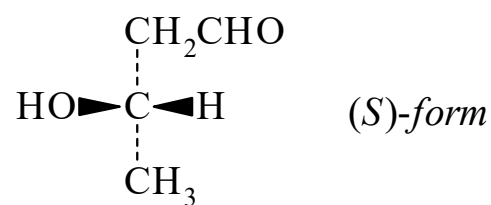




>>Entry Name: 3-Hydroxybutanal, 9CI

Synonym(s): β -Hydroxybutyraldehyde. Aldol. Acetaldol



CAS Registry Number: 107-89-1

Related CAS Registry Numbers(s): 39562-58-8

Molecular Formula: $\text{C}_4\text{H}_8\text{O}_2$

Molecular Weight: 88.106

Accurate Mass: 88.05243

Percentage Composition: C 54.53%; H 9.15%; O 36.32%

Hazard & Toxicity: Fl. p. 83/66° (oc), autoignition temp. 245/250°. Skin and eye irritant. LD₅₀ (rat, orl) 2180 mg/kg. LD₅₀ (rbt, skn) 140 mg/kg

Rare Chemicals Library: S42682-2

>>Variant: (*S*)-form

Molecular Formula: $\text{C}_4\text{H}_8\text{O}_2$

Molecular Weight: 88.106

Accurate Mass: 88.05243

Percentage Composition: C 54.53%; H 9.15%; O 36.32%

>>Derivative: Di-Me acetal

CAS Registry Number: 86146-07-8

Boiling Point: Bp₂₅ 87°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -13.1$ (c, 1.1 in CHCl_3)

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

Molecular Formula: $\text{C}_4\text{H}_8\text{O}_2$

Molecular Weight: 88.106

Accurate Mass: 88.05243

Percentage Composition: C 54.53%; H 9.15%; O 36.32%

Physical Description: Syrupy liq.

Boiling Point: Bp₂₀ 83°

Solubility: Misc. H_2O , EtOH

Density: d^{16} 1.11

Other Data: Dec. at 85° $\rightarrow$ 2-Butenal [HHW33-L](#) + H_2O

>>Derivative: Oxime

CAS Registry Number: 82521-17-3

Molecular Formula: $\text{C}_4\text{H}_9\text{NO}_2$

Molecular Weight: 103.121

Accurate Mass: 103.063329

Percentage Composition: C 46.59%; H 8.80%; N 13.58%; O 31.03%

Boiling Point: Bp₁₁ 117-118°

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 18295-45-9

Melting Point: Mp 93-95°

>>Derivative: Ac

CAS Registry Number: 26391-36-6

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_3$

Molecular Weight: 130.143

Accurate Mass: 130.062995

Percentage Composition: C 55.37%; H 7.74%; O 36.88%

Boiling Point: Bp₁₈ 87-89°