



Accurate Mass: 108.043596
Percentage Composition: C 44.44%; H 3.73%; N 51.83%
Physical Description: Cryst. (H₂O)
Melting Point: Mp 174-175°
Aldrich: 15304-4
Fluka: 9338

>>Derivative: *N*³-Ac, Et ester

CAS Registry Number: 15250-36-9
Molecular Formula: C₈H₁₁N₃O₃
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: C₆H₆N₄O
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. (H₂O)
Melting Point: Mp 221-222°

>>Derivative: *N*¹-Phenyl, Et ester

CAS Registry Number: 16078-71-0
Molecular Formula: C₁₂H₁₃N₃O₂
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: C₄H₅N₃O₂
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: C₇H₁₁N₃O₂
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. (CH₂Cl₂/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: C₅H₆N₄
Molecular Weight: 122.129
Accurate Mass: 122.059246
Percentage Composition: C 49.17%; H 4.95%; N 45.88%
Physical Description: Cryst. (CH₂Cl₂/petrol or EtOH)
Melting Point: Mp 135-136° (126°)