



>>Entry Name: 4-Heptanone, 9CI, 8CI

ENTRY UNDER REVIEW

Synonym(s): Dipropyl ketone. Butyrone. FEMA 2546

CAS Registry Number: 123-19-3

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

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: Scent constit. of urine of red fox *Vulpes vulpes*

Use/Importance: Flavouring ingredient

Physical Description: Refractive liq. with a penetrating odour and burning taste

Melting Point: Mp -32.6°

Boiling Point: Bp $142-144^\circ$

Solubility: Insol. H_2O , sol. EtOH, Et_2O

Density: d^{20}_4 0.81

Refractive Index: n^{20}_D 1.4019

Hazard & Toxicity: Flammable, fl. p. 49° . LD₅₀ (rat,orl) 3730 mg/kg

Aldrich: 10174-5

Fluka: 43570

Sigma: H5387

>>Derivative: Oxime

CAS Registry Number: 1188-63-2

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%

Use/Importance: Used for extraction separation of Ag, Au, Pd (CHCl_3); photometric detn. of Pd

Physical Description: Cryst.

Melting Point: Mp $187-188^\circ$

Boiling Point: Bp₇₇₂ 196°

Solubility: Sol. CHCl_3

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 1655-41-0

Melting Point: Mp 75°

References:

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