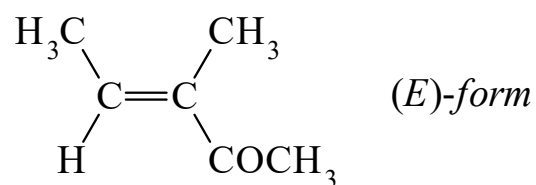




>>Entry Name: 3-Methyl-3-penten-2-one, 9CI

Synonym(s): 2-Acetyl-2-butene



CAS Registry Number: 565-62-8

Molecular Formula: C₆H₁₀O

Molecular Weight: 98.144

Accurate Mass: 98.073165

Percentage Composition: C 73.43%; H 10.27%; O 16.30%

Boiling Point: Bp 138°. Bp₈₅ 75°

pKa Value: pK_a -3.42 (H₂SO₄ aq.)

Refractive Index: n_D²⁰ 1.4508

Fluka: 68567

>>Variant: (E)-form

CAS Registry Number: 1567-73-3

Molecular Formula: C₆H₁₀O

Molecular Weight: 98.144

Accurate Mass: 98.073165

Percentage Composition: C 73.43%; H 10.27%; O 16.30%

Physical Description: Liq.

Boiling Point: Bp 147° (125°)

>>Derivative: Oxime

CAS Registry Number: 16750-76-8

Molecular Formula: C₆H₁₁NO

Molecular Weight: 113.159

Accurate Mass: 113.084064

Percentage Composition: C 63.69%; H 9.80%; N 12.38%; O 14.14%

Physical Description: Needles

Melting Point: Mp 75-76°

Other Data: This deriv. (also semicarbazone and dinitrophenylhydrazone) assumed to be of the *E*-form

>>Derivative: Semicarbazone

Physical Description: Needles

Melting Point: Mp 201°

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 200°

>>Variant: (Z)-form

CAS Registry Number: 1567-72-2

Molecular Formula: C₆H₁₀O

Molecular Weight: 98.144

Accurate Mass: 98.073165

Percentage Composition: C 73.43%; H 10.27%; O 16.30%

Physical Description: Liq.

Boiling Point: Bp 124°

References:

Hinkel, L.E. *et al.*, *J.C.S.*, 1931, 814, (*synth*)

McGreer, D.E. *et al.*, *Can. J. Chem.*, 1965, **43**, 1398; 1971, **49**, 105, (*synth*, *ir*, *pmr*)

Hasbrouck, R.W. *et al.*, *J.O.C.*, 1973, **38**, 2103, (*synth*)

Lambert, J.B. *et al.*, *J.O.C.*, 1990, **55**, 3460, (*synth*, *pmr*)

Boldrini, G. *et al.*, *J.O.C.*, 1991, **56**, 5820, (*synth*, *ir*, *pmr*)

Kawasaki, T. *et al.*, *J.C.S. Perkin I*, 1993, 1777, (*synth*, *ir*, *pmr*)