



>>Entry Name: 5-Methyl-3-hexen-2-one, 9CI

ENTRY UNDER REVIEW

Synonym(s): Isobutylideneacetone. FEMA 3409

CAS Registry Number: 5166-53-0

$\text{H}_3\text{CCOCH}=\text{CHCH}(\text{CH}_3)_2$

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}$

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Biological Source: Occ. in the oil of *Carphephorus* spp.

Hazard & Toxicity: LD₅₀ (rat, orl) 1680 mg/kg. LD₅₀ (rbt, skn) 450 mg/kg

Aldrich: 18760-7

>>Variant: (E)-form

CAS Registry Number: 1821-29-0

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}$

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Use/Importance: Flavouring ingredient

Boiling Point: Bp₅₀ 77.5°

Density: d²² 0.84

Refractive Index: n_D²² 1.4395

Other Data: The (Z)-form was erroneously reported in the earlier lit.(1930)

>>Derivative: Semicarbazone

Melting Point: Mp 126°

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 170.5°

References:

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Sheikh, Y.M. *et al.*, *Org. Mass Spectrom.*, (Suppl.), 1970, **4**, 273, (ms)

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