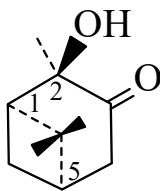




>>Entry Name: **2-Hydroxy-3-pinanone**

Synonym(s): 2-Hydroxy-2,6,6-trimethylbicyclo[3.1.1]heptan-3-one, 9Cl. Oxypinone. Oxypinocamphone



(1*R*,2*R*,5*R*)-*form*

CAS Registry Number: 10136-65-9

Molecular Formula: C₁₀H₁₆O₂

Molecular Weight: 168.235

Accurate Mass: 168.11503

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Hazard & Toxicity: LD₅₀ (mus, scu) 500 mg/kg

>>Variant: (1*R*,2*R*,5*R*)-form

CAS Registry Number: 24047-72-1

Molecular Formula: C₁₀H₁₆O₂

Molecular Weight: 168.235

Accurate Mass: 168.11503

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Melting Point: Mp 37-39°

Boiling Point: Bp 245°

Optical Rotation: [α]_D²⁰+39 (c, 0.5 in CHCl₃)

Aldrich: 40041-6

>>Variant: (1*S*,2*R*,5*S*)-form

CAS Registry Number: 20536-50-9

Molecular Formula: C₁₀H₁₆O₂

Molecular Weight: 168.235

Accurate Mass: 168.11503

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Physical Description: Oil

Boiling Point: Bp_{0.15} 53-55°

Optical Rotation: [α]_D²⁵+90.41 (c, 5 in CHCl₃)

>>Derivative: Ac

Physical Description: Cryst. (pentane)

Melting Point: Mp 50-51°

Optical Rotation: [α]_D²⁵-0.33 (c, 12 in CHCl₃)

>>Variant: (1*S*,2*S*,5*S*)-form

CAS Registry Number: 1845-25-6

Molecular Formula: C₁₀H₁₆O₂

Molecular Weight: 168.235

Accurate Mass: 168.11503

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Use/Importance: Used in asymmetric synth. of amino acids

Physical Description: Prisms (pentane)

Melting Point: Mp 31-32°

Boiling Point: Bp₁₇ 113-115°

Optical Rotation: [α]_D²⁵-38.9 (c, 2.64 in CHCl₃)

Aldrich: 38034-2

Fluka: 56205