



>>Entry Name: 3-Hydroxy-3-methyl-2-butanone, 9CI

Synonym(s): 2-Methyl-3-oxo-2-butanol. Trimethylketol. Dimethylacetylcarbinol. 3-Oxo-*tert*-amyl alcohol

CAS Registry Number: 115-22-0

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

Molecular Formula: $\text{C}_5\text{H}_{10}\text{O}_2$

Molecular Weight: 102.133

Accurate Mass: 102.06808

Percentage Composition: C 58.80%; H 9.87%; O 31.33%

Physical Description: Liq. with sweet odour

Boiling Point: Bp 137.8-139°. Bp₂₁ 46-47°

Aldrich: H3960-4

Fluka: 55619

>>Derivative: Oxime

CAS Registry Number: 7431-25-6

Molecular Formula: $\text{C}_5\text{H}_{11}\text{NO}_2$

Molecular Weight: 117.147

Accurate Mass: 117.078979

Percentage Composition: C 51.26%; H 9.46%; N 11.96%; O 27.31%

Physical Description: Leaflets (petrol)

Melting Point: Mp 86-87°

>>Derivative: Phenylhydrazone

Physical Description: Plates (EtOH)

Melting Point: Mp 83-85°

>>Derivative: Semicarbazone

Physical Description: Cryst. (CHCl_3 /petrol)

Melting Point: Mp 165°

>>Derivative: Benzoyl

CAS Registry Number: 21478-65-9

Molecular Formula: $\text{C}_{12}\text{H}_{14}\text{O}_3$

Molecular Weight: 206.241

Accurate Mass: 206.094295

Percentage Composition: C 69.89%; H 6.84%; O 23.27%

Boiling Point: Bp_{0.05} 73°

>>Derivative: Me ether, oxime

CAS Registry Number: 15403-10-8

Molecular Formula: $\text{C}_6\text{H}_{13}\text{NO}_2$

Molecular Weight: 131.174

Accurate Mass: 131.094629

Percentage Composition: C 54.94%; H 9.99%; N 10.68%; O 24.39%

Physical Description: Prisms (petrol)

Melting Point: Mp 92-93°

Boiling Point: Bp 190°

Solubility: Sol. H_2O

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 421A, (*ir*)

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Gaines, J.R. *et al.*, *J.O.C.*, 1963, **28**, 1032, (*synth*)

Thomsen, A.D. *et al.*, *Acta Chem. Scand.*, 1971, **25**, 1576, (*synth*)

Lee, V. *et al.*, *J.O.C.*, 1975, **40**, 381, (*synth*)

Büchi, G. *et al.*, *J.A.C.S.*, 1978, **100**, 294, (*synth*)