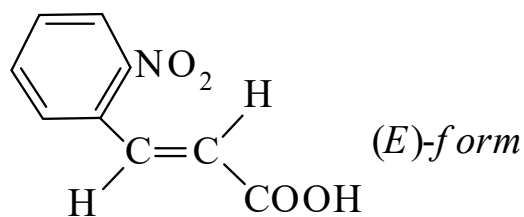




>>Entry Name: 3-(2-Nitrophenyl)-2-propenoic acid, 9Cl

Synonym(s): *o*-Nitrocinnamic acid, 8Cl. 3-*o*-Nitrophenylacrylic acid



CAS Registry Number: 612-41-9

Related CAS Registry Numbers(s): 2001-33-4 52162-78-4

Molecular Formula: C₉H₇NO₄

Molecular Weight: 193.159

Accurate Mass: 193.037509

Percentage Composition: C 55.96%; H 3.65%; N 7.25%; O 33.13%

Aldrich: N1640-1

Fluka: 74130

Sigma: N1631

>>Variant: (*E*)-form

CAS Registry Number: 1013-96-3

Molecular Formula: C₉H₇NO₄

Molecular Weight: 193.159

Accurate Mass: 193.037509

Percentage Composition: C 55.96%; H 3.65%; N 7.25%; O 33.13%

Physical Description: Needles (EtOH)

Melting Point: Mp 240°

pKa Value: p*K*_a 4.15 (25°)

>>Derivative: Me ester

CAS Registry Number: 39228-29-0

Molecular Formula: C₁₀H₉NO₄

Molecular Weight: 207.185

Accurate Mass: 207.053159

Percentage Composition: C 57.97%; H 4.38%; N 6.76%; O 30.89%

Physical Description: Needles (MeOH aq.)

Melting Point: Mp 73°

Boiling Point: Bp₁₅ 187-189°

>>Derivative: Et ester

CAS Registry Number: 24393-59-7

Molecular Formula: C₁₁H₁₁NO₄

Molecular Weight: 221.212

Accurate Mass: 221.068809

Percentage Composition: C 59.73%; H 5.01%; N 6.33%; O 28.93%

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 44°

>>Derivative: Chloride

Molecular Formula: C₉H₆ClNO₃

Molecular Weight: 211.604

Accurate Mass: 211.003621

Percentage Composition: C 51.09%; H 2.86%; Cl 16.75%; N 6.62%; O 22.68%

Melting Point: Mp 64.5°

>>Derivative: Amide