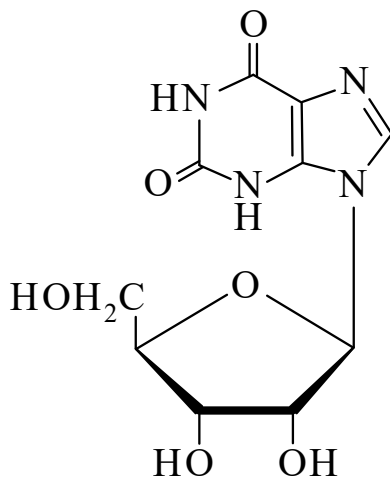




>>Entry Name: Xanthosine, 8Cl

Synonym(s): 3,9-Dihydro-9-β-D-ribofuranosyl-1*H*-purine-2,6-dione, 9Cl. 9-β-D-Ribofuranosylxanthine



CAS Registry Number: 146-80-5

Related CAS Registry Numbers(s): 5968-90-1

Molecular Formula: C₁₀H₁₂N₄O₆

Molecular Weight: 284.228

Accurate Mass: 284.075686

Percentage Composition: C 42.26%; H 4.26%; N 19.71%; O 33.77%

Physical Description: Prismatic cryst. (H₂O)

Optical Rotation: $[\alpha]_D^{30} -51.2$ (c, 8.0 in 0.3*M* NaOH)

Solubility: Spar. sol. cold H₂O; v. sol. hot H₂O

pKa Value: p*K*_{a1} 5.67; p*K*_{a3} 12.85 (25°)

Other Data: λ_{max} 253 nm (ε 8 790) (H₂O). Dec. on heating with no distinct melting range

>>Derivative: 3'-Phosphate

Synonym(s): 3'-Xanthylic acid, 9Cl, 8Cl

CAS Registry Number: 21089-32-7

Molecular Formula: C₁₀H₁₃N₄O₉P

Molecular Weight: 364.208

Accurate Mass: 364.042018

Percentage Composition: C 32.98%; H 3.60%; N 15.38%; O 39.54%; P 8.50%

Melting Point: Mp 200° (as brucine salt)

Optical Rotation: $[\alpha]_D^{20} -61.66$ (c, 5.0 in NaOH)

>>Derivative: 5'-Phosphate

Synonym(s): Xanthosine 5'-(dihydrogen phosphate), 9Cl. 5'-Xanthylic acid, 8Cl. Xanthosine monophosphate. Xanthosine 5'-phosphate. XMP

CAS Registry Number: 523-98-8

Extra CAS Registry Numbers(s): 25899-70-1

Molecular Formula: C₁₀H₁₃N₄O₉P

Molecular Weight: 364.208

Accurate Mass: 364.042018

Percentage Composition: C 32.98%; H 3.60%; N 15.38%; O 39.54%; P 8.50%

Use/Importance: Inhibitor of isoforms I and II of human inosine 5'-monophosphate dehydrogenase

Physical Description: No phys. props. reported

>>Derivative: 5'-Triphosphate

CAS Registry Number: 6253-56-1

Extra CAS Registry Numbers(s): 50801-64-4 90011-94-2

Molecular Formula: C₁₀H₁₅N₄O₁₅P₃

Molecular Weight: 524.168

Accurate Mass: 523.974682

Percentage Composition: C 22.91%; H 2.88%; N 10.69%; O 45.79%; P 17.73%

Physical Description: No phys. props. reported