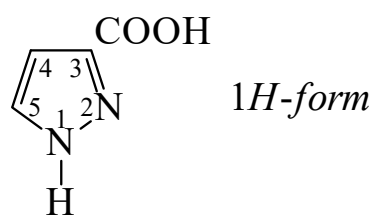




>>Entry Name: 3(5)-Pyrazolecarboxylic acid, 9CI



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%

Biological Source: Isol. from the sponge *Tedania adhelans*

Physical Description: Prisms (H₂O)

Melting Point: Mp 293 dec.°

Solubility: Sol. EtOH; mod. sol. Et₂O, AcOH; insol. CHCl₃, C₆H₆

>>Derivative: Me ester

CAS Registry Number: 15366-34-4

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. (C₆H₆)

Melting Point: Mp 139-140°

Solubility: Sol. MeOH; spar. sol. petrol

>>Derivative: Et ester

CAS Registry Number: 5932-27-4

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: Cryst. (hexane/EtOAc)

Melting Point: Mp 158-159°

Rare Chemicals Library: S94043-7

>>Derivative: Amide

CAS Registry Number: 33064-36-7

Molecular Formula: C₄H₅N₃O

Molecular Weight: 111.103

Accurate Mass: 111.043262

Percentage Composition: C 43.24%; H 4.54%; N 37.82%; O 14.40%

Melting Point: Mp 203-204°

>>Derivative: Nitrile

Synonym(s): 3-Cyanopyrazole

CAS Registry Number: 33064-34-5

Molecular Formula: C₄H₃N₃

Molecular Weight: 93.088

Accurate Mass: 93.032697

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

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 76-77°

>>Variant: 1*H*-form

CAS Registry Number: 1621-91-6

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%

Rare Chemicals Library: S94529-3