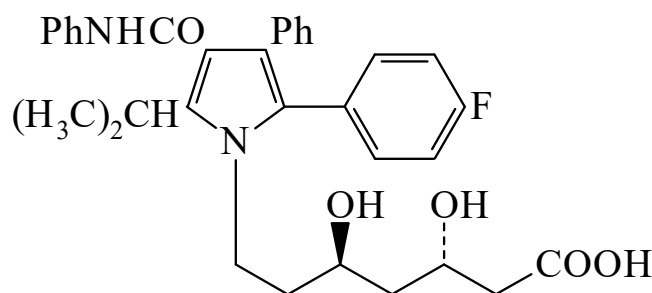




>>Entry Name: Atorvastatin, BAN, INN

Synonym(s): 2-(4-Fluorophenyl)- β , δ -dihydroxy-5-(1-methylethyl)-3-phenyl-4-[(phenylamino)carbonyl]-1*H*-pyrrole-1-heptanoic acid. Lipitor. Torvast. Totalip. Xarator. CI 981. PDI 34298



CAS Registry Number: 134523-00-5

Related CAS Registry Numbers(s): 110862-48-1

Molecular Formula: C₃₃H₃₅FN₂O₅

Molecular Weight: 558.648

Accurate Mass: 558.253001

Percentage Composition: C 70.95%; H 6.31%; F 3.40%; N 5.01%; O 14.32%

Biological Use/Importance: HMG-CoA reductase inhibitor. Antihypercholesterolaemic agent

Development Status: Marketed drug. Launched Dec 1996. Worldwide 3rd best selling prescription drug (\$5.03 bn) (Pfizer) (2000, Pharma Business)

Calculated Log P Data: Log P 4.66 (calc)

Other Data: Interconversion between lactone and hydroxy forms

>>Variant: (3'*R*,5'*R*)-form

Molecular Formula: C₃₃H₃₅FN₂O₅

Molecular Weight: 558.648

Accurate Mass: 558.253001

Percentage Composition: C 70.95%; H 6.31%; F 3.40%; N 5.01%; O 14.32%

>>Derivative: Ca salt (2:1)

Synonym(s): Atorvastatin calcium, USAN

CAS Registry Number: 134523-03-8

Physical Description: Amorph. solid

>>Derivative: Lactone

Synonym(s): 5-(4-Fluorophenyl)-2-(1-methylethyl)-*N*,4-diphenyl-1-[2-(tetrahydro-4-hydroxy-6-oxo-2*H*-pyran-2-yl)ethyl]-1*H*-pyrrole-3-carboxamide, 9CI

CAS Registry Number: 125995-03-1

Molecular Formula: C₃₃H₃₃FN₂O₄

Molecular Weight: 540.633

Accurate Mass: 540.242436

Percentage Composition: C 73.31%; H 6.15%; F 3.51%; N 5.18%; O 11.84%

Physical Description: Foam

Optical Rotation: $[\alpha]_D^{23} +25.5$ (c, 0.51 in CHCl₃) (94.6% op)

References:

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Baumann, K.L. *et al.*, *Tet. Lett.*, 1992, **33**, 2279; 2283, (*synth, pmr*)
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Dostal, L.A. *et al.*, *Teratology*, 1994, **50**, 387, (*tox*)
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