Aflatoxin B1

Other names:	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- AFB1 Cyclopenta(c)furo(3',2':4,5)furo(2,3-h)(1)benzopyran-1,11-dione, 2,3,6a,9a-tetrahydro-4-methoxy- 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]chro
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)1
InchiKey:	OQIQSTLJSLGHID-UHFFFAOYSA-N
Formula:	C17H12O6
SMILES:	COc1cc2c(c3oc(=O)c4c(c13)CCC4=O)C1C=COC1O2
Mol. weight [g/mol]:	312.27
CAS:	1162-65-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.63		Crippen Method
logp	2.276		Crippen Method
mcvol	201.210	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1162658&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume