



>>Derivative: 1-Benzyl, Et ester

CAS Registry Number: 21377-11-7

Molecular Formula: C₁₃H₁₅N₃O₂

Molecular Weight: 245.28

Accurate Mass: 245.116427

Percentage Composition: C 63.66%; H 6.16%; N 17.13%; O 13.05%

Physical Description: Needles (EtOH)

Melting Point: Mp 115-116°

>>Variant: 2*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: 2-Ac, Et ester

CAS Registry Number: 14333-81-4

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 74-76°

>>Derivative: 2-Me, Et ester

CAS Registry Number: 31037-02-2

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. (C₆H₆/petrol)

Melting Point: Mp 101°

>>Derivative: 2-Me, amide

CAS Registry Number: 18213-75-7

Molecular Formula: C₅H₈N₄O

Molecular Weight: 140.144

Accurate Mass: 140.069811

Percentage Composition: C 42.85%; H 5.75%; N 39.98%; O 11.42%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 237-239°

>>Derivative: 2-Me, nitrile

Synonym(s): 5-Amino-4-cyano-1-methylpyrazole

CAS Registry Number: 5334-41-8

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. (H₂O)

Melting Point: Mp 222-223°

>>Derivative: 2-Me, *N*³-Ac

CAS Registry Number: 92914-76-6

Molecular Formula: C₇H₉N₃O₃

Molecular Weight: 183.166

Accurate Mass: 183.064392

Percentage Composition: C 45.90%; H 4.95%; N 22.94%; O 26.20%

Physical Description: Cryst. (Me₂CO aq.)

Melting Point: Mp 194.5-195°