



>>Entry Name: 4-Oxo-4-phenyl-2-butenic acid, 9CI

Synonym(s): 3-Benzoyl-2-propenoic acid. β -Benzoylacrylic acid

CAS Registry Number: 583-06-2

PhCOCH=CHCOOH

Molecular Formula: C₁₀H₈O₃

Molecular Weight: 176.171

Accurate Mass: 176.047345

Percentage Composition: C 68.18%; H 4.58%; O 27.25%

>>Variant: (*E*)-form

CAS Registry Number: 17812-07-6

Molecular Formula: C₁₀H₈O₃

Molecular Weight: 176.171

Accurate Mass: 176.047345

Percentage Composition: C 68.18%; H 4.58%; O 27.25%

Melting Point: Mp 96-96.5°

Solubility: Sol. hot H₂O

Aldrich: 45247-5

>>Derivative: Oxime

Molecular Formula: C₁₀H₉NO₃

Molecular Weight: 191.186

Accurate Mass: 191.058244

Percentage Composition: C 62.82%; H 4.74%; N 7.33%; O 25.11%

Melting Point: Mp 168 dec.°

>>Derivative: Me ester

CAS Registry Number: 19522-25-9

Molecular Formula: C₁₁H₁₀O₃

Molecular Weight: 190.198

Accurate Mass: 190.062995

Percentage Composition: C 69.46%; H 5.30%; O 25.24%

Melting Point: Mp 30-32°

Boiling Point: Bp₅ 150°

>>Derivative: Et ester

CAS Registry Number: 15121-89-8

Molecular Formula: C₁₂H₁₂O₃

Molecular Weight: 204.225

Accurate Mass: 204.078645

Percentage Composition: C 70.58%; H 5.92%; O 23.50%

Boiling Point: Bp₂₅ 184-185°

Density: d 1.11

Refractive Index: n_D²⁰ 1.5430

Other: Kaneka J-3

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 229°

>>Variant: ($\pm$)-form

Molecular Formula: C₁₀H₈O₃

Molecular Weight: 176.171

Accurate Mass: 176.047345

Percentage Composition: C 68.18%; H 4.58%; O 27.25%