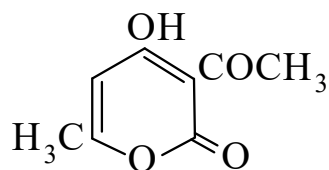




>>Entry Name: 3-Acetyl-4-hydroxy-6-methyl-2*H*-pyran-2-one, 9CI

ENTRY UNDER REVIEW

Synonym(s): Dehydroacetic acid. Dehydracetic acid



CAS Registry Number: 771-03-9

Extra CAS Registry Numbers(s): 85-25-6 520-45-6

Molecular Formula: C₈H₈O₄

Molecular Weight: 168.149

Accurate Mass: 168.04226

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Biological Source: Isol. from *Solandra nitida*

Use/Importance: Fungicide used against moulds on fresh and dried fruit. Now superseded. Used as a 1% aq. soln. for separation and gravimetric detn. of Pd

Physical Description: Rhombic needles or plates (EtOH)

Melting Point: Mp 109°

Boiling Point: Bp 270°. Bp₅ 132-133°

Solubility: Sol. H₂O, EtOH, Me₂CO, Et₂O

pKa Value: pK_a 5.12 (25°)

UV: [neutral] λ_{max} 223 (); 308 () (MeOH) (Berdy)

Hazard & Toxicity: LD₅₀ (rat, orl) 500 mg/kg

Fluka: 30740

>>Derivative: Na salt

CAS Registry Number: 4418-26-2

Melting Point: Mp 284-287°

Fluka: 30750

Sigma: D3500

>>Derivative: Oxime

Molecular Formula: C₈H₉NO₄

Molecular Weight: 183.163

Accurate Mass: 183.053159

Percentage Composition: C 52.46%; H 4.95%; N 7.65%; O 34.94%

Melting Point: Mp 153-154°

>>Derivative: Anilide

Molecular Formula: C₁₄H₁₃NO₃

Molecular Weight: 243.262

Accurate Mass: 243.089544

Percentage Composition: C 69.12%; H 5.39%; N 5.76%; O 19.73%

Melting Point: Mp 115°

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