



>>Entry Name: 4-Hydroxy-2-butanone, 9CI
Synonym(s): 3-Oxo-1-butanol. Acetonylcarbinol

CAS Registry Number: 590-90-9
H3CCOCH2CH2OH

Molecular Formula: C4H8O2
Molecular Weight: 88.106
Accurate Mass: 88.05243
Percentage Composition: C 54.53%; H 9.15%; O 36.32%
Source/Synthesis: Present in tobacco smoke
Boiling Point: Bp₃₀ 109-110°. Bp₁₁ 90°
Solubility: Misc. H₂O, EtOH, Et₂O

>>Derivative: Ac

CAS Registry Number: 10150-87-5
Molecular Formula: C6H10O3
Molecular Weight: 130.143
Accurate Mass: 130.062995
Percentage Composition: C 55.37%; H 7.74%; O 36.88%
Boiling Point: Bp₃₀ 125-130°
Aldrich: 27451-8

>>Derivative: Ac, semicarbazone

Physical Description: Prisms (MeOH)
Melting Point: Mp 207 dec.°

>>Derivative: Oxime

CAS Registry Number: 42875-72-9
Molecular Formula: C4H9NO2
Molecular Weight: 103.121
Accurate Mass: 103.063329
Percentage Composition: C 46.59%; H 8.80%; N 13.58%; O 31.03%
Boiling Point: Bp₂₀ 125-130°

References:

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 742D, (*ir*)
Morgan, G.T. *et al.*, *J.C.S.*, 1932, 2669, (*synth*)
Fetizon, M. *et al.*, *Chem. Comm.*, 1969, 1102, (*synth*)
Ueno, Y. *et al.*, *Tet. Lett.*, 1976, 4597, (*synth*, *pmr*)