



pKa Value: pK_{a1} 4.24

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

CAS Registry Number: 10250-61-0

Molecular Formula: $C_7H_{10}N_2O_2$

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 71.5-72.5°

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

CAS Registry Number: 5744-51-4

Molecular Formula: $C_8H_{12}N_2O_2$

Molecular Weight: 168.195

Accurate Mass: 168.089878

Percentage Composition: C 57.13%; H 7.19%; N 16.66%; O 19.02%

Physical Description: Cryst. (Et₂O/ petrol)

Melting Point: Mp 40-42°

Rare Chemicals Library: S94036-4

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

CAS Registry Number: 54384-74-6

Molecular Formula: $C_6H_9N_3O$

Molecular Weight: 139.157

Accurate Mass: 139.074562

Percentage Composition: C 51.79%; H 6.52%; N 30.20%; O 11.50%

Melting Point: Mp 177-178°

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

Synonym(s): 3-Cyano-1,5-dimethylpyrazole

Molecular Formula: $C_6H_7N_3$

Molecular Weight: 121.141

Accurate Mass: 121.063997

Percentage Composition: C 59.49%; H 5.82%; N 34.69%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 68-69°

>> **Derivative:** *N*-Et

Synonym(s): 1-Ethyl-5-methyl-1*H*-pyrazole-3-carboxylic acid

CAS Registry Number: 50920-46-2

Molecular Formula: $C_7H_{10}N_2O_2$

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. (H₂O or C₆H₆)

Melting Point: Mp 136-137°

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

CAS Registry Number: 50920-45-1

Molecular Formula: $C_9H_{14}N_2O_2$

Molecular Weight: 182.222

Accurate Mass: 182.105528

Percentage Composition: C 59.32%; H 7.74%; N 15.37%; O 17.56%

Physical Description: Liq.

Boiling Point: Bp₁₂ 154°

Density: d_4^{20} 1.079

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

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