



>>Entry Name: 4-Nitro-3(5)-pyrazolecarboxylic acid

CAS Registry Number: 5334-40-7

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%

Physical Description: Solid

Melting Point: Mp 204 dec.°

Aldrich: 41484-0

>>Derivative: Me ester

CAS Registry Number: 138786-86-4

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%

Physical Description: Solid (as hydrochloride)

Melting Point: Mp 205-208 dec.° (hydrochloride)

>>Derivative: Et ester

CAS Registry Number: 55864-87-4

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: Cryst. (C_6H_6 /petrol)

Melting Point: Mp 124-126°

>>Derivative: Chloride

Molecular Formula: $C_4H_2ClN_3O_3$

Molecular Weight: 175.531

Accurate Mass: 174.978469

Percentage Composition: C 27.37%; H 1.15%; Cl 20.20%; N 23.94%; O 27.34%

Physical Description: Cream solid

Melting Point: Mp 192-193 dec.°

>>Derivative: Amide

CAS Registry Number: 65190-36-5

Molecular Formula: $C_4H_4N_4O_3$

Molecular Weight: 156.101

Accurate Mass: 156.028341

Percentage Composition: C 30.78%; H 2.58%; N 35.89%; O 30.75%

Physical Description: Cryst. (H_2O)

Melting Point: Mp 291-293°

>>Derivative: Phenylhydrazide

Physical Description: Yellowish scales (EtOH)

Melting Point: Mp 193-194°

>>Derivative: Nitrile

Synonym(s): 3-Cyano-4-nitropyrazole

CAS Registry Number: 61241-07-4

Molecular Formula: $C_4H_2N_4O_2$

Molecular Weight: 138.085

Accurate Mass: 138.017776

Percentage Composition: C 34.79%; H 1.46%; N 40.57%; O 23.17%

Physical Description: Plates (H_2O)

Melting Point: Mp 162-163°