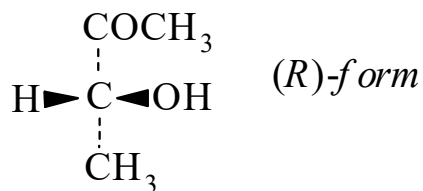




>>Entry Name: 3-Hydroxy-2-butanone, 9CI, 8CI

ENTRY UNDER REVIEW

Synonym(s): Acetoin. Dimethylketol. Methylacetylcarbinol. 1-Hydroxyethyl methyl ketone. Acetylmethylcarbinol. FEMA 2008



CAS Registry Number: 513-86-0

Molecular Formula: C₄H₈O₂

Molecular Weight: 88.106

Accurate Mass: 88.05243

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

Biological Source: Constit. of beer, wine, fresh or cooked apple, fresh or cooked leek, corn, honey, cocoa, butter, cheeses, roasted coffee and other foodstuffs

Use/Importance: Flavouring ingredient, low oral tox.

Aldrich: A1795-1

Fluka: 540

Supelco: S48-2008

>>Variant: (R)-form

CAS Registry Number: 53584-56-8

Molecular Formula: C₄H₈O₂

Molecular Weight: 88.106

Accurate Mass: 88.05243

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

Biological Source: Constit. of butter and produced by many microorganisms

Boiling Point: Bp 142.7-143.2°. Bp₂₀ 49.2°

Optical Rotation: [α]_D²⁰ -58 (neat)

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 114-116°

Optical Rotation: [α]_D²⁵ -12 (c, 2.765 in CHCl₃)

>>Derivative: Semicarbazone

Melting Point: Mp 188°

>>Variant: (S)-form

CAS Registry Number: 78183-56-9

Molecular Formula: C₄H₈O₂

Molecular Weight: 88.106

Accurate Mass: 88.05243

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

Boiling Point: Bp 142-144°. Bp₂₃ 51°

Other Data: Not obt. optically pure

>>Derivative: Semicarbazone

Melting Point: Mp 187°