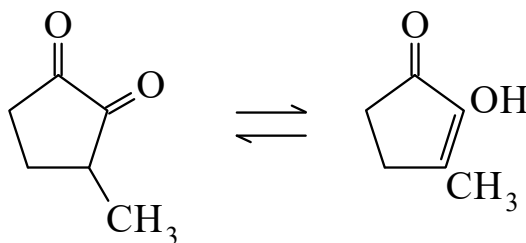




>>Entry Name: 3-Methyl-1,2-cyclopentanedione, 9CI

ENTRY UNDER REVIEW

Synonym(s): Cyclotene. Corylone. FEMA 2700



CAS Registry Number: 765-70-8

Molecular Formula: C₆H₈O₂

Molecular Weight: 112.128

Accurate Mass: 112.05243

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Biological Source: Constit. of coffee and many other foods. Comly. obt. by isoln. from beechwood tar

Use/Importance: Important flavouring ingredient. Occasionally used as an intensifier in perfumery. Enol-form predominates in non-polar solvs. and solid state

Physical Description: Cryst. + 2H₂O with caramel odour

Melting Point: Mp 78-79° (hydrate). Mp 106.5-107° (anhyd.)

Aldrich: 17850-0

Fluka: 66550

>>Derivative: Dihydrazone

Molecular Formula: C₆H₁₂N₄

Molecular Weight: 140.188

Accurate Mass: 140.106196

Percentage Composition: C 51.41%; H 8.63%; N 39.97%

Melting Point: Mp 143°

>>Derivative: Dioxime

CAS Registry Number: 41330-47-6

Molecular Formula: C₆H₁₀N₂O₂

Molecular Weight: 142.157

Accurate Mass: 142.074228

Percentage Composition: C 50.69%; H 7.09%; N 19.71%; O 22.51%

Melting Point: Mp 148-149 dec.°

>>Derivative: Bisemicarbazone

Melting Point: Mp 280°

>>Derivative: Bis(thiosemicarbazone)

Synonym(s): 2,2'-(3-Methyl-1,2-cyclopentanediyldiene)bishydrazinecarbothioamide, 9CI

CAS Registry Number: 15899-61-3

Molecular Formula: C₈H₁₄N₆S₂

Molecular Weight: 258.371

Accurate Mass: 258.072134

Percentage Composition: C 37.19%; H 5.46%; N 32.53%; S 24.82%

Use/Importance: Used as 0.06% soln. in DMF/Me₂CO for photometric detn. of Zn ($\lambda_{\max}$ 415 nm, ϵ 10000), Bi ($\lambda_{\max}$ 420 nm, ϵ 11000), Cd, Hg, Cu, Co; as soln. in EtOH for photometric detn. of Pb and Ag ($\lambda_{\max}$ 430 nm, ϵ 10000, pH8)

Physical Description: Yellow cryst.

Melting Point: Mp 240°

Solubility: Sol. EtOH, CHCl₃, DMF, Me₂CO

>>Variant: Enol-form

Synonym(s): 2-Hydroxy-3-methyl-2-cyclopenten-1-one