



Formula: C<sub>21</sub>H<sub>23</sub>NO<sub>5</sub>

MW: 369.42

CAS: 482-74-6

TNP NUMBER: TNP00336

MDL NUMBER: MFCD00046960

IUPAC: 11,12-dimethoxy-7-methyl-4H,6H,8H,9H,15H-benzo[1'',2''-4',5']azecino[9',8'-3,4]benzo[d]1,3-dioxolen-14-one

Smiles: c12cc(c(cc1CCN(Cc1c(CC2=O)ccc2c1OCO2)C)OC)OC

ACCEPTORS: 5

DONORS: 0

ROTATION BONDS: 2

N+O: 6

Chiral Centers: 0

LogP: 2.63

LogS: -4.46

LIPINSKI: 4

Monograph Number: 0002635

Title: Cryptopine

CAS Registry Number: 482-74-6

CAS Name:

4,6,7,13-Tetrahydro-9,10-dimethoxy-5-methylbenzo[e]-1,3-dioxolo[4,5-l][2]benzazecin-12(5H)-one

Additional Names: cryptocavine

Molecular Formula: C<sub>21</sub>H<sub>23</sub>NO<sub>5</sub>

Molecular Weight: 369.41.

Percent Composition: C 68.28%, H 6.28%, N 3.79%, O 21.66%

Literature References: Occurs in opium (0.003-0.03%). Has been found in *Corydalis sempervirens* (L.) Pers., and in *Dicentra* spp., Fumariaceae: Manske, Can. J. Res. 8, 407 (1933); 7, 265 (1932); 15B, 274 (1937). Structure: Perkin, J. Chem. Soc. 115, 713 (1919). Synthesis: Haworth, Perkin, *ibid.* 1926, 1769. Crystal structure: S. R. Hall, F. R. Ahmed, Acta Crystallogr. B24, 346 (1968).

Properties: Crystallizes as six-sided prisms or plates from benzene, mp 220-221. d 1.35. Almost insol in water and ether. Soluble in chloroform, acetic acid. One part dissolves in 455 parts alc or 80 parts boiling alc. Sparingly sol in most other organic solvents. May be crystallized from hot alc, benzene, petr ether, methyl ethyl ketone, isoamyl alcohol, acetophenone, pyridine, or an alcohol-pyridine mixture. The salts tend to oil out, but can be crystallized by warming, redissolving, and slow cooling.

Melting point: mp 220-221

Density: d 1.35

Synonyms:

CRYPTOPINE;benzo(e)-1,3-dioxolo(4,5-l)(2)benzazecin-12(5h)-one,4,6,7,13-tetrahydro-9,10-d; cryptocavine;cryptopin;imethoxy-5-methyl-;kryptocavin;4,6,7,13-Tetrahydro-9,10-dimethoxy-5-methylbenzo(e)-1,3-dioxolo(4,5-l)(2)benzazecin-12(5H)-one;Kryptopine

CAS:482-74-6

MF:C<sub>21</sub>H<sub>23</sub>NO<sub>5</sub>

MW:369.41

EINECS:207-584-8

Product Categories: Cryptopine

Chemical Properties: Stability:Stable. Incompatible with strong oxidizing agents.

Safety Information: RIDADR 1544 HazardClass 6.1(b) PackingGroup III Cryptopine

Usage And Synthesis: Cryptopine

