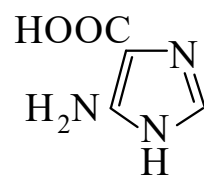




>>Entry Name: 5-Amino-1*H*-imidazole-4-carboxylic acid, 9CI

Synonym(s): 5-Amino-4-glyoxalinecarboxylic acid. 4-Amino-1*H*-imidazole-5-carboxylic acid



CAS Registry Number: 4919-04-4

Related CAS Registry Numbers(s): 60104-30-5

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%

>>Derivative: Et ester

CAS Registry Number: 21190-16-9

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: Needles (EtOAc/EtOH)

Melting Point: Mp 180-181°

>>Derivative: Et ester; hydrochloride

Melting Point: Mp 190-191°

>>Derivative: Et ester, *N*-Ac

CAS Registry Number: 21189-96-8

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)

Melting Point: Mp 217-218°

>>Derivative: Et ester, *N*-benzoyl

CAS Registry Number: 21190-00-1

Molecular Formula: C₁₃H₁₃N₃O₃

Molecular Weight: 259.264

Accurate Mass: 259.095692

Percentage Composition: C 60.23%; H 5.05%; N 16.21%; O 18.51%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 188-189°

>>Derivative: Amide

CAS Registry Number: 360-97-4

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%

Use/Importance: Intermed. in purine biosynth.

Physical Description: Cryst. (EtOH)

Melting Point: Mp 170-171°

Hazard & Toxicity: Exp. tumourigenic data