



>>Entry Name: **1*H*-Pyrazole-3,5-dicarboxylic acid**, 9CI

CAS Registry Number: 3112-31-0

Molecular Formula: C₅H₄N₂O₄

Molecular Weight: 156.098

Accurate Mass: 156.017108

Percentage Composition: C 38.47%; H 2.58%; N 17.95%; O 41.00%

Melting Point: Mp 360°

Aldrich: P5680-1

Fluka: 82640

>>**Derivative:** Monohydrate

Physical Description: Needles (HCl aq.)

Melting Point: Mp 287-290 dec.°

>>**Derivative:** Di-Me ester

CAS Registry Number: 4077-76-3

Molecular Formula: C₇H₈N₂O₄

Molecular Weight: 184.151

Accurate Mass: 184.048408

Percentage Composition: C 45.66%; H 4.38%; N 15.21%; O 34.75%

Physical Description: Plates (Et₂O)

Melting Point: Mp 151-155°

>>**Derivative:** Di-Et ester

CAS Registry Number: 37687-24-4

Molecular Formula: C₉H₁₂N₂O₄

Molecular Weight: 212.205

Accurate Mass: 212.079708

Percentage Composition: C 50.94%; H 5.70%; N 13.20%; O 30.16%

Physical Description: Cryst. (C₆H₆/EtOAc)

Melting Point: Mp 49-51°

Aldrich: 38759-2

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

Molecular Formula: C₉H₁₀N₂O₅

Molecular Weight: 226.188

Accurate Mass: 226.058973

Percentage Composition: C 47.79%; H 4.46%; N 12.38%; O 35.37%

Melting Point: Mp 84.5-85°

>>**Derivative:** *N*-Me

CAS Registry Number: 75092-39-6

Molecular Formula: C₆H₆N₂O₄

Molecular Weight: 170.124

Accurate Mass: 170.032758

Percentage Composition: C 42.36%; H 3.55%; N 16.47%; O 37.62%

Physical Description: Prisms (H₂O)

Melting Point: Mp 266-268° (249.5-250° dec.)

>>**Derivative:** *N*-Me, 3-Me ester

CAS Registry Number: 117860-55-6

Molecular Formula: C₇H₈N₂O₄

Molecular Weight: 184.151

Accurate Mass: 184.048408

Percentage Composition: C 45.66%; H 4.38%; N 15.21%; O 34.75%

Physical Description: Needles (MeOH aq.)

Melting Point: Mp 129-130.5°