



Melting Point: Mp 88-89°

Boiling Point: Bp₂₂ 210°

>>Derivative: 1-Ph, *tert*-butyl ester

CAS Registry Number: 2055-51-8

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%

Melting Point: Mp 100°

>>Derivative: 1-Ph, amide

CAS Registry Number: 2055-53-0

Molecular Formula: C₉H₈N₄O

Molecular Weight: 188.188

Accurate Mass: 188.069811

Percentage Composition: C 57.44%; H 4.28%; N 29.77%; O 8.50%

Melting Point: Mp 229-231°

>>Derivative: 1-Ph, nitrile

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

CAS Registry Number: 61456-87-9

Molecular Formula: C₉H₆N₄

Molecular Weight: 170.173

Accurate Mass: 170.059246

Percentage Composition: C 63.52%; H 3.55%; N 32.92%

Physical Description: Needles (CCl₄)

Melting Point: Mp 123°

>>Derivative: 1-Benzyl, Me ester

CAS Registry Number: 76003-76-4

Molecular Formula: C₁₁H₁₁N₃O₂

Molecular Weight: 217.227

Accurate Mass: 217.085127

Percentage Composition: C 60.82%; H 5.10%; N 19.34%; O 14.73%

Melting Point: Mp 104°

>>Derivative: 1-Hydroxy, Et ester

CAS Registry Number: 137156-41-3

Molecular Formula: C₅H₇N₃O₃

Molecular Weight: 157.129

Accurate Mass: 157.048742

Percentage Composition: C 38.22%; H 4.49%; N 26.74%; O 30.55%

Use/Importance: Coupling reagent for peptide synth.

Melting Point: Mp 110-112°

>>Variant: 2*H*-form

Molecular Formula: C₃H₃N₃O₂

Molecular Weight: 113.076

Accurate Mass: 113.022527

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

>>Derivative: 2-Me

CAS Registry Number: 63062-88-4

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%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 141-142°