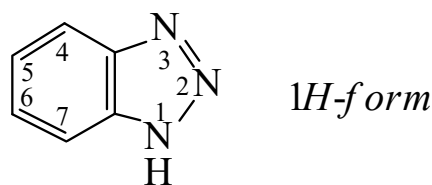




>>Entry Name: **Benzotriazole**

Synonym(s): Aziminobenzene (obsol.). 1,2,3-Triazaindene



CAS Registry Number: 95-14-7

Related CAS Registry Numbers(s): 273-02-9 22257-44-9

Molecular Formula: C₆H₅N₃

Molecular Weight: 119.126

Accurate Mass: 119.048347

Percentage Composition: C 60.50%; H 4.23%; N 35.27%

General Statement: 1*H*-Form predominates (>99.9%)

Use/Importance: Used for pptn. separation and gravimetric detn. of Ag, Cd, Co, Ni, Zn. The benzotriazolyl group is an extremely versatile substituent showing props. of leaving group, electron donor and ability to promote adjacent proton loss. Used in enamine synthesis

Physical Description: Needles (C₆H₆)

Melting Point: Mp 100°

Solubility: Sol. C₆H₆

pKa Value: p*K*_{a1} 1.6; p*K*_{a2} 8.64 (20°)

Hazard & Toxicity: Can detonate during vac. dist. Severe eye and skin irritant. LD₅₀ (rat, orl) 600 mg/kg

Aldrich: B1140-0

Fluka: 12799

Sigma: B1254

>>Variant: 1*H*-form

Molecular Formula: C₆H₅N₃

Molecular Weight: 119.126

Accurate Mass: 119.048347

Percentage Composition: C 60.50%; H 4.23%; N 35.27%

>>Derivative: *N*-Ac

CAS Registry Number: 18773-93-8

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%

Melting Point: Mp 51°

>>Derivative: *N*-Benzoyl

CAS Registry Number: 4231-62-3

Molecular Formula: C₁₃H₉N₃O

Molecular Weight: 223.234

Accurate Mass: 223.074562

Percentage Composition: C 69.95%; H 4.06%; N 18.82%; O 7.17%

Melting Point: Mp 112°

>>Derivative: *N*-Chlorocarbonyl

Synonym(s): 1*H*-Benzotriazole-1-carbonyl chloride. 1-Chlorocarbonylbenzotriazole

CAS Registry Number: 65095-13-8

Molecular Formula: C₇H₄ClN₃O

Molecular Weight: 181.581

Accurate Mass: 181.004289

Percentage Composition: C 46.30%; H 2.22%; Cl 19.52%; N 23.14%; O 8.81%

Use/Importance: Synthetic reagent

Physical Description: Cryst. (petrol)

Melting Point: Mp 54-55°

>>Derivative: *N*-Hydroxy