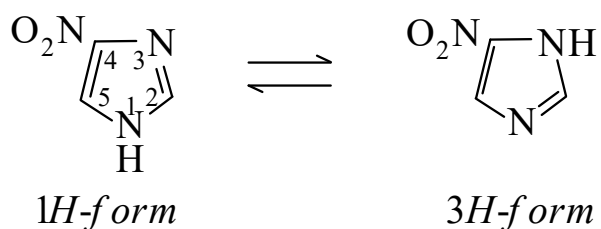




>>Entry Name: 4(5)-Nitroimidazole

Synonym(s): 4-Nitroiminazole. 4-Nitroglyoxaline



Related CAS Registry Numbers(s): 36877-68-6

Molecular Formula: $C_3H_3N_3O_2$

Molecular Weight: 113.076

Accurate Mass: 113.022527

Percentage Composition: C 31.87%; H 2.67%; N 37.16%; O 28.30%

Physical Description: Prisms (EtOH)

Melting Point: Mp 312-313°

pKa Value: pK_{a1} -0.16; pK_{a2} 9.2 (DMF aq.)

>>Variant: 1*H*-form

CAS Registry Number: 3034-38-6

Molecular Formula: $C_3H_3N_3O_2$

Molecular Weight: 113.076

Accurate Mass: 113.022527

Percentage Composition: C 31.87%; H 2.67%; N 37.16%; O 28.30%

Aldrich: 14161-5

Fluka: 73400

Rare Chemicals Library: S80227-1

Sigma: N9508

>>Derivative: 1-Me

Synonym(s): 1-Methyl-4-nitro-1*H*-imidazole

CAS Registry Number: 3034-41-1

Molecular Formula: $C_4H_5N_3O_2$

Molecular Weight: 127.102

Accurate Mass: 127.038177

Percentage Composition: C 37.80%; H 3.96%; N 33.06%; O 25.18%

Physical Description: Needles (H₂O)

Melting Point: Mp 133-134°

Hazard & Toxicity: Mutagenic props.

Rare Chemicals Library: S91529-7

>>Derivative: 1-Nitro

Synonym(s): 1,4-Dinitro-1*H*-imidazole

Molecular Formula: $C_3H_2N_4O_4$

Molecular Weight: 158.073

Accurate Mass: 158.007606

Percentage Composition: C 22.80%; H 1.28%; N 35.44%; O 40.49%

Melting Point: Mp 92°

>>Variant: 3*H*-form

Molecular Formula: $C_3H_3N_3O_2$

Molecular Weight: 113.076

Accurate Mass: 113.022527

Percentage Composition: C 31.87%; H 2.67%; N 37.16%; O 28.30%

>>Derivative: *N*-Me

Synonym(s): 1-Methyl-5-nitro-1*H*-imidazole