



>>Entry Name: 2,4-Pentanedione, 9CI, 8CI

Synonym(s): Acetylacetone. Diacetylmethane. 4-Hydroxy-3-penten-2-one

CAS Registry Number: 123-54-6

Related CAS Registry Numbers(s): 10556-94-2 17272-66-1

$\text{H}_3\text{CCOCH}_2\text{COCH}_3 \leftrightarrow \text{H}_3\text{CC}(\text{OH})=\text{CHCOCH}_3$

Molecular Formula: $\text{C}_5\text{H}_8\text{O}_2$

Molecular Weight: 100.117

Accurate Mass: 100.05243

Percentage Composition: C 59.98%; H 8.05%; O 31.96%

Biological Source: Isol. from ethereal oil of *Pinus sylvestris*

Use/Importance: Protecting reagent for aminoacids. Cleaves phenylhydrazones and semicarbazones, intermed. in heterocyclic synth. Forms many metal complexes. Used for extraction and separation of Al, Be, Ce, Co, Ga, In, Fe(III), Mo, U, V

Physical Description: Liq.

Boiling Point: $\text{Bp}_{746} 139^\circ$

Solubility: Sol. dil. HCl; spar. sol. hot H_2O ; misc. org. solvs.

Density: $d_4^{25} 0.927$

Hazard & Toxicity: Flammable, fl. p. 34° , autoignition temp. 340° . Skin and severe eye irritant. LD_{50} (rat, orl) 55 mg/kg. Exp. neurotoxic. Repeated exposure to low concs. may be cumulative

Aldrich: P775-4

Fluka: 909

Sigma: A3636

>>Variant: Oxo-form

Molecular Formula: $\text{C}_5\text{H}_8\text{O}_2$

Molecular Weight: 100.117

Accurate Mass: 100.05243

Percentage Composition: C 59.98%; H 8.05%; O 31.96%

Melting Point: $\text{Mp } -23^\circ$

pKa Value: $\text{pK}_a -6.1$ (H_2SO_4)

>>Derivative: Imine

Synonym(s): 4-Imino-2-pentanone, 9CI. 4-Amino-3-penten-2-one. Fluoral P

CAS Registry Number: 870-74-6

Molecular Formula: $\text{C}_5\text{H}_9\text{NO}$

Molecular Weight: 99.132

Accurate Mass: 99.068414

Percentage Composition: C 60.58%; H 9.15%; N 14.13%; O 16.14%

Physical Description: Cryst. (EtOAc)

Melting Point: $\text{Mp } 43^\circ$ (40°)

Rare Chemicals Library: S36623-4

>>Derivative: Monoanil

Synonym(s): 4-(Phenylimino)-2-pentanone, 9CI. 4-Anilino-3-penten-2-one

CAS Registry Number: 880-12-6

Molecular Formula: $\text{C}_{11}\text{H}_{13}\text{NO}$

Molecular Weight: 175.23

Accurate Mass: 175.099714

Percentage Composition: C 75.40%; H 7.48%; N 7.99%; O 9.13%

Physical Description: Cryst. (petrol)

Melting Point: $\text{Mp } 51-53^\circ$

Boiling Point: $\text{Bp } 285-286^\circ$

Rare Chemicals Library: S53251-7