



Formula: C<sub>20</sub>H<sub>17</sub>NO<sub>6</sub>

MW: 367.36

CAS: 485-49-4

TNP NUMBER: TNP00509

MDL NUMBER: MFCD00067279

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

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

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 Ca<sup>2+</sup>-activated K<sup>+</sup> currents. *Neurosci. Lett.* 231, 13, (1997)  
Strobaek, D., et al., Pharmacological characterization of small-conductance Ca<sup>2+</sup>-activated K<sup>+</sup> 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

ACCEPTORS: 6

DONORS: 0

ROTATION BONDS: 1

N+O: 7

Chiral Centers: 2

LogP: 2.62

LogS: -4.34

LIPINSKI: 4

Synonyms:

(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;(+) -BICUCULLINE;(+) -BICUCULLINE;BICUCULLINE;D-BICUCULLINE;5-g)isoquinolin-5-yl)-, (r-(r\*,s\*))-lo(;bicucullin

CAS:485-49-4

MF:C20H17NO6

MW:367.35

EINECS:207-619-7

Product Categories: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 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) 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 (+)-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

