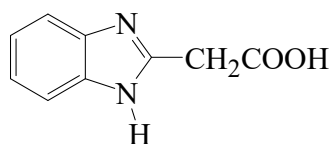




>>Entry Name: **1*H*-Benzimidazole-2-acetic acid**, 9CI



CAS Registry Number: 13570-08-6

Molecular Formula: C₉H₈N₂O₂

Molecular Weight: 176.174

Accurate Mass: 176.058578

Percentage Composition: C 61.36%; H 4.58%; N 15.90%; O 18.16%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 117°

pKa Value: p*K*_a 7.2 (25°,dioxan aq.)

>>**Derivative:** Hydrochloride

Melting Point: Mp 271-272°

>>**Derivative:** Me ester

CAS Registry Number: 49672-05-1

Molecular Formula: C₁₀H₁₀N₂O₂

Molecular Weight: 190.201

Accurate Mass: 190.074228

Percentage Composition: C 63.15%; H 5.30%; N 14.73%; O 16.82%

pKa Value: p*K*_a 6.78 (25°,H₂O)

>>**Derivative:** Et ester

CAS Registry Number: 14741-71-0

Molecular Formula: C₁₁H₁₂N₂O₂

Molecular Weight: 204.228

Accurate Mass: 204.089878

Percentage Composition: C 64.69%; H 5.92%; N 13.72%; O 15.67%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 129°

>>**Derivative:** Amide

CAS Registry Number: 60792-56-5

Molecular Formula: C₉H₉N₃O

Molecular Weight: 175.19

Accurate Mass: 175.074562

Percentage Composition: C 61.70%; H 5.18%; N 23.99%; O 9.13%

Melting Point: Mp 245-247°

pKa Value: p*K*_a 7.46 (25°,H₂O)

>>**Derivative:** Nitrile

Synonym(s): 2-(Cyanomethyl)-1*H*-benzimidazole

CAS Registry Number: 4414-88-4

Molecular Formula: C₉H₇N₃

Molecular Weight: 157.174

Accurate Mass: 157.063997

Percentage Composition: C 68.78%; H 4.49%; N 26.73%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 210-211°

>>**Derivative:** *N*-Me

Molecular Formula: C₁₀H₁₀N₂O₂

Molecular Weight: 190.201

Accurate Mass: 190.074228

Percentage Composition: C 63.15%; H 5.30%; N 14.73%; O 16.82%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 75° (dec.)