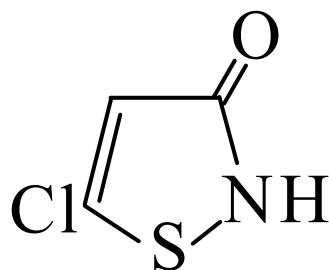




>>Entry Name: 5-Chloro-3(2H)-isothiazolone, 9Cl

Synonym(s): 5-Chloro-4-isothiazolin-3-one, 8Cl. 5-Chloro-3-hydroxyisothiazole. 5-Chloro-3-isothiazolol



CAS Registry Number: 33311-80-7

Related CAS Registry Numbers(s): 26530-03-0

Molecular Formula: C₃H₂ClNOS

Molecular Weight: 135.574

Accurate Mass: 134.954561

Percentage Composition: C 26.58%; H 1.49%; Cl 26.15%; N 10.33%; O 11.80%; S 23.65%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 95-96°

>>Derivative: N-Me

Synonym(s): 5-Chloro-2-methyl-3(2H)-isothiazolone. Kathon CG 5243

CAS Registry Number: 26172-55-4

Molecular Formula: C₄H₄ClNOS

Molecular Weight: 149.6

Accurate Mass: 148.970211

Percentage Composition: C 32.11%; H 2.69%; Cl 23.70%; N 9.36%; O 10.69%; S 21.43%

Use/Importance: Industrial microbiocide and antifouling agent

Physical Description: Cryst. (petrol)

Melting Point: Mp 54-55°

>>Derivative: N-Et

CAS Registry Number: 33344-74-0

Molecular Formula: C₅H₆ClNOS

Molecular Weight: 163.627

Accurate Mass: 162.985861

Percentage Composition: C 36.70%; H 3.70%; Cl 21.67%; N 8.56%; O 9.78%; S 19.60%

Boiling Point: Bp_{0.5} 64°

Refractive Index: n_D^{24.5} 1.5698

>>Derivative: N-Ph

CAS Registry Number: 19389-32-3

Molecular Formula: C₉H₆ClNOS

Molecular Weight: 211.671

Accurate Mass: 210.985861

Percentage Composition: C 51.07%; H 2.86%; Cl 16.75%; N 6.62%; O 7.56%; S 15.15%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 118-120°

References:

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Miller, G.A. et al., J. Het. Chem., 1971, **8**, 581-586, (N-Et, N-Ph, synth, uv, pmr)

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Beeley, N.R.A. et al., J.C.S. Perkin I, 1994, 2245-2251, (synth, ir, pmr)