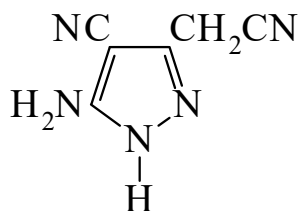




>>Entry Name: 5-Amino-4-cyano-1*H*-pyrazole-3-acetonitrile, 9Cl

Synonym(s): 5-Amino-4-cyano-3-cyanomethylpyrazole



CAS Registry Number: 54711-21-6

Molecular Formula: C₆H₅N₅

Molecular Weight: 147.139

Accurate Mass: 147.054495

Percentage Composition: C 48.98%; H 3.42%; N 47.60%

Physical Description: Needles (H₂O)

Melting Point: Mp 197-198°

Rare Chemicals Library: S34097-9

Other: PB A20150

>>Derivative: *N*⁵-Ac

Molecular Formula: C₈H₇N₅O

Molecular Weight: 189.176

Accurate Mass: 189.06506

Percentage Composition: C 50.79%; H 3.73%; N 37.02%; O 8.46%

Melting Point: Mp 276° (AcOH)

>>Derivative: 1-Me

CAS Registry Number: 53871-49-1

Molecular Formula: C₇H₇N₅

Molecular Weight: 161.166

Accurate Mass: 161.070145

Percentage Composition: C 52.17%; H 4.38%; N 43.45%

Physical Description: Needles (H₂O)

Melting Point: Mp 178°

>>Derivative: 1-Ph

CAS Registry Number: 7152-40-1

Molecular Formula: C₁₂H₉N₅

Molecular Weight: 223.237

Accurate Mass: 223.085795

Percentage Composition: C 64.56%; H 4.06%; N 31.37%

Physical Description: Needles (EtOH)

Melting Point: Mp 166°

Rare Chemicals Library: S45313-7

>>Derivative: 1-Ph; *N*⁵-Ac

Molecular Formula: C₁₄H₁₁N₅O

Molecular Weight: 265.274

Accurate Mass: 265.09636

Percentage Composition: C 63.39%; H 4.18%; N 26.40%; O 6.03%

Melting Point: Mp 168°

References:

Taylor, E.C. *et al.*, *J.A.C.S.*, 1959, **81**, 2452, (*synth, derivs*)