



>>Entry Name: 4-Heptenal, 9CI

ENTRY UNDER REVIEW

CAS Registry Number: 62238-34-0

H3CCH2CH=CHCH2CH2CHO

Molecular Formula: C₇H₁₂O

Molecular Weight: 112.171

Accurate Mass: 112.088815

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

>>Variant: (*E*)-form

CAS Registry Number: 929-22-6

Molecular Formula: C₇H₁₂O

Molecular Weight: 112.171

Accurate Mass: 112.088815

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

Biological Source: Constit. of black Hemiptera bugs

Use/Importance: Oil with nauseous odour

Boiling Point: Bp 112-113°

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Dull-orange needles (EtOH)

Melting Point: Mp 120°

>>Variant: (*Z*)-form

Synonym(s): FEMA 3289

CAS Registry Number: 6728-31-0

Molecular Formula: C₇H₁₂O

Molecular Weight: 112.171

Accurate Mass: 112.088815

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

Biological Source: Component of butter. Widespread trace constit. of food flavours

Use/Importance: Flavouring agent. Used in cream and butter flavourings

Physical Description: Liq. with creamy odour

Boiling Point: Bp₁₂ 42-44°

Refractive Index: n_D²⁰ 1.4343

Aldrich: W32890-1

References:

Mukerji, S.K. *et al.*, *Tet. Lett.*, 1966, 2479, (*synth*)

Stetter, H. *et al.*, *Synthesis*, 1975, 379, (*synth*)