



>>Entry Name: 3-Phenyl-2-propynoic acid, 9CI

Synonym(s): Phenylpropionic acid

CAS Registry Number: 637-44-5

PhC≡CCOOH

Molecular Formula: C₉H₆O₂

Molecular Weight: 146.145

Accurate Mass: 146.03678

Percentage Composition: C 73.97%; H 4.14%; O 21.90%

Melting Point: Mp 135-136°

Aldrich: P3120-5

Fluka: 78982

Sigma: P2021

>>Derivative: Me ester

CAS Registry Number: 4891-38-7

Molecular Formula: C₁₀H₈O₂

Molecular Weight: 160.172

Accurate Mass: 160.05243

Percentage Composition: C 74.99%; H 5.03%; O 19.98%

Physical Description: Light yellow cryst.

Melting Point: Mp 25°

Boiling Point: Bp₁ 95-96°

>>Derivative: Et ester

CAS Registry Number: 2216-94-6

Molecular Formula: C₁₁H₁₀O₂

Molecular Weight: 174.199

Accurate Mass: 174.06808

Percentage Composition: C 75.84%; H 5.79%; O 18.37%

Boiling Point: Bp 260-270°

Aldrich: E4530-9

Fluka: 78985

>>Derivative: Chloride

CAS Registry Number: 7299-58-3

Molecular Formula: C₉H₅ClO

Molecular Weight: 164.591

Accurate Mass: 164.002892

Percentage Composition: C 65.68%; H 3.06%; Cl 21.54%; O 9.72%

Boiling Point: Bp_{0.1} 46°

>>Derivative: Dimethylamide

CAS Registry Number: 26218-50-8

Molecular Formula: C₁₁H₁₁NO

Molecular Weight: 173.214

Accurate Mass: 173.084064

Percentage Composition: C 76.28%; H 6.40%; N 8.09%; O 9.24%

Physical Description: Cryst.

Melting Point: Mp 100°

>>Derivative: Hydrazide

CAS Registry Number: 27412-70-0

Molecular Formula: C₉H₈N₂O

Molecular Weight: 160.175

Accurate Mass: 160.063663

Percentage Composition: C 67.49%; H 5.03%; N 17.49%; O 9.99%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 114-115°