



>>Entry Name: 3-Methyl-2,4-pentanedione, 9CI
Synonym(s): Methylacetylacetone. 1,1-Diacetylene

CAS Registry Number: 815-57-6
H3CCH(COCH3)2

Molecular Formula: C6H10O2
Molecular Weight: 114.144
Accurate Mass: 114.06808
Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Boiling Point: Bp 170-172°. Bp₆₀ 86°
Density: d₄²⁰ 0.976
pKa Value: pK_{a1} 10.87 (25°)
Refractive Index: n_D²⁰ 1.4437
Other Data: Forms salts with many metals

Aldrich: 28285-5

>>Derivative: Dioxime

CAS Registry Number: 24760-83-6
Molecular Formula: C6H12N2O2
Molecular Weight: 144.173
Accurate Mass: 144.089878
Percentage Composition: C 49.99%; H 8.39%; N 19.43%; O 22.19%
Melting Point: Mp 132°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 661C, (nmr)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 512A, (ir)
v. Auwers, K. *et al.*, *Annalen*, 1922, **426**, 227, (synth)
Kelso, R.G. *et al.*, *J.A.C.S.*, 1955, **77**, 1751, (synth)
Org. Synth., 1971, **51**, 90, (synth)
Org. Synth., Coll. Vol., 5, 1973, 785, (synth)