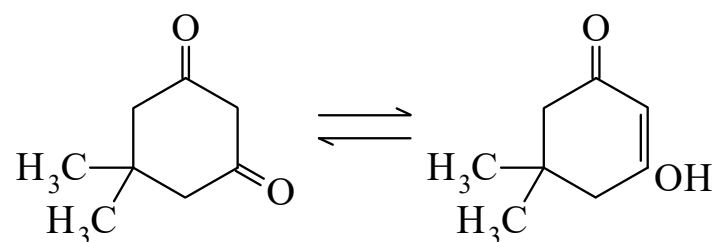




>>Entry Name: 5,5-Dimethyl-1,3-cyclohexanedione, 9CI

Synonym(s): 5,5-Dimethyldihydroresorcinol. Methone. Dimedone. 3-Hydroxy-5,5-dimethyl-2-cyclohexen-1-one



CAS Registry Number: 126-81-8

Related CAS Registry Numbers(s): 3471-13-4 82531-23-5

Type of Compound Code(s): PS8300 PM6450 PA0900

Molecular Formula: C₈H₁₂O₂

Molecular Weight: 140.182

Accurate Mass: 140.08373

Percentage Composition: C 68.55%; H 8.63%; O 22.83%

General Statement: Enolised β-diketone. Exists in aq. soln. mainly as enol tautomer

Use/Importance: Characterising reagent for carbonyl compds., protecting agent for NH₂ groups. Used in photometric detn. of CN⁽⁻⁾

Physical Description: Monoclinic needles or prisms

Melting Point: Mp 148.5-149°

Solubility: Sol. CHCl₃, C₆H₆; spar. sol. petrol, H₂O

pKa Value: pK_{a1} 5.27 (25°)

Aldrich: D15330-3

Fluka: 38490

Sigma: D3504

>>Derivative: Monooxime

CAS Registry Number: 31933-48-9

Molecular Formula: C₈H₁₃NO₂

Molecular Weight: 155.196

Accurate Mass: 155.094629

Percentage Composition: C 61.91%; H 8.44%; N 9.03%; O 20.62%

Physical Description: Cryst.

Melting Point: Mp 115°

>>Derivative: Dioxime

CAS Registry Number: 37110-24-0

Type of Compound Code(s): PS8300 PA1400 PM6850

Molecular Formula: C₈H₁₄N₂O₂

Molecular Weight: 170.211

Accurate Mass: 170.105528

Percentage Composition: C 56.45%; H 8.29%; N 16.46%; O 18.80%

Use/Importance: Used as 0.5% soln. in EtOH for photometric detn. of Co (λ_{max} 400 nm, ε 23000)

Physical Description: Prisms + 2H₂O

Melting Point: Mp 176° (anhyd.). Mp 170°

Solubility: Sol. alkaline aq. solns., alcohols, CHCl₃

>>Derivative: Bisthiosemicarbazone

CAS Registry Number: 79811-20-4

Type of Compound Code(s): PA4950 PM7120 PS8300 PA2700 PA2050 PA1900 PA1850 PA1250 PA0550

Molecular Formula: C₁₀H₁₈N₆S₂

Molecular Weight: 286.424

Accurate Mass: 286.103434

Percentage Composition: C 41.93%; H 6.33%; N 29.34%; S 22.39%

Use/Importance: Used as 0.01M soln. of hydrochloride in 0.1M HClO₄ for photometric detn. of ClO₃⁽⁻⁾ (λ_{max} 417 nm, ε 18600, 70% HClO₄ medium), BrO₃⁽⁻⁾ (λ_{max} 415 nm), IO₃⁽⁻⁾, IO₄⁽⁻⁾, NO₂⁽⁻⁾, Pb, Zn

Physical Description: Yellow cryst. (EtOH) (as hydrochloride)

Melting Point: Mp 187-189° (as hydrochloride)

Solubility: Sol. acids, EtOH, DMF

Other Data: Reg. no. refers to hydrochloride