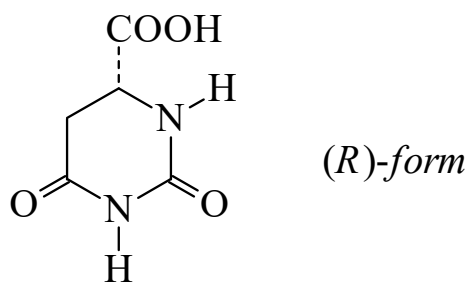




>>>Entry Name: Hexahydro-2,6-dioxo-4-pyrimidinecarboxylic acid, 9CI

Synonym(s): Dihydroorotic acid. Hydroorotic acid



CAS Registry Number: 155-54-4

Molecular Formula: $C_5H_6N_2O_4$

Molecular Weight: 158.113

Accurate Mass: 158.032758

Percentage Composition: C 37.98%; H 3.82%; N 17.72%; O 40.48%

Rare Chemicals Library: S94164-6

>>>Variant: (R)-form

Synonym(s): D-form

CAS Registry Number: 5988-53-4

Molecular Formula: $C_5H_6N_2O_4$

Molecular Weight: 158.113

Accurate Mass: 158.032758

Percentage Composition: C 37.98%; H 3.82%; N 17.72%; O 40.48%

Melting Point: Mp 266 dec.°

Optical Rotation: $[\alpha]_D^{26} -34.29$ (c, 2.49 in 2.5% $NaHCO_3$ aq.)

>>>Derivative: 1-Me

Melting Point: Mp 221-222°

Optical Rotation: $[\alpha]_D -37$ (c, 0.5 in DMF)

>>>Derivative: 3-Et

Melting Point: Mp 160-161°

Optical Rotation: $[\alpha]_D -42.6$ (c, 0.5 in DMF)

>>>Variant: (S)-form

Synonym(s): L-form

CAS Registry Number: 5988-19-2

Molecular Formula: $C_5H_6N_2O_4$

Molecular Weight: 158.113

Accurate Mass: 158.032758

Percentage Composition: C 37.98%; H 3.82%; N 17.72%; O 40.48%

Use/Importance: Key intermed. in pyrimidine biosynth. from aspartic acid

Melting Point: Mp 266 dec.°

Optical Rotation: $[\alpha]_D^{25} +33.2$ (c, 1.99 in 1% $NaHCO_3$ aq.)

Aldrich: 28559-5

Sigma: D7128

>>>Derivative: 1-Me

Molecular Formula: $C_6H_8N_2O_4$

Molecular Weight: 172.14

Accurate Mass: 172.048408

Percentage Composition: C 41.86%; H 4.68%; N 16.27%; O 37.18%

Melting Point: Mp 219-221°

Optical Rotation: $[\alpha]_D +37.5$ (c, 0.5 in DMF)