



>>Entry Name: 4-Hydroxy-4-methyl-2-pentanone, 9CI

Synonym(s): Diacetone alcohol. Acetonyldimethylcarbinol. Pyranton A

CAS Registry Number: 123-42-2

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

Molecular Formula: $\text{C}_6\text{H}_{12}\text{O}_2$

Molecular Weight: 116.16

Accurate Mass: 116.08373

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

Biological Source: Isol. from the arctic bramble *Rubus arcticus*, from green algae and from the sleepy grass sp. *Stipa vaseyi*. Prod. by *Streptomyces olivaceus*. Prod. from acetone in the presence of base

Use/Importance: Solvent, preservative in pharmaceutical preparations. Used in brake fluids and surface coatings, low acute tox.

Biological Use/Importance: Hypnotic

Physical Description: Oil

Melting Point: Mp -44°

Boiling Point: Bp 164° . Bp₁₁ $63-64^\circ$

Solubility: Sol. H_2O

Hazard & Toxicity: Skin, mucous membrane and severe eye irritant. Inhalation causes headache, nausea, eye and pulmonary effects. Exp. hepatotoxic. Flammable, fl. p. 55/59/64°, autoignition temp. 603/643°. OES: long-term 50 ppm; short-term 75 ppm

Aldrich: H4154-4

Fluka: 31450

>>Derivative: Oxime

CAS Registry Number: 17918-67-1

Molecular Formula: $\text{C}_6\text{H}_{13}\text{NO}_2$

Molecular Weight: 131.174

Accurate Mass: 131.094629

Percentage Composition: C 54.94%; H 9.99%; N 10.68%; O 24.39%

Melting Point: Mp $104-105^\circ$ (58.5°)

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 95122-53-5

Melting Point: Mp $198-199^\circ$

>>Derivative: Me ether

Synonym(s): 4-Methoxy-4-methyl-2-pentanone. Pentoxone

CAS Registry Number: 107-70-0

Molecular Formula: $\text{C}_7\text{H}_{14}\text{O}_2$

Molecular Weight: 130.186

Accurate Mass: 130.09938

Percentage Composition: C 64.58%; H 10.84%; O 24.58%

Use/Importance: Solvent for lacquers and resins

Boiling Point: Bp₂₂ 95° . Bp₁₀ 48°

References:

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