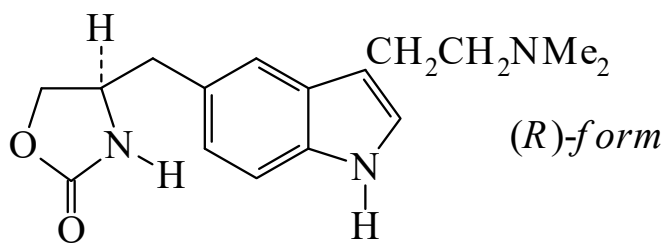




>>Entry Name: Zolmitriptan, BAN, INN, USAN

Synonym(s): 4-[[3-[2-(Dimethylamino)ethyl]-1*H*-indol-5-yl]methyl]-2-oxazolidinone, 9Cl. *N,N*-Dimethyl-2-[5-(2-oxo-1,3-oxazolidin-4-ylmethyl)-1*H*-indol-3-yl]ethanamine. Zomig, 311C90



Related CAS Registry Numbers(s): 139264-24-7

Molecular Formula: C₁₆H₂₁N₃O₂

Molecular Weight: 287.361

Accurate Mass: 287.163377

Percentage Composition: C 66.88%; H 7.37%; N 14.62%; O 11.14%

Biological Use/Importance: 5-Hydroxytryptamine (5HT_{1D}) receptor agonist. Potential antimigraine agent

Development Status: Marketed drug. Approved for clinical use in Sweden (1999). Approved by FDA (1997)

Solubility: Sol. H₂O (> 2g per 100 cm³)

pK_a Value: pK_a 9.64

>>Variant: (*R*)-form

CAS Registry Number: 139264-25-8

Molecular Formula: C₁₆H₂₁N₃O₂

Molecular Weight: 287.361

Accurate Mass: 287.163377

Percentage Composition: C 66.88%; H 7.37%; N 14.62%; O 11.14%

Physical Description: Solid (EtOAc)

Melting Point: Mp 130° (as hydrochloride)

Optical Rotation: [α]_D²¹+5.15 (c, 0.77 in MeOH) (hydrochloride)

Other Data: CAS no. refers to hydrochloride

>>Variant: (*S*)-form

CAS Registry Number: 139264-17-8

Molecular Formula: C₁₆H₂₁N₃O₂

Molecular Weight: 287.361

Accurate Mass: 287.163377

Percentage Composition: C 66.88%; H 7.37%; N 14.62%; O 11.14%

Physical Description: Cryst. +1 2-propanol + 0.5 H₂O (2-propanol)

Melting Point: Mp 139-141° (solvate)

Optical Rotation: [α]_D²²-5.79 (c, 0.5 in MeOH)

Other Data: Pharmacol. active isomer

>>Derivative: Hydrochloride

CAS Registry Number: 139264-19-0

Physical Description: Solid (2-propanol)

Melting Point: Mp 118-120°

Optical Rotation: [α]_D²³-9.35 (c, 0.31 in H₂O)

>>Derivative: Succinate

CAS Registry Number: 139264-20-3

Physical Description: Solid

Melting Point: Mp 122-123°

>>Derivative: Maleate

CAS Registry Number: 139264-18-9

Physical Description: Solid (EtOH)

Melting Point: Mp 151-152°