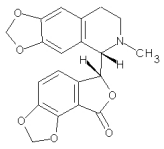

Formula: C20H17NO6

MW: 367.36

CAS: 485-49-4

MDL: MFCD00067279

TNP: TNP00509

(r-(r*,s*))-6-(5,6,7,8-tetrahydro-6-methyl-1,3-dioxolo(4,5-g)isoquinolin-5-yl)-furo(3,4-e)-1,3-benzodioxol-8(6h)-one;
[R-(R*,S*)]-6-(5,6,7,8-TETRAHYDRO-6-METHYL-1,3-DIOXOLO[4,5-G]ISOQUINOLIN-5-YL)FURO[3,4-E]-1,3-BENZODIOXOL-8(6H)-ONE; (+)-BICUCULINE; (+)-BIC

LogP: -8.63

LogS: -1.15

Acceptors: 6

Donors: 0

Rotation Bonds: 1

Chiral Centers: 2

N+O: 7

LIPINSKY: 4

Info: Alkaloid naturally occurring in the d-form; found in Dicentra cucullaria (L.) Bernh., Adlumia fungosa (ait.), Greene, Fuariaceae, and several Corydalis species

IUPAC: (6R)-6-((5S)-6-methyl(5,6,7,8-tetrahydro-2H-1,3-dioxolano[4,5-g]isoquinolin-5-yl))-6-hydro-2H-1,3-dioxoleno[4,5-e]isobenzofuran-8-one

Smiles: c12c(c3C(O[C@H](c3cc2)([C@@H]2(c3cc4OCOc4cc3CCN2C)))=O)OCO1

REFERENCE: Reference Avoli, M., et al., Functional and pharmacological properties of GABA-mediated inhibition in the human neocortex. Can. J. Physiol. Pharmacol. 75, 526, (1997) Johnson, S.W., Seutin, V., Bicuculline methiodide potentiates NMDA-dependent burst firing in rat dopamine neurons by blocking apamin-sensitive Ca2+-activated K+ currents. Neurosci. Lett. 231, 13, (1997) Strobaek, D., et al., Pharmacological characterization of small-conductance Ca2+-activated K+ channels stably expressed in HEK 293 cells. Br. J. Pharmacol. 129, 991, (2000) abstract Chebib, M., Johnston, G.A., The 'ABC' of GABA receptors: a brief review. Clin. Exp. Pharmacol. Physiol. 26, 937, (1999) Merck Merck 13,1207

SOURCE: Alkaloid naturally occurring in the d-form; found in Dicentra cucullaria (L.) Bernh., Adlumia fungosa (ait.), Greene, Fuariaceae, and several Corydalis species

ACTIVITY: GABAa receptor antagonist.

Specification: Alkaloids; Intermediates & Fine Chemicals; Pharmaceuticals; GABA/Glycine receptor; GABA (+)-Bicuculline Chemical Properties:

mp 193-197 C storage temp. 0-6C Merck 13,1207 CAS DataBase Reference485-49-4(CAS DataBase Reference) EPA Substance Registry SystemFuro[3,4-e]-1,3- benzodioxol-8(6H)-one, 6-[(5S)-5,6,7,8-tetrahydro- 6-methyl-1,3-dioxolo[4,5- g]isoquinolin-5-yl]-, (6R)-(485-49-4) Safety Information Hazard Codes T,N,Xn Risk Statements 23/24/25-50-36/37/38-20/21/22 Safety Statements 36/37-45-61-36-26 RIDADR UN 1544 6.1/PG 2 WGK Germany 3 RTECS LV0909840 F 10-23 HazardClass 6.1(b) PackingGroup III (R-(R*,S*))-6-(5,6,7,8-Tetrahydro-6-methyl-1,3-dioxolo(4,5-g)isoquinolin-5-yl)-furo(3,4-e)-1,3-benzodioxol-8(6H)-one English (+)-Bicuculline Usage And Synthesis Chemical Properties:

Pale Yellow Solid UsageAlkaloid naturally occurring in the d-form. Shows GABA antagonist activity. Biological ActivityClassical GABA A antagonist. (+)-Bicuculline

Merck 13 Reference: Monograph Number: 0001207

Title: Bicuculline

CAS Registry Number: 485-49-4

CAS Name:
(6R)-6-[(5S)-5,6,7,8-Tetrahydro-6-methyl-1,3-dioxolo[4,5-g]isoquinolin-5-yl]furo[3,4-e]-1,3-benzodioxol-8(6H)-one

Molecular Formula: C20H17NO6

Molecular Weight: 367.35.

Percent Composition: C 65.39%, H 4.66%, N 3.81%, O 26.13%

Literature References: Alkaloid naturally occurring in the d-form; found in Dicentra cucullaria (L.) Bernh., Adlumia fungosa (Ait.) Greene, Fumariaceae, and several Corydalis species: Manske, Can. J. Res. 7, 265 (1932); 8, 210, 407 (1933); 9, 436 (1933); Edwards, Handa, Can. J. Chem. 39, 1801 (1961). Synthesis of dl-form: Groenewoud, Robinson, J. Chem. Soc. 1936, 199. Resolution of isomers: Haworth et al., Nature 165, 529 (1950). Stereoisomer of adlumidine, q.v., and of capnoidine: Manske, J. Am. Chem. Soc. 72, 3207 (1950). Preliminary stereochemical studies: Safe, Moir, Can. J. Chem. 42, 160 (1964). Revised stereochemistry: Blaha et al., Collect. Czech. Chem. Commun. 29, 2328 (1964); Snatzke et al., Tetrahedron 25, 5059 (1969). Crystal and molecular structure: Gorinsky, Moss, J. Cryst. Mol. Struct. 3, 299 (1973). Shows GABA (q.v.) antagonist activity: Curtis et al., Nature 226, 1222 (1970).

Properties: Elongated plates from chloroform-methanol, mp 215; also reported as mp 177, solidifies and remelts 193-195: Manske, Can. J. Res. 21B, 13 (1943). uv max (acidified ethanol): 225, 296, 324 nm (e 36700, 6390, 5870). [a]D25 +130.5 (CHCl3). pKa 4.84. Sol in benzene, chloroform, ethyl acetate. Sparingly sol in alc and ether.

Melting point: mp 215; mp 177

pKa: pKa 4.84

Optical Rotation: [a]D25 +130.5 (CHCl3)

Absorption maximum: uv max (acidified ethanol): 225, 296, 324 nm (e 36700, 6390, 5870)