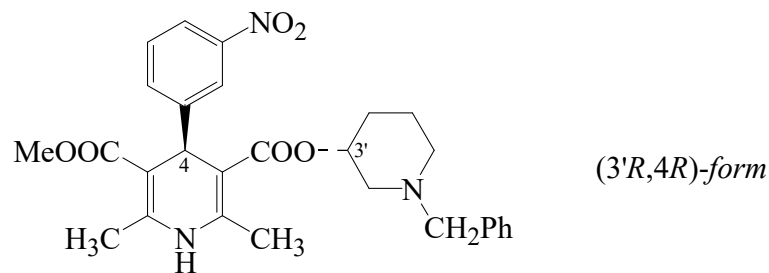




>>Entry Name: Benidipine, INN

Synonym(s): Methyl 1-(phenylmethyl)-3-piperidinyl 1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-3,5-pyridinedicarboxylate, 9Cl. Coniel. Nakadipine



CAS Registry Number: 91599-75-6

Related CAS Registry Numbers(s): 85387-35-5 119009-45-9 119065-61-1

Molecular Formula: C₂₈H₃₁N₃O₆

Molecular Weight: 505.569

Accurate Mass: 505.221287

Percentage Composition: C 66.52%; H 6.18%; N 8.31%; O 18.99%

General Statement: Benidipine applies to the (3'*RS*,4*RS*)-form

Use/Importance: Calcium antagonist. Antihypertensive agent

Development Status: Launched 1991 (Japan)

Calculated Log P Data: Log P 5.11 (uncertain value) (calc)

>>Variant: (3'*R*,4*R*)-form

CAS Registry Number: 119065-60-0

Molecular Formula: C₂₈H₃₁N₃O₆

Molecular Weight: 505.569

Accurate Mass: 505.221287

Percentage Composition: C 66.52%; H 6.18%; N 8.31%; O 18.99%

Optical Rotation: $[\alpha]_{\text{D}}^{23} -88.9$ (c, 0.62 in Me₂CO)

>>Derivative: Hydrochloride

CAS Registry Number: 129262-07-3

Extra CAS Registry Numbers(s): 119065-62-2

Optical Rotation: $[\alpha]_{\text{D}}^{21} -110.2$ (c, 0.24 in Me₂CO)

>>Variant: (3'*S*,4*S*)-form

CAS Registry Number: 119009-44-8

Molecular Formula: C₂₈H₃₁N₃O₆

Molecular Weight: 505.569

Accurate Mass: 505.221287

Percentage Composition: C 66.52%; H 6.18%; N 8.31%; O 18.99%

Optical Rotation: $[\alpha]_{\text{D}}^{23} +87.7$ (c, 0.57 in Me₂CO)

>>Derivative: Hydrochloride

CAS Registry Number: 129262-08-4

Extra CAS Registry Numbers(s): 119009-46-0

Physical Description: Solid (Me₂CO/Et₂O)

Optical Rotation: $[\alpha]_{\text{D}}^{21} +113.6$ (c, 0.5 in Me₂CO)

Other Data: More pharmacol. active diastereoisomer

>>Variant: (3'*RS*,4*RS*)-form

CAS Registry Number: 105979-17-7

Molecular Formula: C₂₈H₃₁N₃O₆

Molecular Weight: 505.569

Accurate Mass: 505.221287

Percentage Composition: C 66.52%; H 6.18%; N 8.31%; O 18.99%

Other Data: Pharmacol. active form