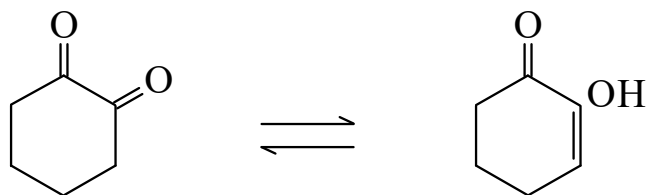




>>Entry Name: 1,2-Cyclohexanedione, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2-Hydroxy-2-cyclohexen-1-one



CAS Registry Number: 765-87-7

Molecular Formula: C₆H₈O₂

Molecular Weight: 112.128

Accurate Mass: 112.05243

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

Use/Importance: Flavour material for food and perfumes. Reagent for sequence anal. of arginyl peptides by ms

Physical Description: Cryst. (petrol)

Melting Point: Mp 38-40°

Boiling Point: Bp 193-195°. Bp₁₇ 85°

Solubility: Mod. sol. H₂O

pKa Value: pK_a 10.3 (20°, 40% enol form)

Hazard & Toxicity: Explosion has resulted when prepd. by HNO₃ oxidn. of cyclohexanol. Irritant

Aldrich: C10140-0

Sigma: C9529

>>Derivative: Dioxime

Synonym(s): Nioxime. Nyoxime

CAS Registry Number: 492-99-9

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%

Use/Importance: Used as 0.01M soln. in EtOH, for extraction-photometric detn. of Ni, Fe(II) (λ_{max} 450 nm, ϵ 18000, CHCl₃)

Physical Description: Needles (H₂O), cryst. (dioxan)

Melting Point: Mp 187-188 dec.°

Solubility: Sol. EtOH, dioxan; sl. sol. H₂O

pKa Value: pK_{a2} 12.16 (25°)

Aldrich: C10200-8

Fluka: 72530

>>Derivative: Bis-2,4-dinitrophenylhydrazone

CAS Registry Number: 1468-24-2

Melting Point: Mp 233-234°

>>Derivative: Bisthiosemicarbazone

see 1,2-Cyclohexanedione bis(thiosemicarbazone), [KNG19-G](#)

>>Derivative: Bis(2-pyridylhydrazone)

see 1,2-Cyclohexanedione bis(2-pyridylhydrazone), [KMX96-B](#)

>>Derivative: Bisbenzoylhydrazone

see 1,2-Cyclohexanedione bisbenzoylhydrazone, [KNG18-F](#)