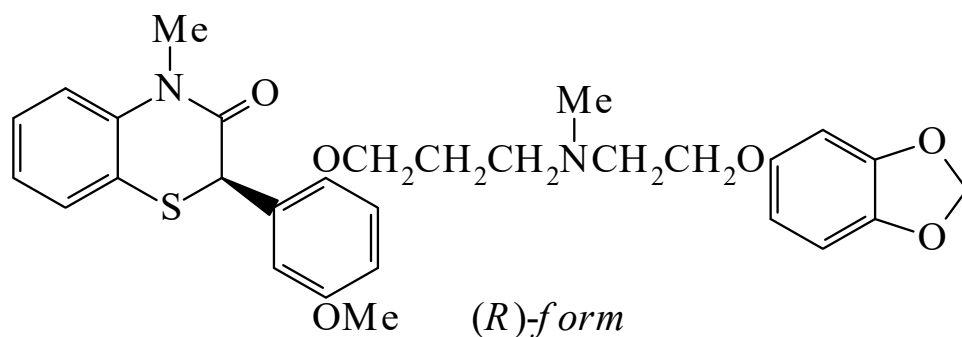




>>Entry Name: Semotiadil, INN

Synonym(s): 2-[2-[3-[[2-(1,3-Benzodioxol-5-yloxy)ethyl]methylamino]propoxy]-5-methoxyphenyl]-4-methyl-2*H*-1,4-benzothiazin-3(4*H*)-one, 9Cl. Sesamodil, JAN



Related CAS Registry Numbers(s): 123388-07-8 123388-25-0

Molecular Formula: C<sub>29</sub>H<sub>32</sub>N<sub>2</sub>O<sub>6</sub>S

Molecular Weight: 536.648

Accurate Mass: 536.198108

Percentage Composition: C 64.91%; H 6.01%; N 5.22%; O 17.89%; S 5.98%

Use/Importance: Calcium antagonist (lacks sodium channel blocking activity). Antihypertensive, antianginal agent

Calculated Log P Data: Log P 4.55 (uncertain value) (calc)

Other Data: Semotiadil refers to (*R*)-form

>>Variant: (*R*)-form

Synonym(s): SD 3211

CAS Registry Number: 116476-13-2

Molecular Formula: C<sub>29</sub>H<sub>32</sub>N<sub>2</sub>O<sub>6</sub>S

Molecular Weight: 536.648

Accurate Mass: 536.198108

Percentage Composition: C 64.91%; H 6.01%; N 5.22%; O 17.89%; S 5.98%

Physical Description: Oil

Other Data: Pharmacol. active isomer

>>Derivative: Fumarate

CAS Registry Number: 116476-14-3

Physical Description: Cryst. (EtOH)

Melting Point: Mp 134-135°

Optical Rotation:  $[\alpha]_D^{25} +195$  (c, 1.0 in DMSO)

>>Variant: (*S*)-form

Synonym(s): Levosemotiadil, INN. SD 3212

CAS Registry Number: 116476-16-5

Molecular Formula: C<sub>29</sub>H<sub>32</sub>N<sub>2</sub>O<sub>6</sub>S

Molecular Weight: 536.648

Accurate Mass: 536.198108

Percentage Composition: C 64.91%; H 6.01%; N 5.22%; O 17.89%; S 5.98%

Use/Importance: Sodium and calcium channel blocker, possesses antiarrhythmic activity

Physical Description: Oil

Calculated Log P Data: Log P 4.55 (uncertain value) (calc)

>>Derivative: Fumarate

Synonym(s): SD 3212

CAS Registry Number: 116476-17-6

Physical Description: Cryst. (EtOH)

Melting Point: Mp 134-135 dec.°

Optical Rotation:  $[\alpha]_D^{25} -195$  (c, 1 in DMSO)