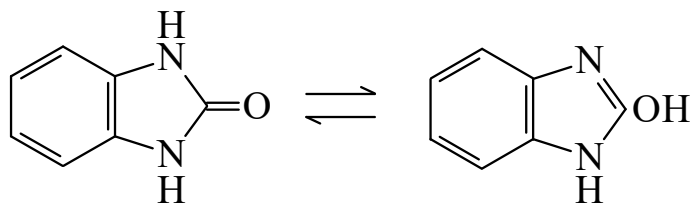




>>Entry Name: **Benzimidazolone**

Synonym(s): 2-Hydroxybenzimidazole. 1,3-Dihydro-2*H*-benzimidazol-2-one, 9CI. Benzimidazolin-2-one, 8CI. *o*-Phenyleneurea. 1*H*-2-Benzimidazolol



CAS Registry Number: 615-16-7

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%

General Statement: Tautomeric. Oxo-form predominates

Physical Description: Plates (H₂O or EtOH)

Melting Point: Mp 312° (300°)

Hazard & Toxicity: LD₅₀ (mus, scu) 620 mg/kg

Aldrich: H1985-9

Fluka: 54602

>>Variant: Oxo-form

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%

>>Derivative: 1-Me

CAS Registry Number: 1849-01-0

Molecular Formula: C₈H₈N₂O

Molecular Weight: 148.164

Accurate Mass: 148.063663

Percentage Composition: C 64.85%; H 5.44%; N 18.91%; O 10.80%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 191-192° (188-189°)

>>Derivative: 1-Et

CAS Registry Number: 10045-45-1

Molecular Formula: C₉H₁₀N₂O

Molecular Weight: 162.191

Accurate Mass: 162.079313

Percentage Composition: C 66.65%; H 6.21%; N 17.27%; O 9.86%

Physical Description: Prisms (EtOAc)

Melting Point: Mp 117-118°

Aldrich: 19401-8

>>Derivative: 1-Benzyl

CAS Registry Number: 28643-53-0

Molecular Formula: C₁₄H₁₂N₂O

Molecular Weight: 224.262

Accurate Mass: 224.094963

Percentage Composition: C 74.98%; H 5.39%; N 12.49%; O 7.13%

Physical Description: Needles (EtOH)

Melting Point: Mp 197-200°