



Synonym(s): 3-Chloro-2-propenenitrile. 3-Chloroacrylonitrile. 1-Chloro-2-cyanoethylene

CAS Registry Number: 3721-38-8

Molecular Formula: C₃H₂ClN

Molecular Weight: 87.508

Accurate Mass: 86.987576

Percentage Composition: C 41.18%; H 2.30%; Cl 40.51%; N 16.01%

Physical Description: Cryst.

Melting Point: Mp 45-46°

Boiling Point: Bp 118°

Hazard & Toxicity: Lachrymator and vesicant

>>Variant: (Z)-form

CAS Registry Number: 1609-93-4

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%

Biological Source: Occurs in *Asparagopsis taxiformis*

Use/Importance: Cotton defoliant and crop desiccant

Physical Description: Cryst. (HCl aq.)

Melting Point: Mp 60.8-61.4°

Boiling Point: Bp_{17.5} 107°

Solubility: Sol. EtOH, Et₂O

pKa Value: pK_{a1} 3.45 (25°)

Hazard & Toxicity: Corrosive, lachrymator

Aldrich: 17740-7

>>Derivative: Me ester

CAS Registry Number: 3510-44-9

Molecular Formula: C₄H₅ClO₂

Molecular Weight: 120.535

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

Physical Description: Liq.

Boiling Point: Bp₇₈ 79-83°

>>Derivative: Chloride

CAS Registry Number: 3721-35-5

Molecular Formula: C₃H₂Cl₂O

Molecular Weight: 124.954

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

Physical Description: Liq.

Boiling Point: Bp₂₆₀ 99-103°

>>Derivative: Amide

CAS Registry Number: 78708-26-6

Molecular Formula: C₃H₄ClNO

Molecular Weight: 105.523

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

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 111-112°

>>Derivative: Ethylamide

CAS Registry Number: 137627-64-6

Molecular Formula: C₅H₈ClNO

Molecular Weight: 133.577

Accurate Mass: 133.029441

Percentage Composition: C 44.96%; H 6.04%; Cl 26.54%; N 10.49%; O 11.98%

Physical Description: Oil