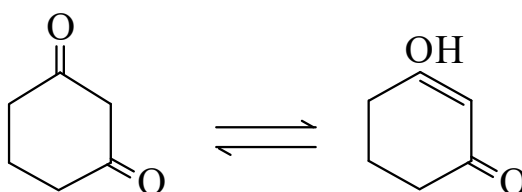




>>Entry Name: 1,3-Cyclohexanedione, 9CI

Synonym(s): Dihydroresorcinol. 3-Hydroxy-2-cyclohexen-1-one



CAS Registry Number: 504-02-9

Molecular Formula: C₆H₈O₂

Molecular Weight: 112.128

Accurate Mass: 112.05243

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

Use/Importance: Fluorogenic derivatising reagent for hplc anal. of aldehydes

Physical Description: Prisms (C₆H₆)

Solubility: Sol. H₂O, EtOH, Me₂CO, CHCl₃, spar. sol. Et₂O

pKa Value: pK_{a1} 5.25 (25°)

Aldrich: C10160-5

Fluka: 29059

Sigma: C0654

>>Derivative: Dioxime

CAS Registry Number: 2802-07-5

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 155-156°

>>Derivative: Phenylhydrazone

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 176-177°

>>Derivative: Bis(phenylthiosemicarbazone)

CAS Registry Number: 77783-17-6

Molecular Formula: C₂₀H₂₂N₆S₂

Molecular Weight: 410.566

Accurate Mass: 410.134734

Percentage Composition: C 58.51%; H 5.40%; N 20.47%; S 15.62%

Use/Importance: Used as 0.1% soln. in DMF for photometric detn. of U(*I*) (λ_{max} 640 nm, ε 18200)

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 216-218°

>>Derivative: Enol Et ether

Synonym(s): 3-Ethoxy-2-cyclohexen-1-one

CAS Registry Number: 5323-87-5

Molecular Formula: C₈H₁₂O₂

Molecular Weight: 140.182

Accurate Mass: 140.08373

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

Physical Description: Liq.

Boiling Point: Bp₆ 104-106°. Bp₁ 76-78°

Aldrich: E445-3

Fluka: 2648