



>>Entry Name: 4-Oxo-4-phenylbutanoic acid, 9CI

Synonym(s): γ -Oxobenzenebutanoic acid. 3-Benzoylpropanoic acid

CAS Registry Number: 2051-95-8

PhCOCH₂CH₂COOH

Molecular Formula: C₁₀H₁₀O₃

Molecular Weight: 178.187

Accurate Mass: 178.062995

Percentage Composition: C 67.41%; H 5.66%; O 26.94%

Use/Importance: Fungicide and bactericide. Reagent used in oligonucleotide synth.

Physical Description: Cryst. (EtOH)

Melting Point: Mp 116°

Other Data: Shows intramolecular H bonding in the solid state

Aldrich: B1380-2

Fluka: 13055

Rare Chemicals Library: S3910-2

Sigma: B0762

>>Derivative: Oxime

CAS Registry Number: 87252-81-1

Molecular Formula: C₁₀H₁₁NO₃

Molecular Weight: 193.202

Accurate Mass: 193.073894

Percentage Composition: C 62.17%; H 5.74%; N 7.25%; O 24.84%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 127.5-128.5°

>>Derivative: Semicarbazone

Melting Point: Mp 181 dec.°

>>Derivative: Me ester

CAS Registry Number: 25333-24-8

Molecular Formula: C₁₁H₁₂O₃

Molecular Weight: 192.214

Accurate Mass: 192.078645

Percentage Composition: C 68.74%; H 6.29%; O 24.97%

Physical Description: Oil

>>Derivative: Et ester

CAS Registry Number: 6270-17-3

Molecular Formula: C₁₂H₁₄O₃

Molecular Weight: 206.241

Accurate Mass: 206.094295

Percentage Composition: C 69.89%; H 6.84%; O 23.27%

Physical Description: Oil

Rare Chemicals Library: S77834-6

>>Derivative: Butyl ester

CAS Registry Number: 29513-56-2

Molecular Formula: C₁₄H₁₈O₃

Molecular Weight: 234.294

Accurate Mass: 234.125595

Percentage Composition: C 71.77%; H 7.74%; O 20.49%

Use/Importance: Carrier for fluorescent whiteners in detergents