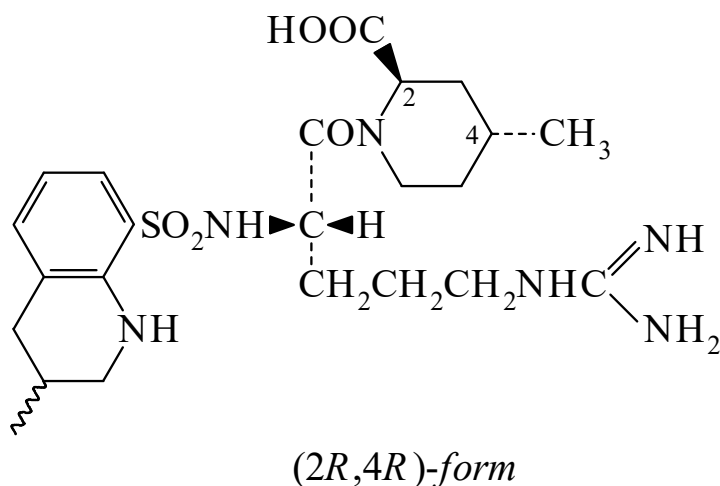




>>Entry Name: Argatroban, INN, JAN, USAN

Synonym(s): 1-[5-[(Aminoiminomethyl)amino]-1-oxo-2-[[[(1,2,3,4-tetrahydro-3-methyl-8-quinolinyl)sulfonyl]amino]pentyl]-4-methyl-2-piperidinecarboxylic acid, 9Cl. Argipidine. MCI 9038. MD 805



CAS Registry Number: 74863-84-6

Related CAS Registry Numbers(s): 141396-28-3 183679-05-2 189264-02-6 189264-03-7 189264-04-8

Molecular Formula: C₂₃H₃₆N₆O₅S

Molecular Weight: 508.641

Accurate Mass: 508.246789

Percentage Composition: C 54.31%; H 7.13%; N 16.52%; O 15.73%; S 6.30%

Use/Importance: Specific reversible thrombin inhibitor, antithrombotic, anticoagulant

Development Status: Launched 1990

>>Variant: (2R,4R)-form

Molecular Formula: C₂₃H₃₆N₆O₅S

Molecular Weight: 508.641

Accurate Mass: 508.246789

Percentage Composition: C 54.31%; H 7.13%; N 16.52%; O 15.73%; S 6.30%

Physical Description: Cryst. + 1 H₂O (EtOH aq.)

Melting Point: Mp 176-180°

Optical Rotation: [α]_D²⁷+76.1 (c, 1 in 0.2M HCl)

Calculated Log P Data: Log P 1.8 (calc)

Other Data: Pharmacol. active isomer

>>Variant: (2R,4S)-form

Molecular Formula: C₂₃H₃₆N₆O₅S

Molecular Weight: 508.641

Accurate Mass: 508.246789

Percentage Composition: C 54.31%; H 7.13%; N 16.52%; O 15.73%; S 6.30%

Physical Description: Cryst. + 1H₂O (EtOH aq.)

Melting Point: Mp 174-176°

Optical Rotation: [α]_D²⁵+43 (c, 1 in 0.1M HCl)

>>Variant: (2S,4R)-form

Molecular Formula: C₂₃H₃₆N₆O₅S

Molecular Weight: 508.641

Accurate Mass: 508.246789

Percentage Composition: C 54.31%; H 7.13%; N 16.52%; O 15.73%; S 6.30%

Physical Description: Cryst. + 1H₂O

Melting Point: Mp 229-232°

Optical Rotation: [α]_D²⁵+35 (c, 1 in 0.1M HCl)

>>Variant: (2S,4S)-form

Molecular Formula: C₂₃H₃₆N₆O₅S

Molecular Weight: 508.641

Accurate Mass: 508.246789

Percentage Composition: C 54.31%; H 7.13%; N 16.52%; O 15.73%; S 6.30%

Physical Description: Cryst. + 1H₂O

Melting Point: Mp 270-272°

Optical Rotation: [α]