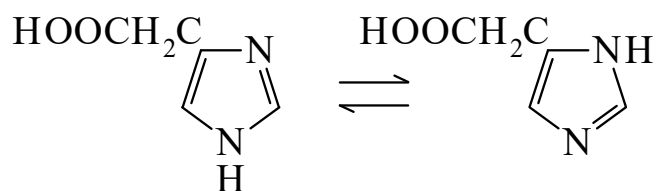




>>Entry Name: 1*H*-Imidazole-4(5)-acetic acid, 9CI



CAS Registry Number: 645-65-8

Related CAS Registry Numbers(s): 4200-48-0 51718-81-1

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%

Biological Source: Isol. from various fungi, e.g. *Polyporus sulphureus*, *Inocybe patouillardii*, *Coprinus atramentarius* and *Phallus impudicus*

Physical Description: Cryst. + 1H₂O

Melting Point: Mp 222 dec.°

>>Derivative: Hydrochloride

CAS Registry Number: 3251-69-2

Melting Point: Mp 223-225°

Aldrich: 21999-1

Fluka: 56770

Sigma: I0375

>>Derivative: Me ester

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. (EtOH) (as picrate)

Melting Point: Mp 167.5-168.5° (picrate)

>>Derivative: Et ester

CAS Registry Number: 28782-45-8

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%

Melting Point: Mp 115-117° (as hydrochloride)

>>Derivative: Nitrile

Synonym(s): 4-(Cyanomethyl)imidazole

CAS Registry Number: 18502-05-1

Molecular Formula: C₅H₅N₃

Molecular Weight: 107.115

Accurate Mass: 107.048347

Percentage Composition: C 56.07%; H 4.70%; N 39.23%

Melting Point: Mp 138-140°

>>Variant: 1*H*-form

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%