



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

CAS Registry Number: 16034-46-1

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 223-224° (219-220°)

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

Molecular Formula: C₇H₁₀N₂O₂

Molecular Weight: 154.168

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

Physical Description: Liq.

Boiling Point: Bp₁₈ 95°

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

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

CAS Registry Number: 1133-77-3

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 183°

pKa Value: p*K*_{a1} 2.7 (20°)

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

CAS Registry Number: 55115-07-6

Molecular Formula: C₁₁H₁₀N₂O₂

Molecular Weight: 202.212

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

Physical Description: Needles

Melting Point: Mp 67°

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

Synonym(s): 5-Cyano-1-phenyl-1*H*-pyrazole

Molecular Formula: C₁₀H₇N₃

Molecular Weight: 169.185

Accurate Mass: 169.063997

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

Physical Description: Liq.

Boiling Point: Bp_{0.625} 95-100° (lit. gives a pressure range)

References: