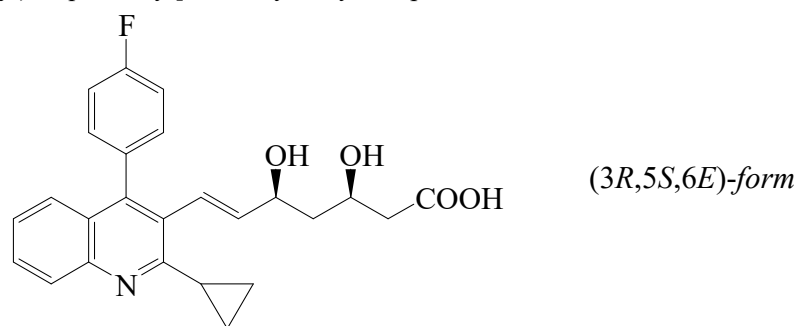




>>Entry Name: Itavastatin, INN

Synonym(s): 7-[2-Cyclopropyl-4-(4-fluorophenyl)-3-quinolinyl]-3,5-dihydroxy-6-heptenoic acid, 9CI



CAS Registry Number: 121659-03-8

Related CAS Registry Numbers(s): 147008-21-7

Molecular Formula: C₂₅H₂₄FNO₄

Molecular Weight: 421.467

Accurate Mass: 421.168937

Percentage Composition: C 71.25%; H 5.74%; F 4.51%; N 3.32%; O 15.18%

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

>>Variant: (3*R*,5*S*,6*E*)-form

CAS Registry Number: 147511-69-1

Molecular Formula: C₂₅H₂₄FNO₄

Molecular Weight: 421.467

Accurate Mass: 421.168937

Percentage Composition: C 71.25%; H 5.74%; F 4.51%; N 3.32%; O 15.18%

>>Derivative: Ca salt

Synonym(s): NK 104

CAS Registry Number: 147526-32-7

Extra CAS Registry Numbers(s): 148885-99-8

>>Derivative: Lactone

Synonym(s): 6-[2-[2-Cyclopropyl-4-(4-fluorophenyl)-3-quinolinyl]ethenyl]tetrahydro-4-hydroxy-2*H*-pyran-2-one

CAS Registry Number: 141750-63-2

Molecular Formula: C₂₅H₂₂FNO₃

Molecular Weight: 403.452

Accurate Mass: 403.158372

Percentage Composition: C 74.43%; H 5.50%; F 4.71%; N 3.47%; O 11.90%

Melting Point: Mp 135-137°

Optical Rotation: [α]_D²⁰ +8.8 (c, 1.01 in CHCl₃) (>98%ee)

>>Variant: (3*ξ*,5*ξ*,6*ξ*)-form

Molecular Formula: C₂₅H₂₄FNO₄

Molecular Weight: 421.467

Accurate Mass: 421.168937

Percentage Composition: C 71.25%; H 5.74%; F 4.51%; N 3.32%; O 15.18%

>>Derivative: Na salt

CAS Registry Number: 121659-04-9

Melting Point: Mp 197-199° (dec.)

>>Derivative: Et ester

CAS Registry Number: 121661-13-0

Extra CAS Registry Numbers(s): 167073-19-0

Molecular Formula: C₂₇H₂₈FNO₄

Molecular Weight: 449.521

Accurate Mass: 449.200237

Percentage Composition: C 72.14%; H 6.28%; F 4.23%; N 3.12%; O 14.24%

Melting Point: Mp 100-104°