



>>Entry Name: 4-Pyrazolecarboxylic acid

CAS Registry Number: 37718-11-9

Molecular Formula: $C_4H_4N_2O_2$

Molecular Weight: 112.088

Accurate Mass: 112.027278

Percentage Composition: C 42.86%; H 3.60%; N 24.99%; O 28.55%

Physical Description: Needles (H_2O)

Melting Point: Mp 275-280°

Aldrich: 30071-3

>>Derivative: Me ester

CAS Registry Number: 51105-90-9

Molecular Formula: $C_5H_6N_2O_2$

Molecular Weight: 126.115

Accurate Mass: 126.042928

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

Melting Point: Mp 136-137°

>>Derivative: Et ester

CAS Registry Number: 37622-90-5

Molecular Formula: $C_6H_8N_2O_2$

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. (petrol/EtOAc)

Melting Point: Mp 78-79° (76-78°)

Boiling Point: Bp₃ 138-140°

Aldrich: 30078-0

>>Derivative: Nitrile

Synonym(s): 4-Cyanopyrazole

CAS Registry Number: 31108-57-3

Molecular Formula: $C_4H_3N_3$

Molecular Weight: 93.088

Accurate Mass: 93.032697

Percentage Composition: C 51.61%; H 3.25%; N 45.14%

Physical Description: Cryst. by subl.

Melting Point: Mp 91-92°

>>Derivative: *N*-Me

Synonym(s): 1-Methyl-1*H*-pyrazole-4-carboxylic acid, 9CI

CAS Registry Number: 5952-92-1

Molecular Formula: $C_5H_6N_2O_2$

Molecular Weight: 126.115

Accurate Mass: 126.042928

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

Physical Description: Needles (EtOH)

Melting Point: Mp 205-206°

Rare Chemicals Library: S93947-1

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

CAS Registry Number: 5952-93-2

Molecular Formula: $C_6H_8N_2O_2$

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. (Et₂O/petrol)

Melting Point: Mp 64°