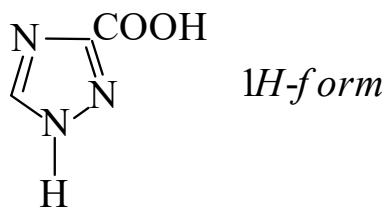




>>Entry Name: 1,2,4-Triazole-3(5)-carboxylic acid, 9CI



**CAS Registry Number:** 4928-87-4

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

**Molecular Weight:** 113.076

**Accurate Mass:** 113.022527

**Percentage Composition:** C 31.87%; H 2.67%; N 37.16%; O 28.30%

**Physical Description:** Fine needles

**Melting Point:** Mp 140 dec.° (gas evol.)

**Rare Chemicals Library:** S1109-7

>>Derivative: Me ester

**CAS Registry Number:** 4928-88-5

**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:** Cryst. (EtOAc)

**Melting Point:** Mp 184 dec.°. Mp 200-201°

>>Derivative: Et ester

**CAS Registry Number:** 64922-04-9

**Molecular Formula:** C<sub>5</sub>H<sub>7</sub>N<sub>3</sub>O<sub>2</sub>

**Molecular Weight:** 141.129

**Accurate Mass:** 141.053827

**Percentage Composition:** C 42.55%; H 5.00%; N 29.77%; O 22.67%

**Physical Description:** Plates (EtOH)

**Melting Point:** Mp 169-171°. Mp 178°

>>Derivative: Amide

**CAS Registry Number:** 3641-08-5

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

**Molecular Weight:** 112.091

**Accurate Mass:** 112.038511

**Percentage Composition:** C 32.15%; H 3.60%; N 49.98%; O 14.27%

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

**Melting Point:** Mp 312°

>>Derivative: Hydrazide

**CAS Registry Number:** 21732-98-9

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

**Molecular Weight:** 127.105

**Accurate Mass:** 127.04941

**Percentage Composition:** C 28.35%; H 3.96%; N 55.10%; O 12.59%

**Physical Description:** Cryst.

**Melting Point:** Mp 277-278°

>>Derivative: Nitrile

**Synonym(s):** 3-Cyano-1,2,4-triazole

**CAS Registry Number:** 3641-10-9

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

**Molecular Weight:** 94.076

**Accurate Mass:** 94.027946

**Percentage Composition:** C 38.30%; H 2.14%; N 59.56%

**Physical Description:** Cryst.

**Melting Point:** Mp 187°