



>>Entry Name: **3-(4-Aminophenyl)-2-propenoic acid**, 9CI

Synonym(s): *p*-Aminocinnamic acid, 8CI

CAS Registry Number: 2393-18-2

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%

Physical Description: Yellow needles

Rare Chemicals Library: S56569-5

>>Variant: (*E*)-form

CAS Registry Number: 17570-30-8

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%

Physical Description: Pale-yellow needles (H₂O)

Melting Point: Mp 175-176 dec.°

>>Derivative: Hydrochloride

CAS Registry Number: 54057-95-3

Melting Point: Mp 265-270°

Aldrich: A4710-9

Fluka: 9673

Sigma: A7896

>>Derivative: Me ester

CAS Registry Number: 66417-26-3

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%

Physical Description: Yellow-brown needles (C₆H₆)

Melting Point: Mp 128-129°

>>Derivative: Et ester

CAS Registry Number: 5048-82-8

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%

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 74°

Rare Chemicals Library: S7760-8

>>Derivative: Nitrile

CAS Registry Number: 77120-14-0

Molecular Formula: C₉H₈N₂

Molecular Weight: 144.176

Accurate Mass: 144.068748

Percentage Composition: C 74.98%; H 5.59%; N 19.43%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 109-110°