



>>Entry Name: 7-Isoquinolinol, 9Cl
Synonym(s): 7-Hydroxyisoquinoline

CAS Registry Number: 7651-83-4

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: Pale yellow plates (EtOH)
Melting Point: Mp 229.5-230.5° (226-227°)
pKa Value: pK_{a1} 5.68; pK_{a2} 8.9 (20°)
Other Data: Sublimes

>>Derivative: N-Oxide

CAS Registry Number: 146607-35-4
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 (EtOH)
Melting Point: Mp 288-290°

>>Derivative: Me ether
Synonym(s): 7-Methoxyisoquinoline

CAS Registry Number: 39989-39-4
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: Needles (petrol)
Melting Point: Mp 49°
Boiling Point: Bp₃₄ 182-186°

>>Derivative: Me ether; hydrochloride

Physical Description: Cryst.
Melting Point: Mp 221°

>>Derivative: Me ether, N-oxide

CAS Registry Number: 146607-34-3
Molecular Formula: C₁₀H₉NO₂
Molecular Weight: 175.187
Accurate Mass: 175.063329
Percentage Composition: C 68.56%; H 5.18%; N 8.00%; O 18.27%
Physical Description: Needles (C₆H₆)
Melting Point: Mp 159-160°

>>Derivative: Et ether
Synonym(s): 7-Ethoxyisoquinoline

CAS Registry Number: 138223-15-1
Molecular Formula: C₁₁H₁₁NO
Molecular Weight: 173.214
Accurate Mass: 173.084064
Percentage Composition: C 76.28%; H 6.40%; N 8.09%; O 9.24%
Physical Description: Liq.
Melting Point: Mp 7-9°
Boiling Point: Bp₂₇ 182-183°

>>Derivative: Et ether; methiodide

Physical Description: Cryst.
Melting Point: Mp 193-194°