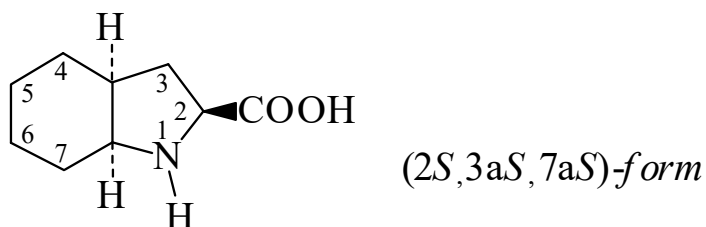




>>Entry Name: Octahydro-1*H*-indole-2-carboxylic acid



Molecular Formula: C₉H₁₅NO₂

Molecular Weight: 169.223

Accurate Mass: 169.110279

Percentage Composition: C 63.88%; H 8.93%; N 8.28%; O 18.91%

>>Variant: (2*S*,3*aS*,7*aS*)-form

CAS Registry Number: 80875-98-5

Molecular Formula: C₉H₁₅NO₂

Molecular Weight: 169.223

Accurate Mass: 169.110279

Percentage Composition: C 63.88%; H 8.93%; N 8.28%; O 18.91%

Melting Point: Mp 268-271 dec.°

Optical Rotation: [α]_D²⁰ -47.7 (c, 1 in MeOH)

>>Derivative: Et ester

CAS Registry Number: 82864-25-3

Molecular Formula: C₁₁H₁₉NO₂

Molecular Weight: 197.277

Accurate Mass: 197.141579

Percentage Composition: C 66.97%; H 9.71%; N 7.10%; O 16.22%

Physical Description: Cryst. (EtOAc) as hydrochloride

Melting Point: Mp 139-140 dec.°

Optical Rotation: [α]_D²⁰ -25.7 (c, 1 in H₂O)

>>Derivative: *tert*-Butyl ester

CAS Registry Number: 80876-00-2

Molecular Formula: C₁₃H₂₃NO₂

Molecular Weight: 225.33

Accurate Mass: 225.172879

Percentage Composition: C 69.30%; H 10.29%; N 6.22%; O 14.20%

Optical Rotation: [α]_D²⁰ -26.3 (c, 1 in MeOH)

>>Variant: (2*S*,3*aR*,7*aR*)-form

Molecular Formula: C₉H₁₅NO₂

Molecular Weight: 169.223

Accurate Mass: 169.110279

Percentage Composition: C 63.88%; H 8.93%; N 8.28%; O 18.91%

Physical Description: Amorph. solid

Melting Point: Mp 115 dec.°

Other Data: Contained 10% of (2*S*,3*aS*,7*aS*)-isomer

References:

Vincent, M. *et al.*, *Tet. Lett.*, 1982, **23**, 1677, (*synth*)

Blankley, C.J. *et al.*, *J. Med. Chem.*, 1987, **30**, 992, (*synth*)