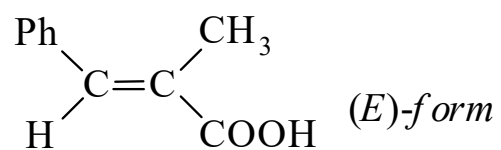




>>Entry Name: 2-Methyl-3-phenyl-2-propenoic acid, 9CI

Synonym(s): α -Methylcinnamic acid. 2-Methyl-3-phenylacrylic acid



CAS Registry Number: 1199-77-5

Molecular Formula: C₁₀H₁₀O₂

Molecular Weight: 162.188

Accurate Mass: 162.06808

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

Aldrich: M3560-6

Fluka: 69738

>>Variant: (*E*)-form

Synonym(s): *trans*-form

CAS Registry Number: 1895-97-2

Molecular Formula: C₁₀H₁₀O₂

Molecular Weight: 162.188

Accurate Mass: 162.06808

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

Physical Description: Prisms (EtOH aq.), needles (petrol)

Melting Point: Mp 74° (needles). Mp 81-82° (prisms) (dimorph.)

>>Derivative: Phenylhydrazine salt

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 64-65°

>>Derivative: Me ester

CAS Registry Number: 22946-43-6

Molecular Formula: C₁₁H₁₂O₂

Molecular Weight: 176.215

Accurate Mass: 176.08373

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

Physical Description: Cryst. (hexane)

Melting Point: Mp 26-27°

Boiling Point: Bp₁₆ 137-138°

>>Derivative: Chloride

CAS Registry Number: 38449-13-7

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%

Physical Description: Needles (Et₂O)

Melting Point: Mp 50°

Boiling Point: Bp₁₂ 126-127°

>>Derivative: Amide

Molecular Formula: C₁₀H₁₁NO

Molecular Weight: 161.203

Accurate Mass: 161.084064

Percentage Composition: C 74.51%; H 6.88%; N 8.69%; O 9.93%

Physical Description: Plates (H₂O)

Melting Point: Mp 128°

Solubility: Spar. sol. EtOH, Et₂O

>>Variant: (*Z*)-form

Synonym(s): *cis*-form. *allo*-form