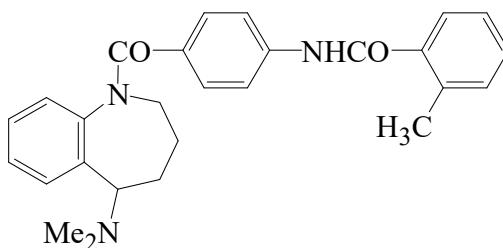




>>Entry Name: *N*-[4-[[5-(Dimethylamino)-2,3,4,5-tetrahydro-1*H*-1-benzazepin-1-yl]carbonyl]phenyl]-2-methylbenzamide, 9Cl
Synonym(s): OPC 31260



CAS Registry Number: 137975-06-5

Related CAS Registry Numbers(s): 138470-70-9 157378-41-1 157378-42-2

Type of Compound Code(s): XA7175

Molecular Formula: C₂₇H₂₉N₃O₂

Molecular Weight: 427.545

Accurate Mass: 427.225977

Percentage Composition: C 75.85%; H 6.84%; N 9.83%; O 7.48%

Biological Use/Importance: Vasopressin V₂ receptor antagonist. Aquaretic agent

>>Variant: (+)-form

Molecular Formula: C₂₇H₂₉N₃O₂

Molecular Weight: 427.545

Accurate Mass: 427.225977

Percentage Composition: C 75.85%; H 6.84%; N 9.83%; O 7.48%

Other Data: Absolute config. not detd.

>>Derivative: Hydrochloride

CAS Registry Number: 138470-68-5

Physical Description: Amorph. solid

Optical Rotation: [α]_D²⁵ +234 (c, 0.2 in MeOH)

Other Data: Opt. rotation as reported in patent, prob. a misprint for +23.4

>>Variant: (-)-form

Molecular Formula: C₂₇H₂₉N₃O₂

Molecular Weight: 427.545

Accurate Mass: 427.225977

Percentage Composition: C 75.85%; H 6.84%; N 9.83%; O 7.48%

>>Derivative: Hydrochloride

CAS Registry Number: 138470-69-6

Physical Description: Amorph. solid

Optical Rotation: [α]_D²⁵ -23.1 (c, 0.2 in MeOH)

>>Variant: (±)-form

CAS Registry Number: 137976-84-2

Molecular Formula: C₂₇H₂₉N₃O₂

Molecular Weight: 427.545

Accurate Mass: 427.225977

Percentage Composition: C 75.85%; H 6.84%; N 9.83%; O 7.48%

Physical Description: Prisms (EtOH)

Melting Point: Mp 207-208°

References:

Pat. Coop. Treaty (WIPO), 1991, Otsuka, 91 05 549; *CA*, **116**, 128686j, (*synth, isomers, pharmacol*)

Yazawa, H. *et al.*, *Br. J. Pharmacol.*, 1996, **117**, 799-804, (*pharmacol*)

Ogawa, H. *et al.*, *J. Med. Chem.*, 1996, **39**, 3547-3555, (*synth, pmr, pharmacol*)

Sato, K. *et al.*, *Nephron*, 1998, **78**, 9-14, (*pharmacol*)