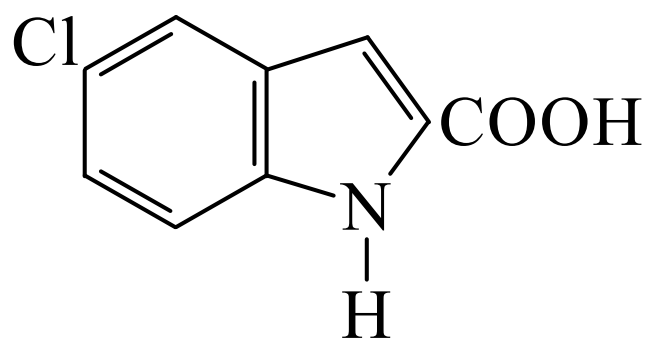




>>Entry Name: 5-Chloro-1*H*-indole-2-carboxylic acid, 9Cl



CAS Registry Number: 10517-21-2

Related CAS Registry Numbers(s): 64507-05-7 87802-11-7 128857-58-9 128857-67-0

Molecular Formula: C₉H₆ClNO₂

Molecular Weight: 195.605

Accurate Mass: 195.008706

Percentage Composition: C 55.26%; H 3.09%; Cl 18.12%; N 7.16%; O 16.36%

Source/Synthesis: Comly. available

Use/Importance: Displays high plasma cholesterol-reducing activity. Useful for treatment of CNS disorders

Physical Description: Cryst. (EtOH)

Melting Point: Mp 289-290 dec.°

pKa Value: pK_a 4.75 (50% EtOH aq.)

Aldrich: C4780-9

Sigma: C5647

>>Derivative: Et ester

CAS Registry Number: 4792-67-0

Molecular Formula: C₁₁H₁₀ClNO₂

Molecular Weight: 223.658

Accurate Mass: 223.040006

Percentage Composition: C 59.07%; H 4.51%; Cl 15.85%; N 6.26%; O 14.31%

Physical Description: Pale yellow needles (C₆H₆/hexane or EtOH)

Melting Point: Mp 167-168°. Mp 171.5-172.5°

Aldrich: 13809-6

>>Derivative: Amide

CAS Registry Number: 21109-01-3

Molecular Formula: C₉H₇ClN₂O

Molecular Weight: 194.62

Accurate Mass: 194.02469

Percentage Composition: C 55.54%; H 3.63%; Cl 18.22%; N 14.39%; O 8.22%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 236-238°

>>Derivative: Hydrazide

CAS Registry Number: 20948-67-8

Molecular Formula: C₉H₈ClN₃O

Molecular Weight: 209.634

Accurate Mass: 209.035589

Percentage Composition: C 51.57%; H 3.85%; Cl 16.91%; N 20.04%; O 7.63%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 269°

>>Derivative: *N*-Me

CAS Registry Number: 59908-47-3

Molecular Formula: C₁₀H₈ClNO₂

Molecular Weight: 209.631

Accurate Mass: 209.024356

Percentage Composition: C 57.30%; H 3.85%; Cl 16.91%; N 6.68%; O 15.26%

Physical Description: Powder

Melting Point: Mp 242-243 dec.°