



>>Entry Name: 4-Aminobenzimidazole
Synonym(s): 1H-Benzimidazol-4-amine, uci
CAS Registry Number: 4331-29-7

Molecular Formula: C₆H₆N₂
Molecular Weight: 133.132
Accurate Mass: 133.063997
Percentage Composition: C 63.14%; H 5.30%; N 31.56%
Physical Description: Prism (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: C₆H₅N₂O
Molecular Weight: 149.132
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: C₆H₅N₂O
Molecular Weight: 149.132
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 I*, 1988, 1939, (oxides)