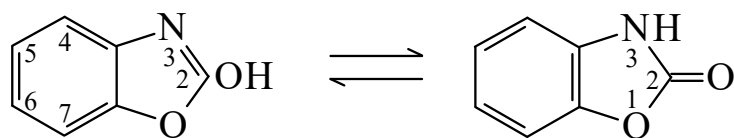




>>Entry Name: 2-Benzoxazolol

ENTRY UNDER REVIEW

Synonym(s): 2(3*H*)-Benzoxazolone, 9Cl. 2-Benzoxazolinone, 8Cl. 2-Hydroxybenzoxazole. BOA



CAS Registry Number: 59-49-4

Molecular Formula: C₇H₅NO₂

Molecular Weight: 135.122

Accurate Mass: 135.032029

Percentage Composition: C 62.22%; H 3.73%; N 10.37%; O 23.68%

General Statement: Tautomeric. *NH*-form predominates

Biological Source: Found in rye seedlings

Melting Point: Mp 141-142°

Solubility: BERDY SOL: Sol. bases, Et₂O; fairly sol. H₂O; poorly sol. hexane

pKa Value: pK_{a1} 8.9 (23°)

UV: [neutral] λ_{max} 270 () (H₂O) (Berdy) [neutral] λ_{max} 275 () (EtOH) (Berdy)

Hazard & Toxicity: LD₅₀ (rat, orl) 700 mg/kg. LD₅₀ (mus, orl) 554 mg/kg

Aldrich: 15705-8

Fluka: 12825

>>Derivative: Monohydrate

Physical Description: Needles (HCl aq.)

Melting Point: Mp 97-98°

>>Variant: *NH*-form

Molecular Formula: C₇H₅NO₂

Molecular Weight: 135.122

Accurate Mass: 135.032029

Percentage Composition: C 62.22%; H 3.73%; N 10.37%; O 23.68%

>>Derivative: *N*-Ac

CAS Registry Number: 24963-28-8

Molecular Formula: C₉H₇NO₃

Molecular Weight: 177.159

Accurate Mass: 177.042594

Percentage Composition: C 61.02%; H 3.98%; N 7.91%; O 27.09%

Melting Point: Mp 95°

Hazard & Toxicity: LD₅₀ (mus, orl) 2730 mg/kg

Rare Chemicals Library: S81541-1

>>Derivative: *N*-Benzoyl

CAS Registry Number: 13787-59-2

Molecular Formula: C₁₄H₉NO₃

Molecular Weight: 239.23

Accurate Mass: 239.058244

Percentage Composition: C 70.29%; H 3.79%; N 5.85%; O 20.06%

Melting Point: Mp 173-174°