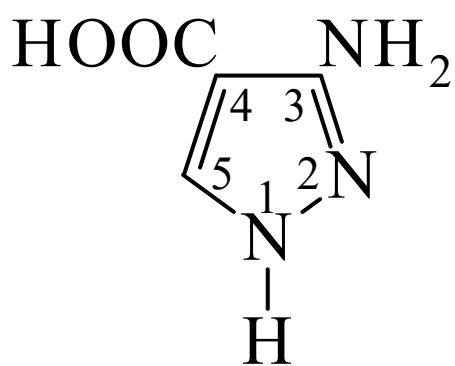




>>Entry Name: 3(5)-Amino-1*H*-pyrazole-4-carboxylic acid, 9CI



CAS Registry Number: 41680-34-6

Related CAS Registry Numbers(s): 5334-31-6 36442-32-7

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. (H₂O)

Melting Point: Mp 120 dec.°

Aldrich: A7740-7

>>Derivative: Me ester

CAS Registry Number: 29097-00-5

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%

Melting Point: Mp 135-136°

>>Derivative: Et ester

CAS Registry Number: 6994-25-8

Molecular Formula: C₆H₉N₃O₂

Molecular Weight: 155.156

Accurate Mass: 155.069477

Percentage Composition: C 46.45%; H 5.85%; N 27.08%; O 20.62%

Physical Description: Cryst. (H₂O or Et₂O)

Melting Point: Mp 102-103°

Aldrich: A4500-9

>>Derivative: Amide

CAS Registry Number: 52906-16-8

Molecular Formula: C₄H₆N₄O

Molecular Weight: 126.118

Accurate Mass: 126.054161

Percentage Composition: C 38.09%; H 4.80%; N 44.42%; O 12.69%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 222-225°

>>Derivative: Anilide

CAS Registry Number: 90399-89-6

Molecular Formula: C₁₀H₁₀N₄O

Molecular Weight: 202.215

Accurate Mass: 202.085461

Percentage Composition: C 59.40%; H 4.98%; N 27.71%; O 7.91%

Melting Point: Mp 198-199°