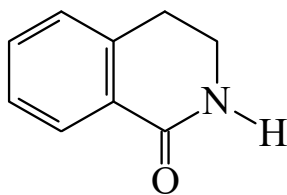




>>Entry Name: 3,4-Dihydro-1(2*H*)-isoquinolinone, 9CI

Synonym(s): 3,4-Dihydroisocarbostyrl. 1-Oxo-1,2,3,4-tetrahydroisoquinoline



CAS Registry Number: 1196-38-9

Molecular Formula: C₉H₉NO

Molecular Weight: 147.176

Accurate Mass: 147.068414

Percentage Composition: C 73.45%; H 6.16%; N 9.52%; O 10.87%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 58°

Boiling Point: Bp_{0.1} 125-127°

>>Derivative: *N*-Ac

CAS Registry Number: 74315-06-3

Molecular Formula: C₁₁H₁₁NO₂

Molecular Weight: 189.213

Accurate Mass: 189.078979

Percentage Composition: C 69.83%; H 5.86%; N 7.40%; O 16.91%

Physical Description: Cryst. (EtOAc/hexane)

Melting Point: Mp 97-98°

>>Derivative: *N*-Benzoyl

CAS Registry Number: 75435-41-5

Molecular Formula: C₁₆H₁₃NO₂

Molecular Weight: 251.284

Accurate Mass: 251.094629

Percentage Composition: C 76.48%; H 5.21%; N 5.57%; O 12.73%

Boiling Point: Bp₂ 210°

>>Derivative: *N*-Me

CAS Registry Number: 6772-65-2

Molecular Formula: C₁₀H₁₁NO

Molecular Weight: 161.203

Accurate Mass: 161.084064

Percentage Composition: C 74.51%; H 6.88%; N 8.69%; O 9.93%

Physical Description: Liq.

Boiling Point: Bp₆ 157°. Bp_{0.4} 118°

>>Derivative: *N*-Hydroxy

Synonym(s): 3,4-Dihydro-2-hydroxy-1(2*H*)-isoquinolinone, 9CI

CAS Registry Number: 116526-30-8

Molecular Formula: C₉H₉NO₂

Molecular Weight: 163.176

Accurate Mass: 163.063329

Percentage Composition: C 66.25%; H 5.56%; N 8.58%; O 19.61%

Biological Source: Prod. by *Streptomyces griseus* 2002-104

Biological Use/Importance: Siderophore. Allergy inhibitor

UV: [neutral] λ_{max} 480 () (H₂O+FeCl₃) (Berdy)

References:

- Schneider, W. *et al.*, *Arch. Pharm. (Weinheim, Ger.)*, 1958, **291**, 560-566, (*synth, N-Me*)
Davies, R.V. *et al.*, *J.C.S. Perkin 1*, 1978, 180-184, (*synth, ir*)
Misra, R.N. *et al.*, *Bioorg. Med. Chem. Lett.*, 1991, **1**, 295-298, (*synth, N-hydroxy*)
Graefe, U. *et al.*, *J. Basic Microbiol.*, 1994, **35**, 351-355, (*isol, N-hydroxy*)
Norman, M.H. *et al.*, *J. Med. Chem.*, 1994, **37**, 2552-2563, (*synth, pmr*)
Kawase, M. *et al.*, *Chem. Pharm. Bull.*, 1997, **45**, 1248-1253, (*N-acyl, derivs, ir, pmr, cmr*)