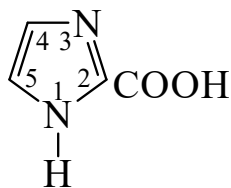




>>Entry Name: **1*H*-Imidazole-2-carboxylic acid**, 9CI



**CAS Registry Number:** 16042-25-4

**Molecular Formula:** C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>O<sub>2</sub>

**Molecular Weight:** 112.088

**Accurate Mass:** 112.027278

**Percentage Composition:** C 42.86%; H 3.60%; N 24.99%; O 28.55%

**Physical Description:** Plates (EtOH aq.)

**Melting Point:** Mp 172-174 (163-164°) dec.°

**Other Data:** Mp dependent on rate of heating

>>Derivative: Me ester

**CAS Registry Number:** 17334-09-7

**Molecular Formula:** C<sub>5</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>

**Molecular Weight:** 126.115

**Accurate Mass:** 126.042928

**Percentage Composition:** C 47.62%; H 4.80%; N 22.21%; O 25.37%

**Physical Description:** Needles (C<sub>6</sub>H<sub>6</sub>/MeOH)

**Melting Point:** Mp 195.5-196°

>>Derivative: Et ester

**CAS Registry Number:** 33543-78-1

**Molecular Formula:** C<sub>6</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>

**Molecular Weight:** 140.141

**Accurate Mass:** 140.058578

**Percentage Composition:** C 51.42%; H 5.75%; N 19.99%; O 22.83%

**Physical Description:** Cryst. (EtOH)

**Melting Point:** Mp 178-179°

>>Derivative: Amide

**CAS Registry Number:** 16093-82-6

**Molecular Formula:** C<sub>4</sub>H<sub>5</sub>N<sub>3</sub>O

**Molecular Weight:** 111.103

**Accurate Mass:** 111.043262

**Percentage Composition:** C 43.24%; H 4.54%; N 37.82%; O 14.40%

**Physical Description:** Needles

**Melting Point:** Mp 295 dec.°

>>Derivative: Nitrile

**Synonym(s):** 2-Cyanoimidazole

**CAS Registry Number:** 31722-49-3

**Molecular Formula:** C<sub>4</sub>H<sub>3</sub>N<sub>3</sub>

**Molecular Weight:** 93.088

**Accurate Mass:** 93.032697

**Percentage Composition:** C 51.61%; H 3.25%; N 45.14%

**Physical Description:** Needles (C<sub>6</sub>H<sub>6</sub>/EtOH)

**Melting Point:** Mp 176-178°

>>Derivative: *N*-Me, Me ester

**CAS Registry Number:** 62366-53-4

**Molecular Formula:** C<sub>6</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>

**Molecular Weight:** 140.141

**Accurate Mass:** 140.058578

**Percentage Composition:** C 51.42%; H 5.75%; N 19.99%; O 22.83%

**Physical Description:** Liq.

**Boiling Point:** Bp<sub>0.1</sub> 80°