. Bp₄ 62-63°

>>Derivative: Ac

Molecular Formula: $\text{C}_{10}\text{H}_{18}\text{O}_3$

Molecular Weight: 186.25

Accurate Mass: 186.125595

Percentage Composition: C 64.49%; H 9.74%; O 25.77%

Physical Description: Oil

Boiling Point: Bp₇ 90-92°

>>Derivative: Oxime

Molecular Formula: $\text{C}_8\text{H}_{17}\text{NO}_2$

Molecular Weight: 159.228

Accurate Mass: 159.125929

Percentage Composition: C 60.35%; H 10.76%; N 8.80%; O 20.10%

Physical Description: Oil

Boiling Point: Bp₁₀ 143°

References:

Org. Synth., Coll. Vol., 2, 1943, 114-116, (*synth*)

Stetter, H. *et al.*, *Synthesis*, 1976, 733-735, (*synth*)

Srinivason, N.S. *et al.*, *Synthesis*, 1979, 520-521, (*synth, ir, pmr, ms*)

Tamao, K. *et al.*, *Tet. Lett.*, 1986, **27**, 65-68, (*synth*)

Org. Synth., Coll. Vol., 7, 1990, 95-99, (*synth, ir, pmr*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 368

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1380