



>>Entry Name: 4-Phenyl-3-butenic acid, 9CI

Synonym(s): Styrylacetic acid

CAS Registry Number: 2243-53-0

Related CAS Registry Numbers(s): 16170-45-9 20068-09-1 60773-92-4

PhCH=CHCH₂COOH

Molecular Formula: C₁₀H₁₀O₂

Molecular Weight: 162.188

Accurate Mass: 162.06808

Percentage Composition: C 74.06%; H 6.21%; O 19.73%

>>Variant: (*E*)-form

CAS Registry Number: 1914-58-5

Molecular Formula: C₁₀H₁₀O₂

Molecular Weight: 162.188

Accurate Mass: 162.06808

Percentage Composition: C 74.06%; H 6.21%; O 19.73%

Physical Description: Needles (H₂O)

Melting Point: Mp 79-81°

Boiling Point: Bp 302°

Aldrich: 15532-2

>>Derivative: K salt

Melting Point: Mp 245 dec.°

>>Derivative: Me ester

CAS Registry Number: 24891-74-5

Molecular Formula: C₁₁H₁₂O₂

Molecular Weight: 176.215

Accurate Mass: 176.08373

Percentage Composition: C 74.98%; H 6.86%; O 18.16%

Boiling Point: Bp₂₀ *ca.*° 185

>>Derivative: Et ester

CAS Registry Number: 1205-84-1

Molecular Formula: C₁₂H₁₄O₂

Molecular Weight: 190.241

Accurate Mass: 190.09938

Percentage Composition: C 75.76%; H 7.42%; O 16.82%

Physical Description: Liq.

Boiling Point: Bp₂ 135-137°

>>Derivative: Chloride

Molecular Formula: C₁₀H₉ClO

Molecular Weight: 180.633

Accurate Mass: 180.034192

Percentage Composition: C 66.49%; H 5.02%; Cl 19.63%; O 8.86%

Melting Point: Mp 41-42°

Boiling Point: Bp_{0.4} 106-108°

>>Derivative: Anhydride

CAS Registry Number: 40418-64-2

Molecular Formula: C₂₀H₁₈O₃

Molecular Weight: 306.36

Accurate Mass: 306.125595

Percentage Composition: C 78.41%; H 5.92%; O 15.67%

Melting Point: Mp 120-121°