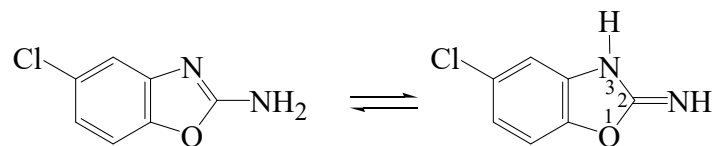




>>>Entry Name: **2-Amino-5-chlorobenzoxazole**

Synonym(s): 5-Chloro-2-benzoxazolamine, 9Cl. **Zoxazolamine**, BAN, INN. Contrazole. Deflexol. Flexin. Miazol. Uri-Boi. Zoxamine. Zoxine. McN 485



CAS Registry Number: 61-80-3

Molecular Formula: C₇H₅ClN₂O

Molecular Weight: 168.582

Accurate Mass: 168.00904

Percentage Composition: C 49.87%; H 2.99%; Cl 21.03%; N 16.62%; O 9.49%

Use/Important: Muscle relaxant

Physical Description: Plates (EtOH aq.)

Development Status: No longer marketed

Melting Point: Mp 182-183° (185-186°)

Hazard & Toxicity: LD₅₀ (rat, orl) 782 mg/kg

Aldrich: A4580-7

Sigma: A3148

>>>Variant: Amino-form

Molecular Formula: C₇H₅ClN₂O

Molecular Weight: 168.582

Accurate Mass: 168.00904

Percentage Composition: C 49.87%; H 2.99%; Cl 21.03%; N 16.62%; O 9.49%

>>>Derivative: Hydrochloride

Physical Description: Needles

Melting Point: Mp 229 dec.°

>>>Derivative: 2-*N*-Benzoyl

Molecular Formula: C₁₄H₉ClN₂O₂

Molecular Weight: 272.69

Accurate Mass: 272.035255

Percentage Composition: C 61.66%; H 3.33%; Cl 13.00%; N 10.27%; O 11.73%

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 213°

>>>Derivative: 2-*N*-Ethoxycarbonyl

Molecular Formula: C₁₀H₉ClN₂O₃

Molecular Weight: 240.645

Accurate Mass: 240.03017

Percentage Composition: C 49.91%; H 3.77%; Cl 14.73%; N 11.64%; O 19.95%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 238 dec.°

>>>Derivative: 2-*N*-Ph

Synonym(s): 2-Anilino-5-chlorobenzoxazole

CAS Registry Number: 79558-94-4

Molecular Formula: C₁₃H₉ClN₂O

Molecular Weight: 244.68

Accurate Mass: 244.04034

Percentage Composition: C 63.82%; H 3.71%; Cl 14.49%; N 11.45%; O 6.54%

Melting Point: Mp 212-213°