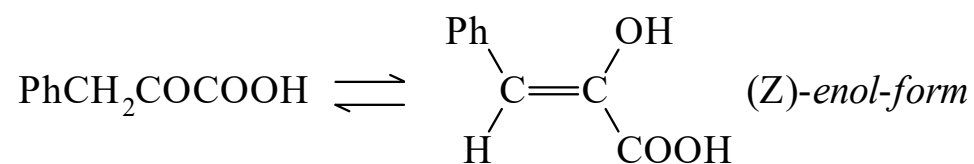




>>Entry Name: 2-Oxo-3-phenylpropanoic acid

ENTRY UNDER REVIEW

Synonym(s):  $\alpha$ -Oxobenzenepranoic acid, 9CI. Phenylpyruvic acid. 2-Hydroxy-3-phenyl-2-propenoic acid, 9CI.  $\alpha$ -Hydroxycinnamic acid



Related CAS Registry Numbers(s): 52178-60-6

Molecular Formula:  $\text{C}_9\text{H}_8\text{O}_3$

Molecular Weight: 164.16

Accurate Mass: 164.047345

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

Biological Source: Occurs in plants, prod. by *Pseudomonas* and other microorganisms

Use/Importance: Substrate for microbial production of phenylalanine

Physical Description: Plates ( $\text{CHCl}_3$ )

Melting Point: Mp 157 dec. $^\circ$

Solubility: Spar. sol. hot  $\text{H}_2\text{O}$

Other Data: Oxidises in air. Reduces boiling Fehling's soln.

>>Derivative: Na salt

CAS Registry Number: 114-76-1

Physical Description: Cryst. +  $1\text{H}_2\text{O}$

Solubility: Insol. EtOH

Other Data: Stable in air.  $\text{H}_2\text{O}$  of cryst. remains at 100 $^\circ$

Aldrich: 33794-3

Fluka: 78200

Sigma: P8001

>>Derivative: Me ester

Synonym(s): Methyl phenylpyruvate

CAS Registry Number: 6362-58-9

Molecular Formula:  $\text{C}_{10}\text{H}_{10}\text{O}_3$

Molecular Weight: 178.187

Accurate Mass: 178.062995

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

Physical Description: Needles

Melting Point: Mp 75 $^\circ$

>>Derivative: Et ester

Synonym(s): Ethyl phenylpyruvate

CAS Registry Number: 6613-41-8

Molecular Formula:  $\text{C}_{11}\text{H}_{12}\text{O}_3$

Molecular Weight: 192.214

Accurate Mass: 192.078645

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

Physical Description: Needles

Melting Point: Mp 45 $^\circ$

Boiling Point: Bp<sub>15</sub> 154.5 $^\circ$

Solubility: Insol.  $\text{H}_2\text{O}$

Other Data: Oxidises in air. Enolic Et esters (*E*)- and (*Z*-) are also known

>>Derivative: Amide

CAS Registry Number: 6362-62-5

Molecular Formula:  $\text{C}_9\text{H}_9\text{NO}_2$

Molecular Weight: 163.176

Accurate Mass: 163.063329

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

Melting Point: Mp 190 $^\circ$

Solubility: Sol. hot EtOH; insol.  $\text{H}_2\text{O}$ ,  $\text{Et}_2\text{O}$ ,  $\text{C}_6\text{H}_6$