



>>Entry Name: **3-(3-Nitrophenyl)-2-propenoic acid**, 9Cl
Synonym(s): *m*-Nitrocinnamic acid, 8Cl. 3-*m*-Nitrophenylacrylic acid

CAS Registry Number: 555-68-0
Related CAS Registry Numbers(s): 1664-58-0 35418-05-4 79432-86-3

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%

Aldrich: 13019-2
Fluka: 74135
Rare Chemicals Library: S7761-6
Sigma: N1881

>>Variant: (*E*)-form

CAS Registry Number: 1772-76-5
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: Yellow needles (EtOH)
Melting Point: Mp 200-201° (193-194°, 196-197°)
pKa Value: pK_a 4.12 (25°)

>>Derivative: Me ester

CAS Registry Number: 659-04-1
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: Pale-yellow prisms (EtOH)
Melting Point: Mp 127°

>>Derivative: Et ester

CAS Registry Number: 621-19-2
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: Prisms (AcOH)
Melting Point: Mp 78-79°

>>Derivative: Amide

Molecular Formula: C₉H₈N₂O₃
Molecular Weight: 192.174
Accurate Mass: 192.053493
Percentage Composition: C 56.25%; H 4.20%; N 14.58%; O 24.98%
Physical Description: Leaflets (MeOH)
Melting Point: Mp 195-196°

>>Variant: (*Z*)-form

CAS Registry Number: 5676-61-9
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
Melting Point: Mp 158°

References: