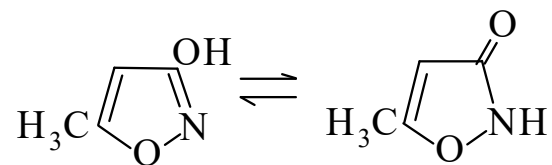




>>Entry Name: 5-Methyl-3-isoxazolol, 8CI

Synonym(s): 5-Methyl-3(2*H*)-isoxazolone, 9CI. 3-Hydroxy-5-methylisoxazole. Tachigaren. Hymexazol. Hydroxyisoxazole, JMAF



CAS Registry Number: 10004-44-1

Molecular Formula: C₄H₅NO₂

Molecular Weight: 99.089

Accurate Mass: 99.032029

Percentage Composition: C 48.49%; H 5.09%; N 14.14%; O 32.29%

Use/Importance: Soil fungicide and plant growth promoter

Physical Description: Needles (hexane), cryst. by subl.

Melting Point: Mp 86° (79-80°)

Solubility: Sol. H₂O

pKa Value: p*K*_a 5.92

Hazard & Toxicity: LD₅₀ (rat, orl) 3112 mg/kg

Sigma: H3275

>>Variant: *OH*-form

Molecular Formula: C₄H₅NO₂

Molecular Weight: 99.089

Accurate Mass: 99.032029

Percentage Composition: C 48.49%; H 5.09%; N 14.14%; O 32.29%

>>Derivative: Me ether

Synonym(s): 3-Methoxy-5-methylisoxazole, 9CI

CAS Registry Number: 16864-45-2

Molecular Formula: C₅H₇NO₂

Molecular Weight: 113.116

Accurate Mass: 113.047679

Percentage Composition: C 53.09%; H 6.24%; N 12.38%; O 28.29%

Physical Description: Liq.

Boiling Point: Bp₃₀ 78°

>>Derivative: Et ether

Synonym(s): 3-Ethoxy-5-methylisoxazole

CAS Registry Number: 127020-20-6

Molecular Formula: C₆H₉NO₂

Molecular Weight: 127.143

Accurate Mass: 127.063329

Percentage Composition: C 56.68%; H 7.13%; N 11.02%; O 25.17%

Physical Description: Oil

>>Variant: *NH*-form

Molecular Formula: C₄H₅NO₂

Molecular Weight: 99.089

Accurate Mass: 99.032029

Percentage Composition: C 48.49%; H 5.09%; N 14.14%; O 32.29%

>>Derivative: 2-Me

Synonym(s): 2,5-Dimethyl-3(2*H*)-isoxazolone, 9CI