



**Aldrich:** 15304-4  
**Fluka:** 9338

>>Derivative:  $N^3$ -Ac, Et ester

**CAS Registry Number:** 15250-36-9  
**Molecular Formula:**  $C_8H_{11}N_3O_3$   
**Molecular Weight:** 197.193  
**Accurate Mass:** 197.080042  
**Percentage Composition:** C 48.73%; H 5.62%; N 21.31%; O 24.34%  
**Physical Description:** Cryst. (EtOH aq.)  
**Melting Point:** Mp 200°

>>Derivative:  $N^3$ -Ac, nitrile

**Molecular Formula:**  $C_6H_6N_4O$   
**Molecular Weight:** 150.14  
**Accurate Mass:** 150.054161  
**Percentage Composition:** C 48.00%; H 4.03%; N 37.32%; O 10.66%  
**Physical Description:** Cryst. ( $H_2O$ )  
**Melting Point:** Mp 221-222°

>>Derivative:  $N^1$ -Phenyl, Et ester

**CAS Registry Number:** 16078-71-0  
**Molecular Formula:**  $C_{12}H_{13}N_3O_2$   
**Molecular Weight:** 231.254  
**Accurate Mass:** 231.100777  
**Percentage Composition:** C 62.33%; H 5.67%; N 18.17%; O 13.84%  
**Melting Point:** Mp 98-100°  
**Aldrich:** 37944-1  
**Rare Chemicals Library:** S34808-2

>>Variant: 1*H*-form

**Molecular Formula:**  $C_4H_5N_3O_2$   
**Molecular Weight:** 127.102  
**Accurate Mass:** 127.038177  
**Percentage Composition:** C 37.80%; H 3.96%; N 33.06%; O 25.18%

>>Derivative: 1-Me, Et ester

**CAS Registry Number:** 21230-43-3  
**Molecular Formula:**  $C_7H_{11}N_3O_2$   
**Molecular Weight:** 169.183  
**Accurate Mass:** 169.085127  
**Percentage Composition:** C 49.70%; H 6.55%; N 24.84%; O 18.91%  
**Physical Description:** Cryst. ( $CH_2Cl_2$ /petrol)  
**Melting Point:** Mp 92-93°

>>Derivative: 1-Me, nitrile

**Synonym(s):** 3-Amino-1-methyl-4-pyrazolecarbonitrile, 9Cl. 3-Amino-4-cyano-1-methylpyrazole

**CAS Registry Number:** 21230-50-2  
**Molecular Formula:**  $C_5H_6N_4$   
**Molecular Weight:** 122.129  
**Accurate Mass:** 122.059246  
**Percentage Composition:** C 49.17%; H 4.95%; N 45.88%  
**Physical Description:** Cryst. ( $CH_2Cl_2$ /petrol or EtOH)  
**Melting Point:** Mp 135-136° (126°)