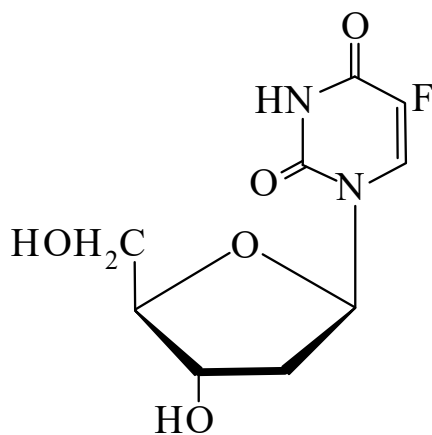




>>Entry Name: **2'-Deoxy-5-fluorouridine**, 9Cl, 8Cl

Synonym(s): 1-(2-Deoxy-β-D-ribofuranosyl)-5-fluorouracil. **Floxuridine**, INN, USAN. Fluoruridinideoxyribose. FUDR. NSC 27640. WR 138720



CAS Registry Number: 50-91-9

Molecular Formula: C₉H₁₁FN₂O₅

Molecular Weight: 246.195

Accurate Mass: 246.065201

Percentage Composition: C 43.91%; H 4.50%; F 7.72%; N 11.38%; O 32.49%

Use/Importance: DNA synthesis inhibitor; antineoplastic agent used in treatment of malignant neoplasms of liver and gastrointestinal tract. Nucleoside transporter substrate

Physical Description: Cryst. (butyl acetate)

Melting Point: Mp 150-151° (145°)

Optical Rotation: [α]_D +37 (H₂O). [α]_D +48.6 (DMF)

Calculated Log P Data: Log P -1.96 (calc)

Other Data: λ_{max} 268 (ε 7 570) (pH 7.2), 270 nm (6 480) (pH 14)

Hazard & Toxicity: LD₅₀ (rat, orl) 215 mg/kg. Exp. reprod. and teratogenic effects. Human systemic effects when used therapeutically

Aldrich: 85665-7

Fluka: 46875

Sigma: F0503

>>Derivative: 3'-Ac

Molecular Formula: C₁₁H₁₃FN₂O₆

Molecular Weight: 288.232

Accurate Mass: 288.075766

Percentage Composition: C 45.84%; H 4.55%; F 6.59%; N 9.72%; O 33.31%

Melting Point: Mp 200-201°

>>Derivative: 5'-Ac

Molecular Formula: C₁₁H₁₃FN₂O₆

Molecular Weight: 288.232

Accurate Mass: 288.075766

Percentage Composition: C 45.84%; H 4.55%; F 6.59%; N 9.72%; O 33.31%

Melting Point: Mp 146°

>>Derivative: 3'-Ac, 5'-mesyl

CAS Registry Number: 27095-26-7

Molecular Formula: C₁₂H₁₅FN₂O₈S

Molecular Weight: 366.323

Accurate Mass: 366.053316

Percentage Composition: C 39.35%; H 4.13%; F 5.19%; N 7.65%; O 34.94%; S 8.75%

Melting Point: Mp 134-134.5°

>>Derivative: 3'-Mesyl

CAS Registry Number: 1549-81-1

Molecular Formula: C₁₀H₁₃FN₂O₇S

Molecular Weight: 324.286

Accurate Mass: 324.042751

Percentage Composition: C 37.04%; H 4.04%; F 5.86%; N 8.64%; O 34.54%; S 9.89%

Melting Point: Mp 158 (161-162°) dec.°