



Formula: C₃₄H₄₇NO₁₁

MW: 645.75

CAS: 302-27-2

TNP NUMBER: TNP00306

MDL NUMBER: MFCD02647022

IUPAC: (1S,5S,6S,8S,16S,4R,9R,13R,14R,18R)-11-ethyl-5,7,14-trihydroxy-6,16,18-trimethoxy-13-(methoxymethyl)-4-phenylcarbonyloxy-11-azahexacyclo[7.7.2.1.0.0.0]nonadec-8-yl acetate

Smiles:

c1ccc(C(O[C@@H]2C3[C@@]4([C@@H](O)[C@@H]([C@]2(CC3[C@]23C5[C@@](COC)([C@@H](C[C@@H]3OC)O)CN(C2[C@H]4[C@@H]5OC)CC)O)OC(=O)C)=O)cc1

REFERENCE: Merck, 13, 120 Ameri, A., The effects of Aconitum alkaloids on the central nervous system. Prog. Neurobiol. 56, 211-235, (1998) abstract Onur, R., et al., Effects of aconitine on neurotransmitter release in the rat neuromuscular junction. Neuropharmacology 34, 1139-1145, (1995) abstract Sawanobori, T., Effects of arrhythmic agents and Mg²⁺ on aconitine-induced arrhythmias. Jpn. Heart J. 5, 709, (1996) Ameri, A. and Simmet, T., Antagonism of the aconitine-induced inexcitability by the structurally related aconitum alkaloids, lappaconitine and ajacine. Brain Res. 842, 332-341, (1999) abstract Seitz, U., and Ameri, A., Different effects on [3H]noradrenaline uptake of the Aconitum alkaloids aconitine, 3-acetylaconitine, lappaconitine, and N-desacetylappaconitine in rat hippocampus. Biochem. Pharmacol. 55, 883-888, (1998) abstract

SOURCE: From Aconitum Napellus L., Ranunculaceae

ACCEPTORS: 11

DONORS: 3

ROTATION BONDS: 4

N+O: 12

Chiral Centers: 15

LogP: 1.91

LogS: -5.36

LIPINSKI: 2

Synonyms:

(1ALPHA,3ALPHA,6ALPHA,14ALPHA,15ALPHA,16BETA)-20-ETHYL-1,6,16-TRIMETHOXY-4-(METHOXYMETHYL)ACONITANE-3,8,13,14,15-PENTOL 8-ACETATE
14-BENZOATE;ACETYLBENZOYLACONINE;ACONITIN;ACONITINE;ACONITANE;ACONITANE-3,8,13,14,15-PENTOL,20-ETHYL-1,6,16-TRIMETHOXY-4-(METHOXYMETHYL)-,8-ACETATE14-BENZOATE,(1ALPHA,3ALPHA,6ALPHA,14ALPHA,15ALPHA,16BETA)-;aconitincristallisat;aconitine(crystalline)

CAS:302-27-2

MF:C34H47NO11

MW:645.74

EINECS:206-121-7

Product Categories:Alkaloids Aconitine

Chemical Properties: mp 200-205 C (dec.) Merck 13,120 NIST Chemistry ReferenceAconitine(302-27-2) T+,Xi Risk Statements 26/28-36/37/38 Safety Statements 24-45-36-26 RIDADR UN 1544 6.1/PG 1 WGK Germany 2 RTECS AR5960000 F 10-34 HazardClass 6.1(a) PackingGroup I Aconitine Aconitine

Usage And Synthesis: Aconitine



