

Product Name : Darunavir ethanolate

Synonyms : TMC-114; UIC-94017

Cat No. : M15408

CAS Number : 635728-49-3

Molecular Formula : C₂₉H₄₃N₃O₈S

Formula Weight : 593.73

Chemical Name : Carbamic acid, N-[(1S,2R)-3-[[[4-aminophenyl)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-, (3R,3aS,6aR)-hexahydrofuro[2,3-b]furan-3-yl ester, compd. with ethanol (1:1)

Description : A potent, selective HIV-1 protease inhibitor that is extremely potent against laboratory HIV-1 strains and primary clinical isolates with IC₅₀ of 3 nM, IC₉₀ of 9 nM; blockes the infectivity and replication of HIV-1(NL4-3) variants with IC₅₀ of 3-29 nM, also potent against multi-PI-resistant clinical HIV-1 variants isolated from patients; used to treat and prevent HIV/AIDS. HIV Infection Approved

Pathway : Microbiology/Virology

Target : HIV

Receptor : WTHIV-1protease

Solubility : 10 mM in DMSO

SMILES : CCO.CC(C)CN(C[C@H]([C@H](CC1=CC=CC=C1)NC(=O)O[C@H]2CO[C@@H]3[C@H]2CCO3)O)S(=O)(=O)C4=CC=C(C=C4)N

Storage : (-20°C)

Stability : ≥ 2 years

Reference :

1. Surleraux DL, et al. J Med Chem. 2005 Mar 24;48(6):1813-22. | 2. Koh Y, et al. Antimicrob Agents Chemother. 2003 Oct;47(10):3123-9. | 3. King NM, et al. J Virol. 2004 Nov;78(21):12012-21.

