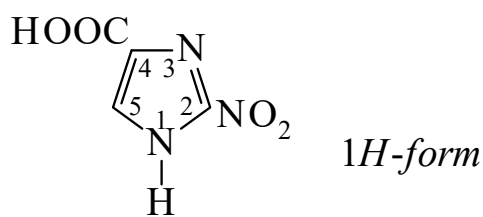




>>Entry Name: 2-Nitro-4(5)-imidazolecarboxylic acid



Related CAS Registry Numbers(s): 76733-64-7 83896-47-3

Molecular Formula: C₄H₃N₃O₄

Molecular Weight: 157.085

Accurate Mass: 157.012357

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

>>Variant: 3H-form

Molecular Formula: C₄H₃N₃O₄

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-2-nitro-1H-imidazole-5-carboxylic acid

CAS Registry Number: 50700-55-5

Molecular Formula: C₅H₅N₃O₄

Molecular Weight: 171.112

Accurate Mass: 171.028007

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

Use/Importance: Displays antimicrobial activity against *Clostridium perfringens* and *E. coli*

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 161-163°

>>Derivative: N-Me, Me ester

CAS Registry Number: 40361-79-3

Molecular Formula: C₆H₇N₃O₄

Molecular Weight: 185.139

Accurate Mass: 185.043657

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

Use/Importance: Displays antimicrobial activity against *Bacteroides fragilis*, *C. perfringens* and *E. coli*

Physical Description: Cryst. (diisopropyl ether/2-propanol or Et₂O/hexane)

Melting Point: Mp 63-65°

Hazard & Toxicity: LD₅₀ (mus, ipr) 500 mg/kg

>>Derivative: N-Me, Et ester

CAS Registry Number: 39070-13-8

Molecular Formula: C₇H₉N₃O₄

Molecular Weight: 199.166

Accurate Mass: 199.059307

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

Use/Importance: Displays antimicrobial activity against *E. coli*, *C. perfringens* and *Trichomonas vaginalis*

Physical Description: Light yellow cryst. (hexane)

Melting Point: Mp 65-66°

>>Derivative: N-Me, hydrazide

CAS Registry Number: 40361-80-6

Molecular Formula: C₅H₇N₅O₃

Molecular Weight: 185.142

Accurate Mass: 185.05489

Percentage Composition: C 32.44%; H 3.81%; N 37.83%; O 25.93%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 141-144 dec.°

References: