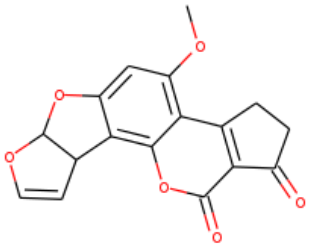
Aflatoxin b1



Other names: 1-Cyclopentene-1-carboxylic acid, 2-(3a,8a-dihydro-4-hydroxy-6-methoxyfuro[2,3-b]benzofuran-5-yl)-5-oxo-, «delta»-lactone; 2,3,6a«alpha»,9a«alpha»-tetrahydro-4-methoxycyclopenta[c]furo[2',3':4,5]furo[2,3-h]chromene-1,11-dione; AFBI; Cyclopenta(c)furo(3',2':4,5)furo(2,3-h)(1)benzopyran-1,11-dione, 2,3,6a,9a-tetrahydro-4-methoxy-; Cyclopenta[c]furo[3',2':4,5]furo[2,3-h][1]benzopyran-1,11-dione, 2,3,6a,9a-tetrahydro-4-methoxy-, (6aR-cis)-; Cyclopenta[c]furo[3',2':4,5]furo[2,3-h][1]benzopyran-1,11-dione, 2,3,6a«alpha»,9a«alpha»-tetrahydro-4-methoxy-.

InChI: InChI=1S/C17H12O6/c1-20-10-6-11-14(8-4-5-21-17(8)22-11)15-13(10)7-2-3-9(18)12(7)16(19)23-15/h4-6,8,17H,2-3H2,1H3

InChI Key: OQIQSTLJSLGHID-UHFFFAOYSA-N

Formula: C17H12O6

SMILES: COc1cc2c(c3oc(=O)c4c(c13)CCC4=O)C1C=COC1O2

Molecular Weight: 312.27

CAS: 1162-65-8

Physical Properties

Property	Value	Unit	Source
$logP_{oct/wat}$	2.28		Crippen Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H12O6/c1-20-10-6-11-14(8-4-5-21-17(8)22-11)15-13(10)7-2-3-9(18)12(7)16(19)23-15/h4-6,8,17H,2-3H2,1H3

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

***logP*$_{oct/wat}$**: Octanol/Water partition coefficient .