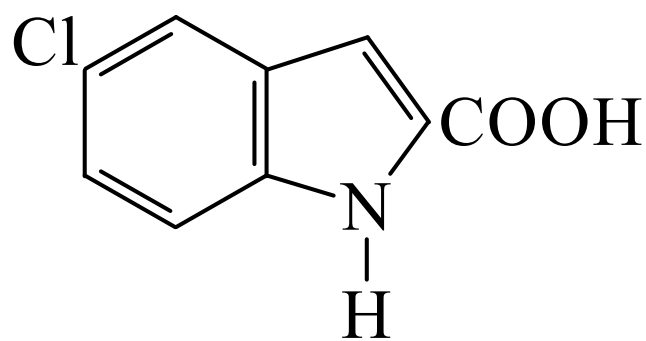




>>Entry Name: 5-Chloro-1*H*-indole-2-carboxylic acid, 9Cl



**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:** C<sub>9</sub>H<sub>6</sub>ClNO<sub>2</sub>

**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<sub>a</sub> 4.75 (50% EtOH aq.)

**Aldrich:** C4780-9

**Sigma:** C5647

>>Derivative: Et ester

**CAS Registry Number:** 4792-67-0

**Molecular Formula:** C<sub>11</sub>H<sub>10</sub>ClNO<sub>2</sub>

**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 (C<sub>6</sub>H<sub>6</sub>/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:** C<sub>9</sub>H<sub>7</sub>ClN<sub>2</sub>O

**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:** C<sub>9</sub>H<sub>8</sub>ClN<sub>3</sub>O

**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:** C<sub>10</sub>H<sub>8</sub>ClNO<sub>2</sub>

**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.°