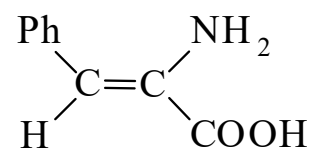




>>Entry Name: 2-Amino-3-phenyl-2-propenoic acid, 9Cl

Synonym(s): α -Aminocinnamic acid, 8Cl. Dehydrophenylalanine



Molecular Formula: C₉H₉NO₂

Molecular Weight: 163.176

Accurate Mass: 163.063329

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

>>Variant: (Z)-form

CAS Registry Number: 65895-01-4

Molecular Formula: C₉H₉NO₂

Molecular Weight: 163.176

Accurate Mass: 163.063329

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

>>Derivative: Me ester

CAS Registry Number: 63096-06-0

Molecular Formula: C₁₀H₁₁NO₂

Molecular Weight: 177.202

Accurate Mass: 177.078979

Percentage Composition: C 67.78%; H 6.26%; N 7.90%; O 18.06%

Melting Point: Mp 37-38°

>>Derivative: Et ester

CAS Registry Number: 61013-56-7

Molecular Formula: C₁₁H₁₃NO₂

Molecular Weight: 191.229

Accurate Mass: 191.094629

Percentage Composition: C 69.09%; H 6.85%; N 7.32%; O 16.73%

Boiling Point: Bp_{0.5} 90-95°

>>Derivative: N-Ac

CAS Registry Number: 55065-02-6

Extra CAS Registry Numbers(s): 5469-45-4

Molecular Formula: C₁₁H₁₁NO₃

Molecular Weight: 205.213

Accurate Mass: 205.073894

Percentage Composition: C 64.38%; H 5.40%; N 6.83%; O 23.39%

Physical Description: Cryst. + 2H₂O (H₂O)

Melting Point: Mp 185-186°

Aldrich: 21385-3

Fluka: 390

Rare Chemicals Library: S17042-9

Sigma: A2399

>>Derivative: N-Ac, Me ester

CAS Registry Number: 60676-51-9

Molecular Formula: C₁₂H₁₃NO₃

Molecular Weight: 219.24

Accurate Mass: 219.089544

Percentage Composition: C 65.74%; H 5.98%; N 6.39%; O 21.89%

Physical Description: Cryst. (C₆H₆ or EtOAc/petrol)

Melting Point: Mp 127-127.5° (115°)