



>>Entry Name: 3-Heptanone, 9CI

ENTRY UNDER REVIEW

Synonym(s): Butyl ethyl ketone. FEMA 2545

CAS Registry Number: 106-35-4

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

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%

Use/Importance: Flavouring ingredient

Physical Description: Liq. with a powerful green, fatty, fruity odour and a melon, banana flavour

Boiling Point: Bp 149-152°

Density: d^{20}_4 0.82

Refractive Index: n^{20}_D 1.4115

Hazard & Toxicity: Flammable. Eye and skin irritant. LD₅₀ (rat, orl) 2760 mg/kg. OES: long-term 50 ppm; short-term 75 ppm (Sk) (current); short-term 100 ppm (Sk) (proposed)

Aldrich: H315-1

Fluka: 3220

Sigma: H6511

>>Derivative: Oxime

CAS Registry Number: 2108-81-8

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: Bp₁ 56°

>>Derivative: Semicarbazone

CAS Registry Number: 3622-67-1

Melting Point: Mp 99-100°. Mp 111°

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 64739-11-3

Melting Point: Mp 70.2°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 409A, (ir)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 637A, (nmr)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 492C, (ir)

Michel, J. *et al.*, *Bull. Soc. Chim. Fr.*, 1968, 4898, (synth)

Collman, J.P. *et al.*, *J.A.C.S.*, 1972, **94**, 1788, (synth)

Olah, G.A. *et al.*, *Synthesis*, 1977, 677, (synth)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 316

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1270-1271

Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, 1992, 201

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, EHA600