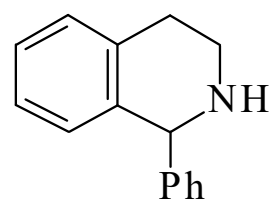




>>Entry Name: 1,2,3,4-Tetrahydro-1-phenylisoquinoline



CAS Registry Number: 22990-19-8

Molecular Formula: C₁₅H₁₅N

Molecular Weight: 209.29

Accurate Mass: 209.120449

Percentage Composition: C 86.08%; H 7.22%; N 6.69%

>>Variant: (R)-form

CAS Registry Number: 180272-45-1

Molecular Formula: C₁₅H₁₅N

Molecular Weight: 209.29

Accurate Mass: 209.120449

Percentage Composition: C 86.08%; H 7.22%; N 6.69%

Physical Description: Cryst.

Melting Point: Mp 84°

Optical Rotation: [α]_D²⁴ -10.2 (c, 0.17 in CHCl₃). [α]_D -12.3 (c, 1.55 in CH₂Cl₂)

>>Variant: (S)-form

CAS Registry Number: 118864-75-8

Molecular Formula: C₁₅H₁₅N

Molecular Weight: 209.29

Accurate Mass: 209.120449

Percentage Composition: C 86.08%; H 7.22%; N 6.69%

Optical Rotation: [α]_D²⁰ +12.2 (c, 0.85 in CH₂Cl₂)

>>Variant: (±)-form

Molecular Formula: C₁₅H₁₅N

Molecular Weight: 209.29

Accurate Mass: 209.120449

Percentage Composition: C 86.08%; H 7.22%; N 6.69%

Physical Description: Prisms (Et₂O)

Melting Point: Mp 97°

Solubility: Spar. sol. EtOH, Et₂O

>>Derivative: N-Me

Molecular Formula: C₁₆H₁₇N

Molecular Weight: 223.317

Accurate Mass: 223.136099

Percentage Composition: C 86.06%; H 7.67%; N 6.27%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 120-130°

>>Derivative: Methiodide

Physical Description: Prisms (EtOH aq.)

Melting Point: Mp 240-243°

References:

Freund, M. *et al.*, *Ber.*, 1909, **42**, 1761, (*synth, resoln*)

v. Binst, G. *et al.*, *J. Het. Chem.*, 1975, **12**, 1165, (*use*)

Wünsch, B. *et al.*, *Eur. J. Org. Chem.*, 1998, 711-718; 1999, 503-517, (*R-form, S-form, synth*)

Wanner, K.Th. *et al.*, *Eur. J. Org. Chem.*, 1998, 2019-2029, (*R-form*)

Pedrosa, R. *et al.*, *J.O.C.*, 2001, **66**, 243-250, (*R-form, ir, pmr, cmr*)