



>>Entry Name: 4-Aminobenzimidazole

Synonym(s): 1*H*-Benzimidazol-4-amine, 9Cl

CAS Registry Number: 4331-29-7

Molecular Formula: C₇H₇N₃

Molecular Weight: 133.152

Accurate Mass: 133.063997

Percentage Composition: C 63.14%; H 5.30%; N 31.56%

Physical Description: Prisms (CHCl₃)

Melting Point: Mp 120-121°

>>Derivative: Hydrochloride (1:2)

CAS Registry Number: 37724-28-0

Physical Description: Cryst. (MeOH)

Melting Point: Mp 247-249 dec.°

>>Derivative: 1-Oxide

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%

Physical Description: Cryst. + 1H₂O (H₂O)

Melting Point: Mp 118-120°

>>Derivative: 1-Oxide; hydrochloride (1:2)

Physical Description: Cryst. (conc. HCl)

Melting Point: Mp 224-226°

>>Derivative: 3-Oxide

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%

Physical Description: Cryst. + 1H₂O (H₂O)

Melting Point: Mp 108-110°

>>Derivative: 3-Oxide; hydrochloride (1:2)

Physical Description: Cryst. (conc. HCl)

Melting Point: Mp 190-192 dec.°

References:

Van der Want, G.M., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1948, **67**, 45, (*synth*)

Fisher, E.C. *et al.*, *J.O.C.*, 1958, **23**, 1944, (*synth*)

Keiser, S. *et al.*, *Pharmazie*, 1972, **27**, 287, (*rev*)

Harvey, I.W. *et al.*, *J.C.S. Perkin 1*, 1988, 1939, (*oxides*)