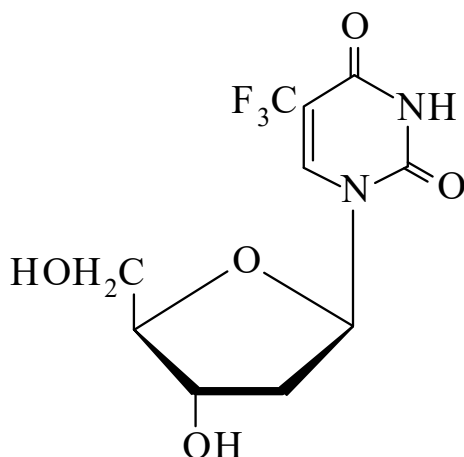




>>Entry Name: 2'-Deoxy-5-(trifluoromethyl)uridine, 8Cl

Synonym(s):  $\alpha,\alpha,\alpha$ -Trifluorothymidine, 9Cl. **Trifluridine**, INN, USAN. Bephen. Thilol. Triherpine. Viromidin. Viroptic. F<sub>3</sub>T. NSC 75520



CAS Registry Number: 70-00-8

**Molecular Formula:** C<sub>10</sub>H<sub>11</sub>F<sub>3</sub>N<sub>2</sub>O<sub>5</sub>

**Molecular Weight:** 296.203

**Accurate Mass:** 296.062007

**Percentage Composition:** C 40.55%; H 3.74%; F 19.24%; N 9.46%; O 27.01%

**Use/Importance:** Ophthalmic antiviral agent. Used in treatment of herpetic keratitis

**Physical Description:** Cryst. (EtOAc)

**Melting Point:** Mp 186-189°

**Optical Rotation:**  $[\alpha]_D^{20} +46.9$  (H<sub>2</sub>O)

**Calculated Log P Data:** Log P -0.97 (calc)

**Hazard & Toxicity:** Mutagenic props. LD<sub>50</sub> (mus, ipr) 1931 mg/kg

**Aldrich:** 32939-8

**Sigma:** T2255

#### References:

*Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **3**, 376A, (nmr)

Heidelberger, C. *et al.*, *J.A.C.S.*, 1962, **84**, 3597, (synth)

Ryan, K.J. *et al.*, *J.O.C.*, 1966, **31**, 1181, (synth)

Cushley, R.J. *et al.*, *J.A.C.S.*, 1968, **90**, 709, (nmr)

Heidelberger, C. *et al.*, *Pharmacol. Ther.*, 1979, **6**, 427, (rev, pharmacol)

Kobayashi, Y. *et al.*, *J.C.S. Perkin 1*, 1980, 2755, (synth)

Carmine, A.A. *et al.*, *Drugs*, 1982, **23**, 329, (rev, pharmacol)

Schwarz, B. *et al.*, *J. Prakt. Chem.*, 1984, **326**, 985, (synth)

Riegel, M.R. *et al.*, *J. Chromatogr.*, 1991, **568**, 467, (hplc)

Tandon, M. *et al.*, *Biochem. Pharmacol.*, 1992, **44**, 2223; 1994, **48**, 1033, (metab)

Harris, D.J., *N. Engl. J. Med.*, 1994, **331**, 481, (use)

*Martindale, The Extra Pharmacopoeia*, 31st edn., Pharmaceutical Press, 1996, 662

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, TKH325