



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

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°. Bp<sub>60</sub> 86°  
Density: d<sub>4</sub><sup>20</sup> 0.976  
pKa Value: pK<sub>a1</sub> 10.87 (25°)  
Refractive Index: n<sub>D</sub><sup>20</sup> 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*)