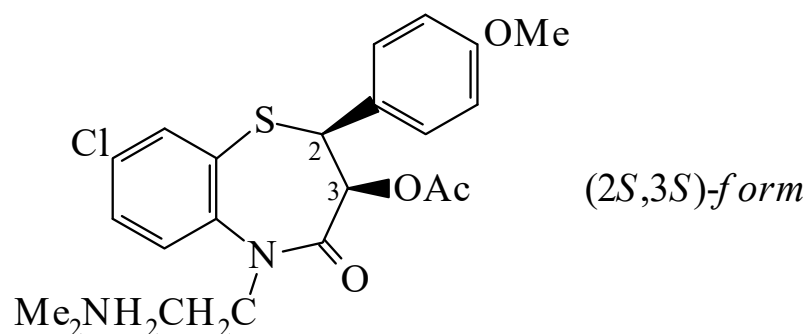




>>Entry Name: Clentiazem, INN

Synonym(s): 3-(Acetyloxy)-8-chloro-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-(4-methoxyphenyl)-1,5-benzothiazepin-4(5H)-one, 9Cl. 8-Chlorodiltiazem. Logna. TA 3090



CAS Registry Number: 111659-76-8

Related CAS Registry Numbers(s): 96125-59-6 104966-77-0 105487-95-4 111659-29-1 111659-55-3 111659-83-7 114177-16-1 114177-22-9 133775-82-3 136726-81-3

Molecular Formula: C₂₂H₂₅ClN₂O₄S

Molecular Weight: 448.969

Accurate Mass: 448.122355

Percentage Composition: C 58.86%; H 5.61%; Cl 7.90%; N 6.24%; O 14.25%; S 7.14%

Use/Importance: Calcium antagonist. Antihypertensive agent. Cerebral vasodilator. Immunosuppressant. Platelet aggregation inhibitor

Calculated Log P Data: Log P 4.45 (uncertain value) (calc)

>>Variant: (2R,3R)-form

Synonym(s): (-)-cis-form

CAS Registry Number: 110284-22-5

Molecular Formula: C₂₂H₂₅ClN₂O₄S

Molecular Weight: 448.969

Accurate Mass: 448.122355

Percentage Composition: C 58.86%; H 5.61%; Cl 7.90%; N 6.24%; O 14.25%; S 7.14%

>>Derivative: Hydrochloride

CAS Registry Number: 96125-52-9

Physical Description: Cryst. + 0.5H₂O (EtOH/Me₂CO)

Melting Point: Mp 127-131°

Optical Rotation: [α]_D²⁰ -93.3 (c, 0.872 in EtOH)

>>Derivative: Maleate (1:1)

CAS Registry Number: 130979-49-6

Physical Description: Cryst. (EtOH)

Melting Point: Mp 160.5-161.5°

Optical Rotation: [α]_D²⁰ -76.8 (c, 1 in MeOH)

>>Variant: (2S,3S)-form

Synonym(s): (+)-cis-form

CAS Registry Number: 96125-53-0

Molecular Formula: C₂₂H₂₅ClN₂O₄S

Molecular Weight: 448.969

Accurate Mass: 448.122355

Percentage Composition: C 58.86%; H 5.61%; Cl 7.90%; N 6.24%; O 14.25%; S 7.14%

Other Data: Pharmacol. active isomer

>>Derivative: Hydrochloride

CAS Registry Number: 114788-20-4

Physical Description: Cryst. + 0.5H₂O (EtOH/Me₂CO)

Melting Point: Mp 128-132°

Optical Rotation: [α]_D²⁰ +92.2 (c, 0.796 in EtOH)

>>Derivative: Maleate (1:1)

Synonym(s): Clentiazem maleate, USAN

CAS Registry Number: 96128-92-6

Physical Description: Cryst. (EtOH)

Melting Point: Mp 160.5-161.5°

Optical Rotation: [α]