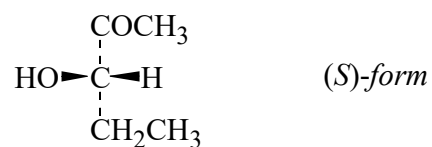




>>Entry Name: 3-Hydroxy-2-pentanone, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2-Oxo-3-pentanol. Acetylethylcarbinol. FEMA 3550



CAS Registry Number: 3142-66-3

Related CAS Registry Numbers(s): 113919-08-7

Molecular Formula: C₅H₁₀O₂

Molecular Weight: 102.133

Accurate Mass: 102.06808

Percentage Composition: C 58.80%; H 9.87%; O 31.33%

>>Variant: (S)-form

CAS Registry Number: 132881-72-2

Molecular Formula: C₅H₁₀O₂

Molecular Weight: 102.133

Accurate Mass: 102.06808

Percentage Composition: C 58.80%; H 9.87%; O 31.33%

Optical Rotation: $[\alpha]_{578}^{15} +52$ (c, 7 in CHCl₃) ($\geq 98\%$ ee)

>>Variant: (±)-form

CAS Registry Number: 118712-30-4

Molecular Formula: C₅H₁₀O₂

Molecular Weight: 102.133

Accurate Mass: 102.06808

Percentage Composition: C 58.80%; H 9.87%; O 31.33%

Use/Importance: Flavouring agent

Physical Description: Liq.

Boiling Point: Bp 147-148°. Bp₃₅ 77°

Density: d₄²⁰ 0.95

>>Derivative: Ac

CAS Registry Number: 20510-66-1

Molecular Formula: C₇H₁₂O₃

Molecular Weight: 144.17

Accurate Mass: 144.078645

Percentage Composition: C 58.32%; H 8.39%; O 33.29%

Boiling Point: Bp₁₃ 68-70°

>>Derivative: Me ether

Synonym(s): 3-Methoxy-2-pentanone

Molecular Formula: C₆H₁₂O₂

Molecular Weight: 116.16

Accurate Mass: 116.08373

Percentage Composition: C 62.04%; H 10.41%; O 27.55%

Boiling Point: Bp₇₆₁ 154-155°

References:

Vénus-Daniloff, E., *Bull. Soc. Chim. Fr.*, 1928, **43**, 582-586, (*synth*)

Bouis, M., *Bull. Soc. Chim. Fr.*, 1932, **51**, 1177-1178, (*synth*)

Singh, M. *et al.*, *J.O.C.*, 1992, **57**, 4263-4270, (*Ac, synth, ir, pmr, cmr*)

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

Bel-Rhlid, R. *et al.*, *Bull. Soc. Chim. Fr.*, 1996, **133**, 1011-1021, (*synth, pmr*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1381