



>>Entry Name: **1*H*-Benzimidazole-5(6)-carboxylic acid**, 9CI

CAS Registry Number: 15788-16-6

Related CAS Registry Numbers(s): 37619-31-1 40159-90-8 66630-79-3 66630-87-3 131020-35-4 131020-50-3 160882-30-4 176646-96-1

Molecular Formula: C₈H₆N₂O₂

Molecular Weight: 162.148

Accurate Mass: 162.042928

Percentage Composition: C 59.26%; H 3.73%; N 17.28%; O 19.73%

Physical Description: Needles (NH₃ aq./AcOH)

Melting Point: Mp 325 dec.°

pKa Value: p*K*_a 3.08 (20°, H₂O)

Aldrich: 29678-3

>>Derivative: Me ester

CAS Registry Number: 26663-77-4

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%

Melting Point: Mp 134-136°. Mp 250 dec.°

>>Derivative: Me ester, hydrochloride

Melting Point: Mp 250°

>>Derivative: Et ester

CAS Registry Number: 58842-61-8

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. (EtOH)

Melting Point: Mp 101-103°

>>Derivative: Amide

Molecular Formula: C₈H₇N₃O

Molecular Weight: 161.163

Accurate Mass: 161.058912

Percentage Composition: C 59.62%; H 4.38%; N 26.07%; O 9.93%

Physical Description: Prisms + H₂O (H₂O)

Melting Point: Mp 247-248°

>>Derivative: Hydrazide

Molecular Formula: C₈H₈N₄O

Molecular Weight: 176.177

Accurate Mass: 176.069811

Percentage Composition: C 54.54%; H 4.58%; N 31.80%; O 9.08%

Physical Description: Needles (EtOH)

Melting Point: Mp 240-248°

>>Variant: 1*H*-form

Molecular Formula: C₈H₆N₂O₂

Molecular Weight: 162.148

Accurate Mass: 162.042928

Percentage Composition: C 59.26%; H 3.73%; N 17.28%; O 19.73%