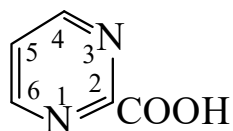




>>Entry Name: 2-Pyrimidinecarboxylic acid, 9CI



**CAS Registry Number:** 31519-62-7

**Molecular Formula:** C<sub>5</sub>H<sub>4</sub>N<sub>2</sub>O<sub>2</sub>

**Molecular Weight:** 124.099

**Accurate Mass:** 124.027278

**Percentage Composition:** C 48.39%; H 3.25%; N 22.57%; O 25.78%

**Physical Description:** Cryst. (H<sub>2</sub>O)

**Melting Point:** Mp 199°

>>Derivative: Me ester

**CAS Registry Number:** 34253-03-7

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

**Molecular Weight:** 138.126

**Accurate Mass:** 138.042928

**Percentage Composition:** C 52.17%; H 4.38%; N 20.28%; O 23.17%

**Physical Description:** Cryst. (H<sub>2</sub>O)

**Melting Point:** Mp 104-105°

>>Derivative: Et ester

**CAS Registry Number:** 42839-08-7

**Molecular Formula:** C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>

**Molecular Weight:** 152.152

**Accurate Mass:** 152.058578

**Percentage Composition:** C 55.26%; H 5.30%; N 18.41%; O 21.03%

**Melting Point:** Mp 64-65°

>>Derivative: Amide

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

**Molecular Weight:** 123.114

**Accurate Mass:** 123.043262

**Percentage Composition:** C 48.78%; H 4.09%; N 34.13%; O 13.00%

**Physical Description:** Cryst. by subl.

**Melting Point:** Mp 167°

**Boiling Point:** Bp<sub>0.01</sub> 140° subl.

>>Derivative: Nitrile

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

**CAS Registry Number:** 14080-23-0

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

**Molecular Weight:** 105.099

**Accurate Mass:** 105.032697

**Percentage Composition:** C 57.14%; H 2.88%; N 39.98%

**Physical Description:** Cryst. by subl.

**Melting Point:** Mp 42-44°

**Boiling Point:** Bp<sub>0.01</sub> 40° subl.

#### References:

Holland, A., *Chem. Ind. (London)*, 1954, 786, (*synth*)

Robba, M., *Ann. Chim. (Paris)*, 1960, **5**, 351, (*derivs*)

Hu, W.-X. *et al.*, *Org. Prep. Proced. Int.*, 1994, **26**, 685, (*nitrile*)