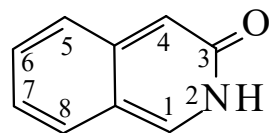




>>Entry Name: **3(2*H*)-Isoquinolinone**

Synonym(s): 3-Hydroxyisoquinoline. 3-Isoquinolinol



CAS Registry Number: 7651-81-2

Molecular Formula: C₉H₇NO

Molecular Weight: 145.16

Accurate Mass: 145.052764

Percentage Composition: C 74.47%; H 4.86%; N 9.65%; O 11.02%

Physical Description: Yellow needles (C₆H₆)

Melting Point: Mp 195-196°

pKa Value: p*K*_{a1} 2.18; p*K*_{a2} 9.62 (20°)

Aldrich: 36895-4

>>Variant: *NH*-form

Molecular Formula: C₉H₇NO

Molecular Weight: 145.16

Accurate Mass: 145.052764

Percentage Composition: C 74.47%; H 4.86%; N 9.65%; O 11.02%

>>Derivative: *N*-Me

Synonym(s): 2-Methyl-3(2*H*)-isoquinolinone

Molecular Formula: C₁₀H₉NO

Molecular Weight: 159.187

Accurate Mass: 159.068414

Percentage Composition: C 75.45%; H 5.70%; N 8.80%; O 10.05%

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 129-136°

>>Variant: *OH*-form

Molecular Formula: C₉H₇NO

Molecular Weight: 145.16

Accurate Mass: 145.052764

Percentage Composition: C 74.47%; H 4.86%; N 9.65%; O 11.02%

>>Derivative: Me ether

Synonym(s): 3-Methoxyisoquinoline

Molecular Formula: C₁₀H₉NO

Molecular Weight: 159.187

Accurate Mass: 159.068414

Percentage Composition: C 75.45%; H 5.70%; N 8.80%; O 10.05%

Physical Description: Cryst. or liq.

Melting Point: Mp 10-12°

References:

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