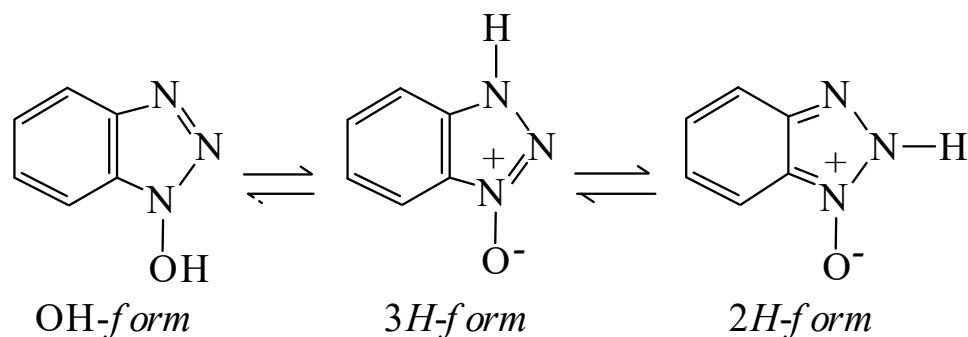




>>Entry Name: 1-Benzotriazolol

Synonym(s): 1-Hydroxybenzotriazole. Benzazimidazole



Related CAS Registry Numbers(s): 123333-53-9

Extra CAS Registry Numbers(s): 80029-43-2

Molecular Formula: C₆H₅N₃O

Molecular Weight: 135.125

Accurate Mass: 135.043262

Percentage Composition: C 53.33%; H 3.73%; N 31.10%; O 11.84%

Use/Importance: Used in peptide synth. Catalyst for acylations and phosphorylations

Physical Description: Needles (anhyd. EtOH/Et₂O)

Melting Point: Mp 155-158° (as hydrate)

Hazard & Toxicity: Exploded on heating above 160° *in vacuo*

>>Variant: OH-form

CAS Registry Number: 2592-95-2

Molecular Formula: C₆H₅N₃O

Molecular Weight: 135.125

Accurate Mass: 135.043262

Percentage Composition: C 53.33%; H 3.73%; N 31.10%; O 11.84%

Aldrich: 36244-1

Fluka: 54802

Sigma: H2006

>>Derivative: 1-O-Benzoyl

Synonym(s): 1-(Benzoyloxy)benzotriazole

CAS Registry Number: 54769-36-7

Molecular Formula: C₁₃H₉N₃O₂

Molecular Weight: 239.233

Accurate Mass: 239.069477

Percentage Composition: C 65.27%; H 3.79%; N 17.56%; O 13.38%

Use/Importance: Selective benzoylating agent for diols

Physical Description: Cryst. (CH₂Cl₂/petrol)

Melting Point: Mp 77-79°

>>Derivative: 1-O-Allyloxycarbonyl

Synonym(s): 1-[[[(2-Propenyloxy)carbonyl]oxy]-1H-benzotriazole, 9CI

CAS Registry Number: 102423-16-5

Molecular Formula: C₁₀H₉N₃O₃

Molecular Weight: 219.199

Accurate Mass: 219.064392

Percentage Composition: C 54.79%; H 4.14%; N 19.17%; O 21.90%

Melting Point: Mp 110-113°

Aldrich: 33415-4

>>Derivative: 1-O-Me

Synonym(s): 1-Methoxybenzotriazole

CAS Registry Number: 22713-34-4

Molecular Formula: C₇H₇N₃O

Molecular Weight: 149.152

Accurate Mass: 149.058912

Percentage Composition: C 56.37%; H 4.73%; N 28.17%; O 10.73%

Melting Point: Mp 88-89°