



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

Synonym(s): Ethylacetylacetone. 3-Ethyl-4-hydroxy-3-penten-2-one

CAS Registry Number: 1540-34-7

Related CAS Registry Numbers(s): 34135-99-4

$\text{H}_3\text{CCH}_2\text{CH}(\text{COCH}_3)_2 \rightleftharpoons \text{H}_3\text{CCH}_2\text{C}(\text{COCH}_3)=\text{C}(\text{CH}_3)\text{OH}$

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}_2$

Molecular Weight: 128.171

Accurate Mass: 128.08373

Percentage Composition: C 65.60%; H 9.44%; O 24.97%

General Statement: About 25% enol form in pure liq., over 40% enol in some solvs. (CCl_4 , C_6H_6)

Boiling Point: Bp 179°. Bp₂₀ 76°

Density: d_4^{20} 0.9568

Refractive Index: n_D^{20} 1.4419

Aldrich: 28297-9

References:

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Morgan, G.T. *et al.*, *J. Soc. Chem. Ind., London*, 1925, **44**, 462, (*synth*)

Johnson, A.W. *et al.*, *J.C.S.*, 1958, 4254, (*synth*)

Yoffe, S.T. *et al.*, *Tetrahedron*, 1962, **18**, 923, (*tautom, ir, uv*)

Ioffe, S.T. *et al.*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1965, 1556; 1968, 2024; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1965, 1523; 1968, 1927, (*tautom, pmr*)

Emsley, J. *et al.*, *J. Mol. Struct.*, 1987, **161**, 193, (*synth, tautom*)

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