



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

CAS Registry Number: 25016-20-0

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.

Melting Point: Mp 155-155.5° (146°). Mp 222°

Solubility: Mod. sol. hot H₂O

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

CAS Registry Number: 17827-61-1

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: Liq.

Boiling Point: Bp₉ 120°

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

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: Liq.

Melting Point: Mp 9-11°

Boiling Point: Bp₁₃ 140-143°

>> **Derivative:** *N*-Ph

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

CAS Registry Number: 4747-46-0

Molecular Formula: C₁₀H₈N₂O₂

Molecular Weight: 188.185

Accurate Mass: 188.058578

Percentage Composition: C 63.83%; H 4.28%; N 14.89%; O 17.00%

Physical Description: Needles (H₂O)

Melting Point: Mp 146°

pKa Value: p*K*_{a1} 3.6 (20°)

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

Molecular Formula: C₁₁H₁₀N₂O₂

Molecular Weight: 202.212

Accurate Mass: 202.074228

Percentage Composition: C 65.34%; H 4.98%; N 13.85%; O 15.82%

Physical Description: Needles

Melting Point: Mp 77°

>> **Derivative:** *N*-Ph, nitrile

Synonym(s): 3-Cyano-1-phenyl-1*H*-pyrazole

CAS Registry Number: 18093-85-1

Molecular Formula: C₁₀H₇N₃

Molecular Weight: 169.185

Accurate Mass: 169.063997

Percentage Composition: C 70.99%; H 4.17%; N 24.84%

Physical Description: Cryst. (Et₂O/petrol)

>> **Variant:** 2*H*-form

Molecular Formula: C₄H₄N₂O₂

Molecular Weight: 112.088

Accurate Mass: 112.027278

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