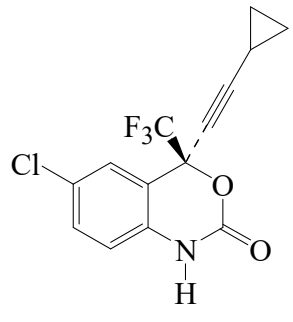
>>**Entry Name: Efavirenz,** INN
Synonym(s): 6-Chloro-4-(cyclopropylethynyl)-1,4-dihydro-4-(trifluoromethyl)-2*H*-3,1-benzoxazin-2-one, 9CI. Sustiva. DMP 266. L 743726



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: $C_{14}H_9ClF_3NO_2$
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)
pKa Value: pK_a 10.2

>>**Variant:** (*S*)-form

CAS Registry Number: 154598-52-4
Molecular Formula: $C_{14}H_9ClF_3NO_2$
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: $[\alpha]_D^{20}$–84.7 (c, 0.5 in $CHCl_3$)
Other Data: Pharmacol. active isomer

References:

Eur. Pat., 1994, *Merck*, 582 455; *CA*, **120**, 270428c, *(synth, pharmacol, isomers)*
Young, S.D. *et al.*, *Antimicrob. Agents Chemother.*, 1995, **39**, 2602-2605, *(pharmacol)*
Pat. Coop. Treaty (WIPO), 1995, *Merck*, 95 20 389; *CA*, **123**, 246802m, *(synth, pharmacol)*
Thompson, A.S. *et al.*, *Tet. Lett.*, 1995, **36**, 8937-8940, *(synth)*
Winslow, D.L. *et al.*, *AIDS*, 1996, **10**, 1205-1209, *(pharmacol)*
Radesca, L.A. *et al.*, *Synth. Commun.*, 1997, **27**, 4373-4384, *(synth)*
Adkins, J.C. *et al.*, *Drugs*, 1998, **56**, 1055-1064, *(rev)*
Graul, A. *et al.*, *Drugs of the Future*, 1998, **23**, 133-141, *(rev, pharmacol)*
Pierce, M.E. *et al.*, *J.O.C.*, 1998, **63**, 8536-8543, *(synth)*
Pedersen, O.S. *et al.*, *Synthesis*, 2000, 479-495, *(rev)*

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