



>>Entry Name: 4(5)-Nitro-2-imidazolecarboxylic acid, 9CI

Related CAS Registry Numbers(s): 16147-98-1 109012-46-6

Molecular Formula: $C_4H_3N_3O_4$

Molecular Weight: 157.085

Accurate Mass: 157.012357

Percentage Composition: C 30.58%; H 1.92%; N 26.75%; O 40.74%

>>Variant: 1*H*-form

Molecular Formula: $C_4H_3N_3O_4$

Molecular Weight: 157.085

Accurate Mass: 157.012357

Percentage Composition: C 30.58%; H 1.92%; N 26.75%; O 40.74%

>>Derivative: *N*-Me

Synonym(s): 1-Methyl-4-nitro-1*H*-imidazole-2-carboxylic acid

CAS Registry Number: 109012-24-0

Molecular Formula: $C_5H_5N_3O_4$

Molecular Weight: 171.112

Accurate Mass: 171.028007

Percentage Composition: C 35.10%; H 2.95%; N 24.56%; O 37.40%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 138 dec.°

>>Derivative: *N*-Me, Et ester

CAS Registry Number: 109012-23-9

Molecular Formula: $C_7H_9N_3O_4$

Molecular Weight: 199.166

Accurate Mass: 199.059307

Percentage Composition: C 42.21%; H 4.55%; N 21.10%; O 32.13%

Physical Description: Pale cream needles (EtOH)

Melting Point: Mp 130-131°

>>Variant: 3*H*-form

Molecular Formula: $C_4H_3N_3O_4$

Molecular Weight: 157.085

Accurate Mass: 157.012357

Percentage Composition: C 30.58%; H 1.92%; N 26.75%; O 40.74%

>>Derivative: *N*-Me

Synonym(s): 1-Methyl-5-nitro-1*H*-imidazole-2-carboxylic acid

CAS Registry Number: 3994-53-4

Molecular Formula: $C_5H_5N_3O_4$

Molecular Weight: 171.112

Accurate Mass: 171.028007

Percentage Composition: C 35.10%; H 2.95%; N 24.56%; O 37.40%

Use/Importance: Useful in treatment of histomoniasis and *Trichomonas vaginalis*

Physical Description: Solid

Melting Point: Mp 84-85 dec.°

>>Derivative: *N*-Me, Me ester

CAS Registry Number: 1563-98-0

Molecular Formula: $C_6H_7N_3O_4$

Molecular Weight: 185.139

Accurate Mass: 185.043657

Percentage Composition: C 38.93%; H 3.81%; N 22.70%; O 34.57%

Physical Description: Solid

Melting Point: Mp 107-110°