



>>Entry Name: 4-Amino-1*H*-pyrazole-3-carboxylic acid, 9CI

Synonym(s): 4-Amino-1*H*-pyrazole-5-carboxylic acid, 9CI

**Molecular Formula:** C<sub>4</sub>H<sub>5</sub>N<sub>3</sub>O<sub>2</sub>

**Molecular Weight:** 127.102

**Accurate Mass:** 127.038177

**Percentage Composition:** C 37.80%; H 3.96%; N 33.06%; O 25.18%

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

**Melting Point:** Mp 212.5 dec.°

**Other Data:** 1-Unsubstituted derivs. tautomeric with the 5-carboxylic acid

>>Derivative: Et ester

**CAS Registry Number:** 55904-61-5

**Molecular Formula:** C<sub>6</sub>H<sub>9</sub>N<sub>3</sub>O<sub>2</sub>

**Molecular Weight:** 155.156

**Accurate Mass:** 155.069477

**Percentage Composition:** C 46.45%; H 5.85%; N 27.08%; O 20.62%

**Melting Point:** Mp 90-92°

>>Derivative: Amide

**CAS Registry Number:** 67221-50-5

**Molecular Formula:** C<sub>4</sub>H<sub>6</sub>N<sub>4</sub>O

**Molecular Weight:** 126.118

**Accurate Mass:** 126.054161

**Percentage Composition:** C 38.09%; H 4.80%; N 44.42%; O 12.69%

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

**Melting Point:** Mp 181-182°

>>Derivative: Nitrile

Synonym(s): 4-Amino-3-cyanopyrazole

**CAS Registry Number:** 68703-67-3

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

**Molecular Weight:** 108.102

**Accurate Mass:** 108.043596

**Percentage Composition:** C 44.44%; H 3.73%; N 51.83%

**Physical Description:** Prisms (H<sub>2</sub>O or by subl.)

**Melting Point:** Mp 143.5-145°

>>Variant: 1*H*-form

**Molecular Formula:** C<sub>4</sub>H<sub>5</sub>N<sub>3</sub>O<sub>2</sub>

**Molecular Weight:** 127.102

**Accurate Mass:** 127.038177

**Percentage Composition:** C 37.80%; H 3.96%; N 33.06%; O 25.18%

>>Derivative: 1-Ph

**CAS Registry Number:** 64299-26-9

**Molecular Formula:** C<sub>10</sub>H<sub>9</sub>N<sub>3</sub>O<sub>2</sub>

**Molecular Weight:** 203.2

**Accurate Mass:** 203.069477

**Percentage Composition:** C 59.11%; H 4.46%; N 20.68%; O 15.75%

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

**Melting Point:** Mp 223-225°