



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

Synonym(s): 3-Chloroacrylic acid

CAS Registry Number: 625-40-1

ClCH=CHCOOH

Molecular Formula: C₃H₃ClO₂

Molecular Weight: 106.508

Accurate Mass: 105.982157

Percentage Composition: C 33.83%; H 2.84%; Cl 33.29%; O 30.04%

>>Variant: (E)-form

CAS Registry Number: 2345-61-1

Molecular Formula: C₃H₃ClO₂

Molecular Weight: 106.508

Accurate Mass: 105.982157

Percentage Composition: C 33.83%; H 2.84%; Cl 33.29%; O 30.04%

Melting Point: Mp 86° (92-94°)

Boiling Point: Bp₁₈ 94°

Solubility: Sol. EtOH, Et₂O; sl. sol. CHCl₃

pKa Value: pK_{a1} 3.79 (25°)

Hazard & Toxicity: Corrosive, lachrymator

Aldrich: C2235-0

Fluka: 22995

>>Derivative: Me ester

Synonym(s): Methyl 3-chloroacrylate

CAS Registry Number: 5135-18-2

Molecular Formula: C₄H₅ClO₂

Molecular Weight: 120.535

Accurate Mass: 119.997807

Percentage Composition: C 39.86%; H 4.18%; Cl 29.41%; O 26.55%

Physical Description: Liq.

Boiling Point: Bp₁₃₁ 74-75°

>>Derivative: Et ester

CAS Registry Number: 16491-00-2

Molecular Formula: C₅H₇ClO₂

Molecular Weight: 134.562

Accurate Mass: 134.013457

Percentage Composition: C 44.63%; H 5.24%; Cl 26.35%; O 23.78%

Physical Description: Liq.

Boiling Point: Bp 143-145°

>>Derivative: Chloride

CAS Registry Number: 3721-36-6

Molecular Formula: C₃H₂Cl₂O

Molecular Weight: 124.954

Accurate Mass: 123.948269

Percentage Composition: C 28.84%; H 1.61%; Cl 56.75%; O 12.80%

Physical Description: Liq.

Boiling Point: Bp 114-116°

>>Derivative: Amide

Synonym(s): 3-Chloroacrylamide

CAS Registry Number: 3533-60-6

Molecular Formula: C₃H₄ClNO

Molecular Weight: 105.523

Accurate Mass: 104.998141

Percentage Composition: C 34.15%; H 3.82%; Cl 33.60%; N 13.27%; O 15.16%

Physical Description: Cryst.

Melting Point: Mp 143.5-145°