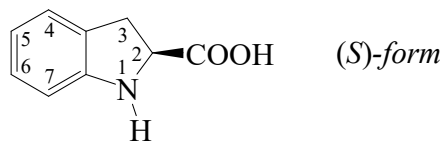




>>Entry Name: 2,3-Dihydro-1*H*-indole-2-carboxylic acid, 9CI

Synonym(s): 2-Indolinecarboxylic acid, 8CI



Related CAS Registry Numbers(s): 78348-24-0

Molecular Formula: C<sub>9</sub>H<sub>9</sub>NO<sub>2</sub>

Molecular Weight: 163.176

Accurate Mass: 163.063329

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

>>Variant: (*S*)-form

CAS Registry Number: 79815-20-6

Molecular Formula: C<sub>9</sub>H<sub>9</sub>NO<sub>2</sub>

Molecular Weight: 163.176

Accurate Mass: 163.063329

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

Melting Point: Mp 177 dec.°

Optical Rotation:  $[\alpha]_{\text{D}}^{20} -114$  (c, 1 in 1*M* HCl)

Aldrich: 34680-2

>>Derivative: Hydrochloride

CAS Registry Number: 82923-76-0

Physical Description: Cryst. + 1H<sub>2</sub>O (Et<sub>2</sub>O/2-propanol)

Melting Point: Mp 133 dec.°

Optical Rotation:  $[\alpha]_{\text{D}} -70$  (c, 1.0 in EtOH)

>>Derivative: Et ester

CAS Registry Number: 79854-42-5

Molecular Formula: C<sub>11</sub>H<sub>13</sub>NO<sub>2</sub>

Molecular Weight: 191.229

Accurate Mass: 191.094629

Percentage Composition: C 69.09%; H 6.85%; N 7.32%; O 16.73%

Physical Description: Cryst. (EtOH/Et<sub>2</sub>O), as hydrochloride

Melting Point: Mp 179-181°

Optical Rotation:  $[\alpha]_{\text{D}} -63$  (c, 1.385 in EtOH)

>>Variant: (±)-form

CAS Registry Number: 16851-56-2

Molecular Formula: C<sub>9</sub>H<sub>9</sub>NO<sub>2</sub>

Molecular Weight: 163.176

Accurate Mass: 163.063329

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

Physical Description: Cryst. (EtOH/Et<sub>2</sub>O)

Melting Point: Mp 120-150 dec.°

Fluka: 57245

>>Derivative: Me ester, *N*-(4-methylbenzenesulfonyl)

Physical Description: Cryst. (Et<sub>2</sub>O/hexane)

Melting Point: Mp 88-90°

>>Derivative: Amide

CAS Registry Number: 16852-04-3

Molecular Formula: C<sub>9</sub>H<sub>10</sub>N<sub>2</sub>O

Molecular Weight: 162.191

Accurate Mass: 162.079313

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

Physical Description: Cryst. (EtOH or by subl.)

Melting Point: Mp 208-209°