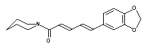

Formula: C17H19NO3

MW: 285.34

CAS: 94-62-2

MDL: MFCD00005839

TNP: TNP00240

1-[5-(1,3-Benzodioxol-5-yl)-1-oxo-2,4-pentadienyl]piperidine;
1-Piperidino-5-(1,3-benzodioxole-5-yl)-2,4-pentadiene-1-one; Piperine

LogP: 1.79

LogS: -3.29

Acceptors: 3

Donors: 0

Rotation Bonds: 3

Chiral Centers: 0

N+O: 4

LIPINSKY: 4

Info: Piperine, from Piper Nigrum (black pepper seeds) 99%

IUPAC: (2E,4E)-5-(2H-benzo[3,4-d]1,3-dioxolen-5-yl)-1-piperidylpenta-2,4-dien-1-one

Smiles: C(N1CCCCC1)(/C=CC=C/c1cc2OCOc2cc1)=O

Specification: piperine

piperine Usage And Synthesis piperine

Merck 13 Reference: Monograph Number: 0007553

Title: Piperine

CAS Registry Number: 94-62-2

CAS Name: 1-[(2E,4E)-5-(1,3-Benzodioxol-5-yl)-1-oxo-2,4-pentadienyl]piperidine

Additional Names: (E,E)-1-piperoylpiperidine

Molecular Formula: C17H19NO3

Molecular Weight: 285.34.

Percent Composition: C 71.56%, H 6.71%, N 4.91%, O 16.82%

Literature References: Isolated from black pepper (Piper nigrum L.); also in P. longum L., P. retrofractum Vahl. (P. officinarum C.D.C.), and P. clusii C.D.C.; in root bark of Piper geniculatum Sw., Piperaceae. Extraction procedure: Cazeneuve, Caillot, Bull. Soc. Chim. [2] 27, 291 (1877). Synthesis: Rugheimer, Ber. 15, 1390 (1882); Newman, Chem. Prod. 16, 379 (1953); Normant, Feugeas, Compt. Rend. 258, 2846 (1964). Spectroscopic structural elucidation and preparative separation of piperine and its stereoisomers isopiperine, isochavicine and chavicine, q.v.: R. De Cleyn, M. Verzele, Bull. Soc. Chim. Belg. 84, 435 (1975). Synthesis of isomers: R. Grewe et al., Ber. 103, 3752 (1970); of piperine and isochavicine: S. Tsuboi et al., Tetrahedron Lett. 1979, 1043. Stereoselective synthesis of piperine: R. A. Olsen, G. O. Spessard, J. Agric. Food Chem. 29, 942 (1981). More toxic to houseflies than pyrethrum: Harvill et al., Contrib. Boyce Thompson Inst. 13, 87 (1943).

Properties: Monoclinic prisms from alcohol, mp 130. Tasteless at first, but burning aftertaste. Neutral to litmus. pK (18): 12.22. Almost insol in water (40 mg/liter at 18), in petr ether. One gram dissolves in 15 ml alcohol, 1.7 ml chloroform, 36 ml ether. Sol in benzene, acetic acid.

Melting point: mp 130

pKa: pK (18): 12.22

Derivative Type: (E,Z)-Form

Additional Names: Isochavicine

Properties: Crystals from chloroform + hexane, mp 89 (Grewe), 103 (De Cleyn). uv max (methanol): 333 nm (e 16300).

Melting point: mp 89 (Grewe), 103 (De Cleyn)

Absorption maximum: uv max (methanol): 333 nm (e 16300)

Derivative Type: (Z,E)-Form

Additional Names: Isopiperine

Properties: Crystals from chloroform + hexane, mp 110 (Grewe), 86 (De Cleyn). uv max (methanol): 332 nm (e 21800).

Melting point: mp 110 (Grewe), 86 (De Cleyn)

Absorption maximum: uv max (methanol): 332 nm (e 21800)

Use: To impart pungent taste to brandy. As insecticide.