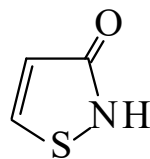




>>Entry Name: **3(2*H*)-Isothiazolone**, 9CI

Synonym(s): 4-Isothiazolin-3-one. 3-Hydroxyisothiazole. 3-Isothiazolol



CAS Registry Number: 1003-07-2

Related CAS Registry Numbers(s): 55965-84-9

Molecular Formula: C₃H₃NOS

Molecular Weight: 101.129

Accurate Mass: 100.993534

Percentage Composition: C 35.63%; H 2.99%; N 13.85%; O 15.82%; S 31.71%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 73-74°

>>Derivative: *S*-Oxide

CAS Registry Number: 31028-29-2

Molecular Formula: C₃H₃NO₂S

Molecular Weight: 117.128

Accurate Mass: 116.988449

Percentage Composition: C 30.76%; H 2.58%; N 11.96%; O 27.32%; S 27.38%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 95-96°

>>Derivative: *S,S*-Dioxide

CAS Registry Number: 26479-40-3

Molecular Formula: C₃H₃NO₃S

Molecular Weight: 133.128

Accurate Mass: 132.983364

Percentage Composition: C 27.07%; H 2.27%; N 10.52%; O 36.05%; S 24.09%

Physical Description: Solid

Melting Point: Mp 118-120 dec.°

>>Derivative: *N*-Me

CAS Registry Number: 2682-20-4

Molecular Formula: C₄H₅NOS

Molecular Weight: 115.156

Accurate Mass: 115.009184

Percentage Composition: C 41.72%; H 4.38%; N 12.16%; O 13.89%; S 27.85%

Use/Importance: Industrial microbiocide and antifouling agent

Physical Description: Cryst. (dichloroethylene)

Melting Point: Mp 48-50°

Boiling Point: Bp_{0.03} 93°

Other Data: V. hygroscopic

>>Derivative: *N*-Me; hydrochloride

CAS Registry Number: 26172-54-3

Physical Description: Solid

Melting Point: Mp 162-166°

Sigma: M6045

>>Derivative: *N*-Octyl

Synonym(s): 2-Octyl-3(2*H*)-isothiazolone, 9CI. **Octhilinone**, ANSI, BSI, ISO. Pancil T. Pancil