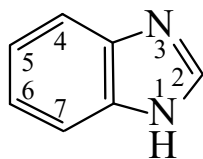




>>Entry Name: **1*H*-Benzimidazole**, 9CI

Synonym(s): Benziminazole. 3-Azaindole. 1,3-Diazaindene. 1,3-Benzodiazole



CAS Registry Number: 51-17-2

Molecular Formula: C₇H₆N₂

Molecular Weight: 118.138

Accurate Mass: 118.053098

Percentage Composition: C 71.17%; H 5.12%; N 23.71%

Physical Description: Plates (H₂O)

Melting Point: Mp 170-172°

pKa Value: p*K*_{a1} 5.53; p*K*_{a2} 12.3 (20°)

Hazard & Toxicity: LD₅₀ (mus, orl) 2910 mg/kg

Aldrich: 19412-3

Fluka: 12250

Sigma: B9131

>>Derivative: 1-Oxide

Synonym(s): Benzimidazole *N*-oxide. 1-Hydroxybenzimidazole

CAS Registry Number: 59118-51-3

Molecular Formula: C₇H₆N₂O

Molecular Weight: 134.137

Accurate Mass: 134.048013

Percentage Composition: C 62.68%; H 4.51%; N 20.88%; O 11.93%

Melting Point: Mp 215°

pKa Value: p*K*_{a1} 2.9; p*K*_{a2} 7.86 (20°)

Other Data: Tautomeric

>>Derivative: 1-Ac

Synonym(s): 1-Acetylbenzimidazole

CAS Registry Number: 18773-95-0

Molecular Formula: C₉H₈N₂O

Molecular Weight: 160.175

Accurate Mass: 160.063663

Percentage Composition: C 67.49%; H 5.03%; N 17.49%; O 9.99%

Physical Description: Needles (C₆H₆)

Melting Point: Mp 113-114°

>>Derivative: 1-Benzoyl

Synonym(s): 1-Benzoylbenzimidazole

CAS Registry Number: 62573-86-8

Molecular Formula: C₁₄H₁₀N₂O

Molecular Weight: 222.246

Accurate Mass: 222.079313

Percentage Composition: C 75.66%; H 4.54%; N 12.60%; O 7.20%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 93°