



>>Entry Name: 3-Oxobutanal, 9CI

ENTRY UNDER REVIEW

Synonym(s): Acetoacetaldehyde. Formylacetone

CAS Registry Number: 625-34-3

$\text{H}_3\text{CCOCH}_2\text{CHO} \leftrightarrow \text{H}_3\text{CCOCH}=\text{CHOH}$

Molecular Formula: $\text{C}_4\text{H}_6\text{O}_2$

Molecular Weight: 86.09

Accurate Mass: 86.03678

Percentage Composition: C 55.81%; H 7.02%; O 37.17%

Solubility: Sol. H_2O

>>Derivative: 1-Ac

CAS Registry Number: 13945-19-2

Molecular Formula: $\text{C}_6\text{H}_8\text{O}_3$

Molecular Weight: 128.127

Accurate Mass: 128.047345

Percentage Composition: C 56.25%; H 6.29%; O 37.46%

Physical Description: Liq.

Boiling Point: $\text{Bp}_{0.5} 40^\circ$

>>Derivative: Di-Me acetal

Synonym(s): 4,4-Dimethoxy-2-butanone, 9CI. FEMA 3381

CAS Registry Number: 5436-21-5

Molecular Formula: $\text{C}_6\text{H}_{12}\text{O}_3$

Molecular Weight: 132.159

Accurate Mass: 132.078645

Percentage Composition: C 54.53%; H 9.15%; O 36.32%

Use/Importance: Synth. Flavouring ingredient

Boiling Point: $\text{Bp}_2 38^\circ$

Aldrich: 38006-7

Fluka: 75830

Sigma: K0750

>>Derivative: Ethylene ketal

Synonym(s): 2-Methyl-1,3-dioxolane-2-acetaldehyde, 9CI. 3,3-(Ethylenedioxy)butanal

CAS Registry Number: 18871-63-1

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_3$

Molecular Weight: 130.143

Accurate Mass: 130.062995

Percentage Composition: C 55.37%; H 7.74%; O 36.88%

Physical Description: Oil

Boiling Point: $\text{Bp}_{13} 80-85^\circ$

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 423B, (*ir*)

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 657B, (*nmr*)

U.S. Pat., 1942, 2 262 817; *CA*, **36**, 1331, (*synth*)

George, W.O. *et al.*, *J.C.S.(B)*, 1968, 132, (*pmr*)

Franke, W.K. *et al.*, *Fette, Seifen, Anstrichm.*, 1980, **82**, 370, (*rev, deriv*)

Lipinski, C.A. *et al.*, *J.O.C.*, 1984, **49**, 566, (*synth*)

Potman, R.P. *et al.*, *J.O.C.*, 1985, **50**, 1955, (*deriv, synth, pmr, ms*)

Yamashita, A. *et al.*, *J.O.C.*, 1989, **54**, 3625, (*ketal*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 630, (*Di-Me acetal*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2073-2074, (*Di-Me acetal*)