



>>Entry Name: 1-Phenyl-1,2-propanedione, 8CI

ENTRY UNDER REVIEW

Synonym(s): Methyl phenyl diketone. Acetylbenzoyl. FEMA 3226

CAS Registry Number: 579-07-7

Ph CO COCH₃

Molecular Formula: C₉H₈O₂

Molecular Weight: 148.161

Accurate Mass: 148.05243

Percentage Composition: C 72.96%; H 5.44%; O 21.60%

Use/Importance: Flavouring ingredient

Physical Description: Yellow oil with a pungent odour

Boiling Point: Bp 222°. Bp₁₂ 102°

Solubility: V. spar. sol. H₂O

Density: d₄²⁰ 1.007

Other Data: Steam-volatile. n_D¹⁰ 1.537

Hazard & Toxicity: Highly flammable, fl. p. <21°

Aldrich: 22303-4

Rare Chemicals Library: S37794-5

Sigma: P2259

>>Derivative: α-Oxime

Synonym(s): α-Isonitroso-α-phenylacetone. Phenyl acetyl ketoxime

CAS Registry Number: 25355-34-4

Molecular Formula: C₉H₉NO₂

Molecular Weight: 163.176

Accurate Mass: 163.063329

Percentage Composition: C 66.25%; H 5.56%; N 8.58%; O 19.61%

Physical Description: Yellow needles (AcOH)

Melting Point: Mp 166-167°

>>Derivative: α-Oxime, Ac

Molecular Formula: C₁₁H₁₁NO₃

Molecular Weight: 205.213

Accurate Mass: 205.073894

Percentage Composition: C 64.38%; H 5.40%; N 6.83%; O 23.39%

Physical Description: Leaflets (EtOH aq.)

Melting Point: Mp 61-62°

>>Derivative: β-Oxime

Synonym(s): α-Isonitrosopropiophenone. Methyl benzoyl ketoxime

CAS Registry Number: 119-51-7

Molecular Formula: C₉H₉NO₂

Molecular Weight: 163.176

Accurate Mass: 163.063329

Percentage Composition: C 66.25%; H 5.56%; N 8.58%; O 19.61%

Physical Description: Needles (H₂O)

Melting Point: Mp 114-115°

Hazard & Toxicity: LD₅₀ (rat, orl) 4240 mg/kg

Aldrich: 22009-4

Rare Chemicals Library: S35465-1

Sigma: I3502