



Formula: C33H40N2O9

MW: 608.69

CAS: 50-55-5

TNP NUMBER: TNP00187

MDL NUMBER: MFCD00066722

IUPAC: 3,8-dimethoxy-4-(methoxycarbonyl)-1,2,3,4,5,11,14,14a,4a,5a-decahydrobenzo[3,4-g]indolo[2,3-a]quinolizin-2-yl 3,4,5-trimethoxybenzoate

Smiles:

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c1cc2c(cc1OC)[nH]c1c2CCN2C1CC1C(C2)CC(C(C1C(OC)=O)OC)OC(c1cc(c(c(c1)OC)OC)OC)=O
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THERAPEUTIC CATEGORY: Antihypertensive

VET THERAP CATEGORY: Hypotensive, Tranquilizer.

SOURCE: Found in Rauwolfia spp.

ACCEPTORS: 9

DONORS: 1

ROTATION BONDS: 8

N+O: 11

Chiral Centers: 6

LogP: 6.02

LogS: -6.6

LIPINSKI: 2

Synonyms: RESERPINE;3,4,5-TRIMETHOXYBENZOYL METHYL
RESERPATE;11,17-DIMETHOXY-18-[(3,4,5-TRIMETHOXYBENZOYL)OXY]YOHIMBAN-16-C
ARBOXYLIC ACID METHYL ESTER;METHYL RESERPATE;METHYL RESERPATE
3,4,5-TRIMETHOXYBENZOIC ACID ESTER;|
-Carpserp;(3beta,16beta,17alpha,18beta,20alpha)-methyleste;,methylester,(3beta,16beta,17alp
ha,18beta,20alpha)-

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EINECS:200-047-9

Product Categories:Miscellaneous Natural Products;Alkaloids;Biochemistry;Indole
Alkaloids;Dopaminergics;Neurotransmitters;Others;Asymmetric Synthesis;Chiral Building
Blocks;Complex Molecules Reserpine

Chemical Properties: mp ~265 C (dec.) refractive index 177 (C=1, DMF) storage temp. 2-8C
Merck 14,8145 BRN 102014 Stability:Stable, but darkens slowly in light. Combustible.
Incompatible with strong acids, reducing agents, oxidizing agents. NIST Chemistry
ReferenceReserpine(50-55-5) EPA Substance Registry SystemYohimban-16-carboxylic acid,
11,17-dimethoxy-18-[(3,4,5- trimethoxybenzoyl)oxy]-, methyl ester, (3.beta.,16.beta.,17.alpha.,
18.beta.,20.alpha.)-(50-55-5) Xn,Xi Risk Statements 22-67-36-10 Safety Statements
22-36/37/39-26 RIDADR 3077 WGK Germany 3 RTECS ZG0350000 F 10-23 PackingGroup II
Hazardous Substances Data50-55-5(Hazardous Substances Data) Reserpine

Usage And Synthesis:

Chemical Properties: off-white crystalline powder General DescriptionWhite or cream to slightly
yellow crystals or crystalline powder. Odorless with a bitter taste. Air & Water
ReactionsInsoluble in water. Reacts slowly with air and water. Darkens slowly on exposure to
light. Reactivity ProfileReserpine is a weak base and can form salts with strong acids.
Incompatible with oxidizing agents and reducing agents. Fire HazardFlash point data for
Reserpine are not available; however, Reserpine is probably combustible. Biological

Activity Binds the vesicular monoamine transporter (VMAT2) and inhibits transport of biogenic amines into adrenal chromaffin granules and synaptic vesicles. Causes depletion of biogenic amine stores. Antihypertensive and antipsychotic. Reserpine

