



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(6*h*)-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(6*H*)-ONE; (+)-BICUCULLINE; (+)-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: (6*R*)-6-((5*S*)-6-methyl(5,6,7,8-tetrahydro-2*H*-1,3-dioxolano[4,5-*g*]isoquinolin-5-yl))-6-hydro-2*H*-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: GABA_A 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 Reference 485-49-4 (CAS DataBase Reference) EPA Substance Registry System Furo[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 Hazard Class 6.1(b) Packing Group 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 Usage Alkaloid naturally occurring in the d-form. Shows GABA antagonist activity. Biological Activity Classical 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). $[\alpha]_{D25} +130.5$ (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: $[\alpha]_{D25} +130.5$ (CHCl₃)

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