



>>Entry Name: 5-Methyl-1*H*-pyrazole-3-carboxylic acid

CAS Registry Number: 402-61-9

Molecular Formula: C₅H₆N₂O₂

Molecular Weight: 126.115

Accurate Mass: 126.042928

Percentage Composition: C 47.62%; H 4.80%; N 22.21%; O 25.37%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 240-241° (236-238°)

>>Derivative: Me ester

CAS Registry Number: 25016-17-5

Molecular Formula: C₆H₈N₂O₂

Molecular Weight: 140.141

Accurate Mass: 140.058578

Percentage Composition: C 51.42%; H 5.75%; N 19.99%; O 22.83%

Physical Description: Cryst.

Melting Point: Mp 75-78°

>>Derivative: Et ester

CAS Registry Number: 4027-57-0

Molecular Formula: C₇H₁₀N₂O₂

Molecular Weight: 154.168

Accurate Mass: 154.074228

Percentage Composition: C 54.54%; H 6.54%; N 18.17%; O 20.76%

Physical Description: Cryst.

Melting Point: Mp 81-82°

>>Derivative: Amide

CAS Registry Number: 4027-56-9

Molecular Formula: C₅H₇N₃O

Molecular Weight: 125.13

Accurate Mass: 125.058912

Percentage Composition: C 47.99%; H 5.64%; N 33.58%; O 12.79%

Physical Description: Cryst.

Melting Point: Mp 178-179°

>>Derivative: Nitrile

Synonym(s): 3-Cyano-5-methylpyrazole

Molecular Formula: C₅H₅N₃

Molecular Weight: 107.115

Accurate Mass: 107.048347

Percentage Composition: C 56.07%; H 4.70%; N 39.23%

Physical Description: Cryst.

Melting Point: Mp 112-113°

>>Variant: 1*H*-form

Molecular Formula: C₅H₆N₂O₂

Molecular Weight: 126.115

Accurate Mass: 126.042928

Percentage Composition: C 47.62%; H 4.80%; N 22.21%; O 25.37%

>>Derivative: *N*-Me

Synonym(s): 1,5-Dimethyl-1*H*-pyrazole-3-carboxylic acid, 9CI