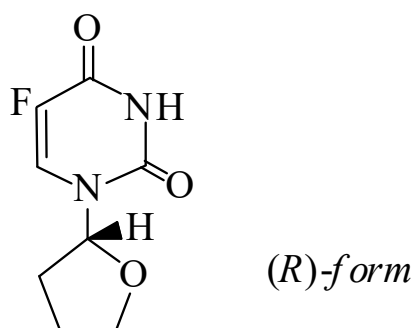




>>Entry Name: Tegafur, BAN, INN, USAN

Synonym(s): 5-Fluoro-1-(tetrahydro-2-furanyl)-2,4(1*H*,3*H*)pyrimidinedione, 9CI. 5-Fluoro-1-(tetrahydro-2-furyl)uracil. Ftorafur. Furflucil. NSC 148958. Many other names



CAS Registry Number: 17902-23-7

Related CAS Registry Numbers(s): 74578-38-4

Molecular Formula: C₈H₉FN₂O₃

Molecular Weight: 200.169

Accurate Mass: 200.059721

Percentage Composition: C 48.00%; H 4.53%; F 9.49%; N 13.99%; O 23.98%

Use/Importance: Antineoplastic agent

Calculated Log P Data: Log P 0.25 (calc)

Hazard & Toxicity: LD₅₀ (rat, orl) 930 mg/kg. Exp. reprod. and teratogenic effects

Aldrich: 20915-5

Sigma: F6256

>>Variant: (*R*)-form

CAS Registry Number: 37076-68-9

Molecular Formula: C₈H₉FN₂O₃

Molecular Weight: 200.169

Accurate Mass: 200.059721

Percentage Composition: C 48.00%; H 4.53%; F 9.49%; N 13.99%; O 23.98%

Melting Point: Mp 174-175.5°

Optical Rotation: [α]_D²³+70 (c, 0.5 in CHCl₃)

>>Variant: (*S*)-form

CAS Registry Number: 55374-30-6

Molecular Formula: C₈H₉FN₂O₃

Molecular Weight: 200.169

Accurate Mass: 200.059721

Percentage Composition: C 48.00%; H 4.53%; F 9.49%; N 13.99%; O 23.98%

Melting Point: Mp 175-177°

Optical Rotation: [α]_D²³-70 (c, 0.5 in CHCl₃)

>>Variant: (±)-form

CAS Registry Number: 65732-47-0

Molecular Formula: C₈H₉FN₂O₃

Molecular Weight: 200.169

Accurate Mass: 200.059721

Percentage Composition: C 48.00%; H 4.53%; F 9.49%; N 13.99%; O 23.98%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 165-166°. Mp 172-173°

Other Data: Component of UFT. 4-Polymorphs. characterised

References: