



>>Entry Name: Heptanal, 9CI, 8CI

ENTRY UNDER REVIEW

Synonym(s): Heptaldehyde. Enanthal. Oenanthal. Enanthole. Oenanthole. Oenanthaldehyde. Enanthaldehyde. FEMA 2540

CAS Registry Number: 111-71-7

Related CAS Registry Numbers(s): 5775-78-0 5784-69-0

$\text{H}_3\text{C}(\text{CH}_2)_5\text{CHO}$

Molecular Formula: $\text{C}_7\text{H}_{14}\text{O}$

Molecular Weight: 114.187

Accurate Mass: 114.104465

Percentage Composition: C 73.63%; H 12.36%; O 14.01%

Biological Source: Found in essential oils of ylang-ylang, clary sage, California orange, bitter orange and others

Use/Importance: Aldehyde and its simple acetals used in perfumery. Flavouring agent

Physical Description: Liq. with fruity odour

Melting Point: Mp -43.3°

Boiling Point: Bp 152.8° . Bp₃₀ 59.6°

Hazard & Toxicity: Low oral toxicity; flammable, fl. p. 35°

Aldrich: W25401-0

Fluka: 75170

Supelco: S48-2540

>>Derivative: Oxime

CAS Registry Number: 629-31-2

Molecular Formula: $\text{C}_7\text{H}_{15}\text{NO}$

Molecular Weight: 129.202

Accurate Mass: 129.115364

Percentage Composition: C 65.07%; H 11.70%; N 10.84%; O 12.38%

Physical Description: Plates (EtOH)

Melting Point: Mp $57-58^\circ$

Boiling Point: Bp 195° . Bp₁₄ 100.5°

>>Derivative: Semicarbazone

CAS Registry Number: 6033-21-2

Physical Description: Cryst. (MeOH)

Melting Point: Mp $108-109^\circ$

>>Derivative: Di-Me acetal

Synonym(s): 1,1-Dimethoxyheptane

CAS Registry Number: 10032-05-0

Molecular Formula: $\text{C}_9\text{H}_{20}\text{O}_2$

Molecular Weight: 160.256

Accurate Mass: 160.14633

Percentage Composition: C 67.45%; H 12.58%; O 19.97%

Boiling Point: Bp 182° . Bp₁₇ 75°

>>Derivative: Di-Et acetal

Synonym(s): 1,1-Diethoxyheptane

CAS Registry Number: 688-82-4

Molecular Formula: $\text{C}_{11}\text{H}_{24}\text{O}_2$

Molecular Weight: 188.309

Accurate Mass: 188.17763

Percentage Composition: C 70.16%; H 12.85%; O 16.99%

Boiling Point: Bp₇₇₄ $204-205^\circ$