

VALSARTAN (CAS number- 137862-53-4)

TAJMTF-YTPOUA7455

Taj Active Pharmaceuticals Ingredients

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Active Pharmaceutical Ingredients
TAJ PHARMACEUTICALS LIMITED INDIA

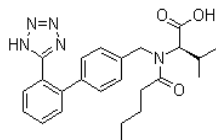


Raw Material / Chemicals Index

Taj Pharmaceuticals Ltd.

VALSARTAN

(CAS NO.137862-53-4)



IUPAC Name: (2S)-3-Methyl-2-[pentanoyl-[[4-[2-(2H-tetrazol-5yl)phenyl]phenyl]methyl]amino]butanoic acid

Molecular Formula: C₂₄H₂₉N₅O₃

Molar mass: 435.5188 g/mol

Density: 1.212 g/cm³

Flash Point: 368 °C

Index of Refraction: 1.586

Boiling Point: 684.9 °C at 760 mmHg

Vapour Pressure: 1.06E-19 mmHg at 25 °C

Melting Point: 116-117 °C

Appearance: white crystalline powder

XLogP3-AA: 4.4

H-Bond Donor: 2

H-Bond Acceptor: 6

Rotatable Bond Count: 10

Tautomer Count: 2

Exact Mass: 435.22704

MonoIsotopic Mass: 435.22704

Topological Polar Surface Area: 112

Heavy Atom Count: 32

Canonical SMILES: CCCCC(=O)N(CC1=CC=C(C=C1)C2=CC=CC=C2C3=NNN=N3)C(C(C)C)C(=O)O

Isomeric SMILES: CCCCC(=O)N(CC1=CC=C(C=C1)C2=CC=CC=C2C3=NNN=N3)[C@@H](C(C)C)C(=O)O

InChI: InChI=1S/C24H29N5O3/c1-4-5-10-21(30)29(22(16(2)3)24(31)32)15-17-11-13-18(14-12-17)19-8-6-7-9-20(19)23-25-27-28-26-23/h6-9,11-14,16,22H,4-5,10,15H2,1-3H3,(H,31,32)(H,25,26,27,28)/t22-/m0/s1

InChIKey: ACWBQPMHZXGDFX-QFIPXVFZSA-N

Product Categories: Active Pharmaceutical Ingredients; Antihypertensive; APIs; Intermediates & Fine Chemicals; Pharmaceuticals; API's

Identifiers

CAS number 137862-53-4

ATC code C09CA03

PubChem 60846

DrugBank APRD00133

Chemical data

Formula C24H29N5O3

Mol. mass 435.519 g/mol

SMILES eMolecules & PubChem

Pharmacokinetic data

Bioavailability 25%

Protein binding 95%

Metabolism

Half life 6 hours

Excretion Renal 30%, biliary 70%

Valsartan is a nonpeptide, orally active, and specific angiotensin II antagonist acting on the AT1 receptor subtype.

Valsartan is chemically described as N-(1-oxopentyl)-N-[[2'-(1H-tetrazol-5-yl) [1,1'-biphenyl]-4-yl]methyl]-L-valine. Its empirical formula is C24H29N5O3, its molecular weight is 435.5.

Valsartan is a white to practically white fine powder. It is soluble in ethanol and methanol and slightly soluble in water. Valsartan is available as tablets for oral administration, containing 40 mg, 80 mg, 160 mg or 320 mg.

Sr. No.	Tests	Specifications	Results
1.	Description	A white or off white crystalline powder.	White crystalline powder
2.	Identification By 1) By IR 2) By HPLC	The IR spectrum of the test should be concordant with IR spectrum of standard which is prepared in same manner. The retention time of the major peak in the chromatogram of the assay preparation corresponds to that in the chromatogram of the standard preparation.	Complies Complies
3.	Solubility	Soluble in Methanol and ethanol.	Complies
4.	Absorbance	Not more than 0.02 at 420 nm (1/20 in methanol)	Complies.
5.	Water content by KF	Not more than 2.0% w/w	1.12%
6.	Residue on Ignition	Not more than 0.1% w/w	0.06%
7.	Heavy Metals	Not more than 10 ppm	Complies
8.	Related substance by HPLC	a)Related compound A : NMT 1.0% b)Related compound B : NMT 0.2% c)Related compound C : NMT 0.1% d)Any other individual impurity : NMT 0.1% e)Total impurity : NMT 0.3%	0.28% 0.07% ND 0.08% 0.28%
9.	Assay (By HPLC)	Should be between 98.0% & 102.0% w/w	99.0% w/w

Specification

Valsartan (CAS NO.137862-53-4) is also named as CGP 48933 ; Diovan ; HSDB 7519 ; UNII-80M03YXJ7I ; Valtan ; Valzaar ; L-Valine, N-(1-oxopentyl)-N-((2'-(1H-tetrazol-5-yl)(1,1'-biphenyl)-4-yl)methyl)- ; N-(p-(o-1H-Tetrazol-5-ylphenyl)benzyl)-N-valeryl-L-valine . It is an angiotensin II receptor antagonist (more commonly called an "ARB", which stands for angiotensin receptor blocker), with particularly high affinity for the type I (AT₁) angiotensin receptor.

Safety Profile



Hazard Codes: Xi

Risk Statements: 36/37/38

R36/37/38:Irritating to eyes, respiratory system and skin.

Safety Statements: 26-37/39

S26: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

S37/39:Wear suitable gloves and eye/face protection.

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