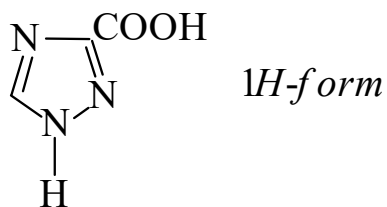




>>Entry Name: 1,2,4-Triazole-3(5)-carboxylic acid, 9CI



CAS Registry Number: 4928-87-4

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%

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: 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. (EtOAc)

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

>>Derivative: Et ester

CAS Registry Number: 64922-04-9

Molecular Formula: C₅H₇N₃O₂

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: C₃H₄N₄O

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. (H₂O)

Melting Point: Mp 312°

>>Derivative: Hydrazide

CAS Registry Number: 21732-98-9

Molecular Formula: C₃H₅N₅O

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: C₃H₂N₄

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°