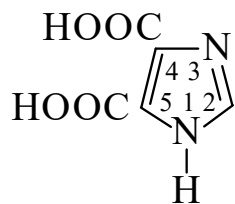




>>Entry Name: 1*H*-Imidazole-4,5-dicarboxylic acid, 9CI



CAS Registry Number: 570-22-9

Molecular Formula: C₅H₄N₂O₄

Molecular Weight: 156.098

Accurate Mass: 156.017108

Percentage Composition: C 38.47%; H 2.58%; N 17.95%; O 41.00%

Melting Point: Mp 288 dec.°

pKa Value: p*K*_{a1} 2.93; p*K*_{a2} 8.04

Hazard & Toxicity: LD₅₀ (mus, ipr) 1800 mg/kg

Aldrich: 24611-5

Fluka: 56757

Rare Chemicals Library: S56643-8

>>Derivative: Di-Me ester

CAS Registry Number: 3304-70-9

Molecular Formula: C₇H₈N₂O₄

Molecular Weight: 184.151

Accurate Mass: 184.048408

Percentage Composition: C 45.66%; H 4.38%; N 15.21%; O 34.75%

Melting Point: Mp 200-203°

Rare Chemicals Library: S2201-3

>>Derivative: Di-Et ester

CAS Registry Number: 1080-79-1

Molecular Formula: C₉H₁₂N₂O₄

Molecular Weight: 212.205

Accurate Mass: 212.079708

Percentage Composition: C 50.94%; H 5.70%; N 13.20%; O 30.16%

Melting Point: Mp 151-152°

>>Derivative: Diamide

>>Derivative: Dihydrazide

CAS Registry Number: 5423-20-1

Molecular Formula: C₅H₈N₆O₂

Molecular Weight: 184.157

Accurate Mass: 184.070874

Percentage Composition: C 32.61%; H 4.38%; N 45.64%; O 17.38%

Melting Point: Mp 375°

>>Derivative: Dinitrile

Synonym(s): 4,5-Dicyanoimidazole

CAS Registry Number: 1122-28-7

Molecular Formula: C₃H₂N₄

Molecular Weight: 118.098

Accurate Mass: 118.027946

Percentage Composition: C 50.85%; H 1.71%; N 47.44%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 172-173°

Aldrich: 32413-2