



>>Entry Name: 2,6-Dimethyl-4-heptanone, 9CI

ENTRY UNDER REVIEW

Synonym(s): Diisopropylacetone. Isovalerone. Diisobutyl ketone. Isobutyl ketone. FEMA 3537

CAS Registry Number: 108-83-8

Type of Compound Code(s): WE2000

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

Molecular Formula:  $\text{C}_9\text{H}_{18}\text{O}$

Molecular Weight: 142.241

Accurate Mass: 142.135765

Percentage Composition: C 76.00%; H 12.75%; O 11.25%

Use/Importance: Flavouring ingredient

Physical Description: Oil

Boiling Point: Bp 165-166°. Bp<sub>11</sub> 56°

Solubility: Sl. sol.  $\text{H}_2\text{O}$ , sol. EtOH

Refractive Index:  $n_D^{20}$  1.4128

**Hazard & Toxicity:** Flammable, fl. p. 49/51°, autoignition temp. 388°. Eye, skin and respiratory tract irritant. High vapour conc. narcotic. Lower conc. may cause headache, nausea. LD<sub>50</sub> (rat, orl) 5750 mg/kg. OES: long-term 25 ppm

Aldrich: 10999-1

Fluka: 38190

>>Derivative: Oxime

CAS Registry Number: 52435-41-3

Molecular Formula:  $\text{C}_9\text{H}_{19}\text{NO}$

Molecular Weight: 157.255

Accurate Mass: 157.146664

Percentage Composition: C 68.74%; H 12.18%; N 8.91%; O 10.17%

Boiling Point: Bp 205-210°. Bp<sub>20</sub> 114-116°

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 92°

>>Derivative: Semicarbazone

Melting Point: Mp 126° (110°)

#### References:

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