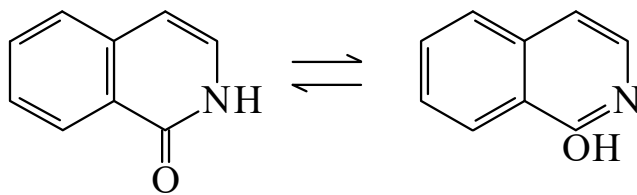




>>Entry Name: **1(2*H*)-Isoquinolinone**, 9CI

Synonym(s): Isocarbostyrl, 8CI. 1-Hydroxyisoquinoline. 1-Isoquinolinol



CAS Registry Number: 491-30-5

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: Needles (H₂O)

Melting Point: Mp 209-210°

pKa Value: p*K*_a −1.2 (20°, H₂SO₄ aq.)

Other Data: Sublimes

Aldrich: 15210-2

Fluka: 55435

>>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*-Ac

Molecular Formula: C₁₁H₉NO₂

Molecular Weight: 187.198

Accurate Mass: 187.063329

Percentage Composition: C 70.58%; H 4.85%; N 7.48%; O 17.09%

Physical Description: Needles (cyclohexane)

Melting Point: Mp 84-86°

>>Derivative: *N*-Benzoyl

Molecular Formula: C₁₆H₁₁NO₂

Molecular Weight: 249.268

Accurate Mass: 249.078979

Percentage Composition: C 77.10%; H 4.45%; N 5.62%; O 12.84%

Physical Description: Needles (heptane)

Melting Point: Mp 147°

>>Derivative: *N*-Me

CAS Registry Number: 4594-71-2

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%

Melting Point: Mp 40°

Boiling Point: Bp₇₂₀ 314-315°

>>Derivative: *N*-Hydroxy

Synonym(s): 2-Hydroxyisocarbostyrl

CAS Registry Number: 21201-50-3

Molecular Formula: C₉H₇NO₂

Molecular Weight: 161.16

Accurate Mass: 161.047679

Percentage Composition: C 67.08%; H 4.38%; N 8.69%; O 19.86%

Physical Description: Needles

Melting Point: Mp 188-189°