



>>Entry Name: 3-(3-Pyridinyl)-2-propenoic acid, 9CI

Synonym(s): 3-(β-Pyridyl)acrylic acid

CAS Registry Number: 1126-74-5

Related CAS Registry Numbers(s): 28447-17-8

Molecular Formula: C₈H₇NO₂

Molecular Weight: 149.149

Accurate Mass: 149.047679

Percentage Composition: C 64.42%; H 4.73%; N 9.39%; O 21.45%

Fluka: 82901

Rare Chemicals Library: S78699-3

>>Variant: (*E*)-form

CAS Registry Number: 19337-97-4

Molecular Formula: C₈H₇NO₂

Molecular Weight: 149.149

Accurate Mass: 149.047679

Percentage Composition: C 64.42%; H 4.73%; N 9.39%; O 21.45%

Melting Point: Mp 236-237°

Aldrich: P6620-3

>>Derivative: Me ester

CAS Registry Number: 61859-84-5

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: Cryst. (EtOH aq.)

Melting Point: Mp 46-47°

Other Data: (*E*)-config. assumed

>>Derivative: Et ester

CAS Registry Number: 59607-99-7

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 18°

Boiling Point: Bp₁ 93-95°

>>Derivative: Nitrile

CAS Registry Number: 54356-27-3

Molecular Formula: C₈H₆N₂

Molecular Weight: 130.149

Accurate Mass: 130.053098

Percentage Composition: C 73.83%; H 4.65%; N 21.52%

Melting Point: Mp 106-107°

>>Variant: (*Z*)-form

Molecular Formula: C₈H₇NO₂

Molecular Weight: 149.149

Accurate Mass: 149.047679

Percentage Composition: C 64.42%; H 4.73%; N 9.39%; O 21.45%

>>Derivative: Et ester

Boiling Point: Bp₁ 120-130°

References: