



>>Entry Name: 2-Heptanone, 9CI

ENTRY UNDER REVIEW

Synonym(s): Methyl pentyl ketone. Amyl methyl ketone. FEMA 2544

CAS Registry Number: 110-43-0

$\text{H}_3\text{C}(\text{CH}_2)_4\text{COCH}_3$

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: Alarm substance of ant *Iridomyrmex pruinosus*. Also a minor consist. of plant oils

Use/Importance: Flavour ingredient

Physical Description: Light-yellow oil with characteristic slightly spicy banana odour

Melting Point: Fp  $-35.5^\circ$

Boiling Point: Bp  $151.45^\circ$ . Bp<sub>21</sub>  $111^\circ$

Density:  $d_4^{20}$  0.82

Refractive Index:  $n_D^{20}$  1.4110

Hazard & Toxicity: Flammable. Skin irritant. LD<sub>50</sub> (rat, orl) 1670 mg/kg. OES: long-term 50 ppm; short-term 100 ppm (Sk)

Aldrich: 12336-6

Fluka: 68592

Sigma: H7883

>>Derivative: Oxime

CAS Registry Number: 5314-31-8

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%

Boiling Point: Bp<sub>7</sub>  $85-87^\circ$

Aldrich: 40815-8

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 2074-03-5

Physical Description: Yellow-orange cryst.

Melting Point: Mp  $73-74^\circ$ . Mp  $89^\circ$

>>Derivative: Semicarbazone

CAS Registry Number: 3622-66-0

Melting Point: Mp  $96-97^\circ$ . Mp  $121-123$  dimorph. $^\circ$

>>Derivative: Di-Et ketal

Synonym(s): 2,2-Diethoxyheptane

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: Bp<sub>18</sub>  $81-83^\circ$

>>Variant:  $\Delta^1$ -Enol-form

Synonym(s): 1-Hepten-2-ol

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%