



>>Entry Name: 3-Acetyl-2,4-pentanedione, 9CI

Synonym(s): Triacetylmethane

CAS Registry Number: 815-68-9

HC(COCH₃)₃

Molecular Formula: C₇H₁₀O₃

Molecular Weight: 142.154

Accurate Mass: 142.062995

Percentage Composition: C 59.14%; H 7.09%; O 33.76%

Boiling Point: Bp₇ 85-86°

Density: d₄²⁰ 1.096

Refractive Index: n_D²⁵ 1.4893

Other Data: Unstable. Completely enolised in aq. soln.

Aldrich: 14738-9

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 663A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 428D, (*ir*)

Forsén, S. *et al.*, *Acta Chem. Scand.*, 1959, **13**, 1383, (*synth, pmr, struct*)

Taylor, E.C. *et al.*, *J.A.C.S.*, 1968, **90**, 2421, (*synth*)

Eck, H. *et al.*, *Annalen*, 1970, **731**, 12, (*synth*)

Boháč, A. *et al.*, *Synthesis*, 1994, 381, (*synth, pmr*)