



>>Entry Name: 2-Oxo-2-phenylacetic acid

Synonym(s): α -Oxobenzeneacetic acid, 9CI. Phenylglyoxylic acid. Benzoylformic acid

CAS Registry Number: 611-73-4

Related CAS Registry Numbers(s): 704-18-7 25327-35-9 25327-36-0

PhCOCOOH

Molecular Formula: C₈H₆O₃

Molecular Weight: 150.134

Accurate Mass: 150.031695

Percentage Composition: C 64.00%; H 4.03%; O 31.97%

Physical Description: Cryst. (CCl₄ or C₆H₆/petrol)

Melting Point: Mp 66°

Boiling Point: Bp₁₂ 147.5°

Other Data: Dec. on dist. at atm. press.

Aldrich: B1305-5

Fluka: 78610

Sigma: B3504

>>Derivative: (E)-Oxime

CAS Registry Number: 25327-35-9

Molecular Formula: C₈H₇NO₃

Molecular Weight: 165.148

Accurate Mass: 165.042594

Percentage Composition: C 58.18%; H 4.27%; N 8.48%; O 29.06%

Physical Description: Prisms (Et₂O), cryst. (Et₂O)

Melting Point: Mp 151 dec.°

>>Derivative: (Z)-Oxime

CAS Registry Number: 25327-36-0

Physical Description: Prisms (Et₂O)

Melting Point: Mp 127 dec.°

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 31334-72-2

Physical Description: Yellow solid

Melting Point: Mp 196-197 dec.°

>>Derivative: Thiosemicarbazone

CAS Registry Number: 18465-40-2

Molecular Formula: C₉H₉N₃O₂S

Molecular Weight: 223.255

Accurate Mass: 223.041547

Percentage Composition: C 48.42%; H 4.06%; N 18.82%; O 14.33%; S 14.36%

Use/Importance: Used as 0.5mM aq. soln. for catalytic detn. of Rh(III)

Physical Description: Cryst.

Solubility: Sol. H₂O, EtOH

>>Derivative: Me ester

Synonym(s): Methyl phenylglyoxylate. Vicure 55

CAS Registry Number: 15206-55-0

Molecular Formula: C₉H₈O₃

Molecular Weight: 164.16

Accurate Mass: 164.047345

Percentage Composition: C 65.85%; H 4.91%; O 29.24%

Physical Description: Oil

Boiling Point: Bp₁₄ 137°. Bp 250-255°

Aldrich: M3050-7

Fluka: 78620