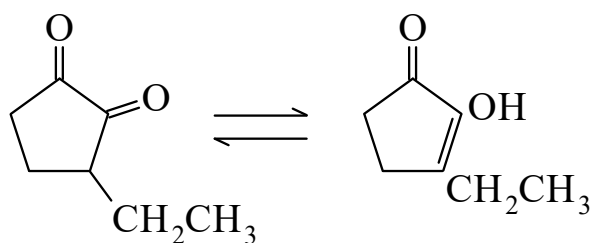




>>Entry Name: 3-Ethyl-1,2-cyclopentanedione, 9CI

ENTRY UNDER REVIEW

Synonym(s): 3-Ethyl-2-hydroxy-2-cyclopenten-1-one, 9CI. FEMA 3152



Molecular Formula: C₇H₁₀O₂

Molecular Weight: 126.155

Accurate Mass: 126.06808

Percentage Composition: C 66.65%; H 7.99%; O 25.36%

General Statement: The two tautomers are apparently capable of separate isolation

Biological Source: Isol. from coffee and tobacco

Use/Importance: Flavouring material, with caramel flavour and flavour enhancing props

>>Variant: Oxo-form

CAS Registry Number: 13494-08-1

Molecular Formula: C₇H₁₀O₂

Molecular Weight: 126.155

Accurate Mass: 126.06808

Percentage Composition: C 66.65%; H 7.99%; O 25.36%

Physical Description: Oil

Melting Point: Fp 20°

Boiling Point: Bp₁ 65-68°

Solubility: Sol. Et₂O

Other Data: λ_{max} 259 nm (log ε 4.04) in EtOH

>>Variant: Enol-form

CAS Registry Number: 21835-01-8

Molecular Formula: C₇H₁₀O₂

Molecular Weight: 126.155

Accurate Mass: 126.06808

Percentage Composition: C 66.65%; H 7.99%; O 25.36%

Physical Description: Cryst. (hexane) with caramel-like odour

Melting Point: Mp 38-40° (42-44°)

Boiling Point: Bp₄ 78-80°

Solubility: Sol. Et₂O

Other Data: Dec. in air

Aldrich: W31521-4

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 26103-86-6

Physical Description: Cryst. (EtOH)

Melting Point: Mp 135-138°

Other Data: Believed to be the 1-DNP of the enol tautomer

>>Derivative: Semicarbazone

CAS Registry Number: 26103-87-7

Physical Description: Cryst. (EtOH)

Melting Point: Mp 232 dec.°

Other Data: Believed to be the 1-semicarbazone of the enol tautomer

References: