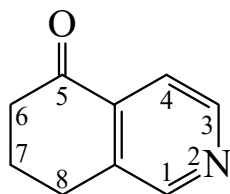




>>Entry Name: 7,8-Dihydro-5(6*H*)-isoquinolinone, 9CI

Synonym(s): 5-Oxo-5,6,7,8-tetrahydroisoquinoline. 5-Oxotetrahydroisoquinoline



CAS Registry Number: 21917-86-2

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. (petrol)

Melting Point: Mp 42-44°

Boiling Point: Bp₄ 113-115°

>>Derivative: Hydrochloride

Physical Description: Cryst.

Melting Point: Mp 235-236°

>>Derivative: Methiodide

Physical Description: Cryst.

Melting Point: Mp 130°

>>Derivative: Oxime

CAS Registry Number: 115787-46-7

Molecular Formula: C₉H₁₀N₂O

Molecular Weight: 162.191

Accurate Mass: 162.079313

Percentage Composition: C 66.65%; H 6.21%; N 17.27%; O 9.86%

Physical Description: Beige cryst.

Melting Point: Mp 173-174°

References:

Sugimoto, N. *et al.*, *Yakugaku Zasshi*, 1956, **76**, 1308; *CA*, **51**, 5076e, (*synth*)

Jones, D.G. *et al.*, *J.C.S.(C)*, 1969, 707, (*synth*, *pmr*)

Epsztajn, J. *et al.*, *J.C.S. Perkin 1*, 1985, 213, (*synth*, *ir*, *pmr*)

Caprathe, B.W. *et al.*, *J. Med. Chem.*, 1991, **34**, 2736, (*synth*, *ir*, *pmr*)

Glassco, W. *et al.*, *J. Med. Chem.*, 1993, **36**, 3381, (*synth*)

Lardenois, P. *et al.*, *Synth. Commun.*, 1996, **26**, 2305, (*synth*, *oxime*)