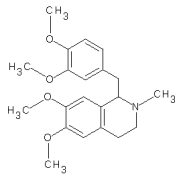

Formula: C21H27NO4

MW: 357.45

CAS: 2688-77-9

MDL: MFCD00006910

TNP: TNP00224

Laudanosine, derivative of

LogP: -2.56

LogS: -2.05

Acceptors: 4

Donors: 0

Rotation Bonds: 6

Chiral Centers: 1

N+O: 5

LIPINSKY: 4

IUPAC: 1-[(3,4-dimethoxyphenyl)methyl]-6,7-dimethoxy-2-methyl-1,2,3,4-tetrahydroisoqu inoline

Smiles: c12C(N(C)CCc1cc(c(c2)OC)OC)Cc1cc(OC)c(cc1)OC

Specification: Laudanosine, derivative of

Laudanosine, derivative of Usage And Synthesis Laudanosine, derivative of

Merck 13 Reference: Monograph Number: 0005396

Title: Laudanosine

CAS Registry Number: 2688-77-9

CAS Name:
(1S)-1-[(3,4-Dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-6,7-dimethoxy-2-methylisoquinoline

Additional Names: 1,2,3,4-tetrahydro-6,7-dimethoxy-2-methyl-1-veratrylisoquinoline; N-methyltetrahydropapaverine

Molecular Formula: C21H27NO4

Molecular Weight: 357.44.

Percent Composition: C 70.56%, H 7.61%, N 3.92%, O 17.90%

Literature References: Occurs in opium (0.0008%). It is the last alkaloid to be separated from morphine extraction mother liquors; occurs as (+)-form. Synthesis: Pictet, Finkelstein, Ber. 42, 1979 (1909); Frydman et al., Tetrahedron 4, 342 (1958); Elliott, J. Heterocycl. Chem. 9, 853 (1972). Asymmetric synthesis: M. Konda et al., Chem. Pharm. Bull. 23, 1025 (1975); of (R)-(-)-laudanosine: M. Konda et al., ibid. 25, 69 (1977); R. E. Gawley, G. A. Smith, Tetrahedron Lett. 29, 301 (1988). Configuration: Leithe, Ber. 64, 2827 (1931); Faltis, Adler, Arch. Pharm. 284, 281 (1951); Corrodi, Hardegger, Helv. Chim. Acta 39, 889 (1956).

Properties: Crystals from light petr (30-60), mp 89. [a]D16 +106 (c = 1.6 in 97% alc); [a]D16 +130 (chloroform); [a]D22 +52.2