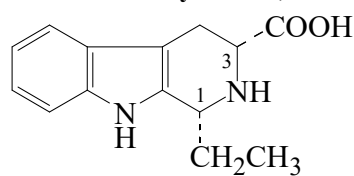




>>Entry Name: 1-Ethyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylic acid, 9Cl



(1*R*,3*R*)-form

CAS Registry Number: 109690-46-2

Molecular Formula: C₁₄H₁₆N₂O₂

Molecular Weight: 244.293

Accurate Mass: 244.121178

Percentage Composition: C 68.83%; H 6.60%; N 11.47%; O 13.10%

>>Variant: (1*R*,3*R*)-form

Synonym(s): (±)-*cis*-form

CAS Registry Number: 98667-08-4

Extra CAS Registry Numbers(s): 134930-19-1

Molecular Formula: C₁₄H₁₆N₂O₂

Molecular Weight: 244.293

Accurate Mass: 244.121178

Percentage Composition: C 68.83%; H 6.60%; N 11.47%; O 13.10%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 236-237°

>>Derivative: Me ester

CAS Registry Number: 75140-14-6

Extra CAS Registry Numbers(s): 123809-90-5

Molecular Formula: C₁₅H₁₈N₂O₂

Molecular Weight: 258.319

Accurate Mass: 258.136828

Percentage Composition: C 69.75%; H 7.02%; N 10.84%; O 12.39%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 112-114°

>>Variant: (1*R*,3*SR*)-form

Synonym(s): (±)-*trans*-form

CAS Registry Number: 98667-09-5

Molecular Formula: C₁₄H₁₆N₂O₂

Molecular Weight: 244.293

Accurate Mass: 244.121178

Percentage Composition: C 68.83%; H 6.60%; N 11.47%; O 13.10%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 242-243°

>>Derivative: Me ester

CAS Registry Number: 73327-08-9

Extra CAS Registry Numbers(s): 123877-71-4

Physical Description: Cryst. (MeOH)

Melting Point: Mp 152.5-153°

References:

Ungemach, F. *et al.*, *J.A.C.S.*, 1980, **102**, 6976-6984, (*Me ester, synth, ir, pmr, cryst struct*)

Ungemach, F. *et al.*, *J.O.C.*, 1981, **46**, 164-168, (*Me ester, synth*)

Saiga, Y. *et al.*, *Chem. Pharm. Bull.*, 1987, **35**, 3705-3712, (*synth, ir, pmr*)