



>>Entry Name: 2,4-Heptadienal, 9CI

CAS Registry Number: 5910-85-0

H3CCH2CH=CHCH=CHCHO

Molecular Formula: C₇H₁₀O

Molecular Weight: 110.155

Accurate Mass: 110.073165

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

>>Variant: (E,E)-form

CAS Registry Number: 4313-03-5

Molecular Formula: C₇H₁₀O

Molecular Weight: 110.155

Accurate Mass: 110.073165

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

Boiling Point: Bp₁₂ 78°. Bp_{0.06} 27-29°

Aldrich: 18054-8

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Purple needles

Melting Point: Mp 157-159°

>>Derivative: Di-Et acetal

Synonym(s): 1,1-Diethoxy-2,4-heptadiene

Molecular Formula: C₁₁H₂₀O₂

Molecular Weight: 184.278

Accurate Mass: 184.14633

Percentage Composition: C 71.70%; H 10.94%; O 17.36%

Boiling Point: Bp₁₂ 96.5-97.5°

>>Derivative: 4R*,5S*-Epoxide

Synonym(s): 3-(3-Ethyloxiranyl)-2-propenal, 9CI. 4,5-Epoxy-2-heptenal

CAS Registry Number: 78307-41-2

Extra CAS Registry Numbers(s): 69511-21-3

Molecular Formula: C₇H₁₀O₂

Molecular Weight: 126.155

Accurate Mass: 126.06808

Percentage Composition: C 66.65%; H 7.99%; O 25.36%

Source/Synthesis: Lipid peroxidation product

>>Variant: (2E,4Z)-form

CAS Registry Number: 4313-02-4

Molecular Formula: C₇H₁₀O

Molecular Weight: 110.155

Accurate Mass: 110.073165

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

Source/Synthesis: Component of black tea aroma

Boiling Point: Bp₁₈ 65°

Refractive Index: n_D²⁵ 1.4990

>>Variant: (2Z,4E)-form

CAS Registry Number: 59121-26-5

Molecular Formula: C₇H₁₀O

Molecular Weight: 110.155

Accurate Mass: 110.073165

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

Physical Description: No phys. props. reported