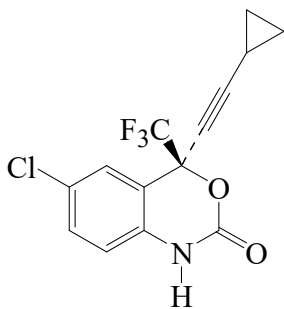




>>Entry Name: Efavirenz, INN

Synonym(s): 6-Chloro-4-(cyclopropylethynyl)-1,4-dihydro-4-(trifluoromethyl)-2H-3,1-benzoxazin-2-one, 9Cl. Sustiva. DMP 266. L 743726



CAS Registry Number: 177530-93-7

Related CAS Registry Numbers(s): 154635-17-3 154801-74-8

Type of Compound Code(s): XA1625 XA2400

Molecular Formula: C₁₄H₉ClF₃NO₂

Molecular Weight: 315.679

Accurate Mass: 315.02739

Percentage Composition: C 53.27%; H 2.87%; Cl 11.23%; F 18.05%; N 4.44%; O 10.14%

Biological Use/Importance: HIV-1 reverse transcriptase inhibitor. Antiviral agent. Used in combination with other antiretroviral agents

Development Status: Launched in the US (1998)

pK_a Value: pK_a 10.2

>>Variant: (S)-form

CAS Registry Number: 154598-52-4

Molecular Formula: C₁₄H₉ClF₃NO₂

Molecular Weight: 315.679

Accurate Mass: 315.02739

Percentage Composition: C 53.27%; H 2.87%; Cl 11.23%; F 18.05%; N 4.44%; O 10.14%

Physical Description: Cryst. (hexane)

Melting Point: Mp 131-132°

Optical Rotation: [α]_D²⁰ -84.7 (c, 0.5 in CHCl₃)

Other Data: Pharmacol. active isomer

References:

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