



>>Entry Name: 2-Heptenal, 9CI

ENTRY UNDER REVIEW

Synonym(s): FEMA 3165

CAS Registry Number: 2463-63-0

Related CAS Registry Numbers(s): 20810-22-4

$\text{H}_3\text{C}(\text{CH}_2)_3\text{CH}=\text{CHCHO}$

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: Isol. from soya bean oil (*Glycine max*)

Use/Importance: Flavouring constit. of many foods

Physical Description: Oil with pungent, green, somewhat fatty odour, pleasant only in extreme dilution

Density: d 0.86

Refractive Index: n_D^{20} 1.4491

>>Variant: (E)-form

CAS Registry Number: 18829-55-5

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%

Boiling Point: Bp 165-167°. Bp₁₅ 61-62°

Aldrich: 25176-3

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 2122-10-3

Melting Point: Mp 132-133°

>>Variant: (Z)-form

CAS Registry Number: 57266-86-1

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%

Boiling Point: Bp₁₆ 64-65°

>>Derivative: Di-Et acetal

Synonym(s): 1,1-Diethoxy-1-heptene

Molecular Formula: $\text{C}_{11}\text{H}_{22}\text{O}_2$

Molecular Weight: 186.294

Accurate Mass: 186.16198

Percentage Composition: C 70.92%; H 11.90%; O 17.18%

Boiling Point: Bp₁₅ 90-92°

References:

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