Aflatoxin G1

Other names:	1H,12H-Furo[3',2':4,5]furo[2,3-h]pyrano[3,4-c][1]benzopyran-1,12-dione, 3,4,7a,10a-tetrahydro-5-methoxy-, (7aR-cis)-, (7aR,cis)3,4,7a,10a-tetrahydro-5-methoxy-1H,12H-furo[3',2':4,5]furo[2,3-h]pyrano[3,4-c]c
Inchi:	InChI=1S/C17H12O7/c1-20-9-6-10-12(8-3-5-22-17(8)23-10)14-11(9)7-2-4-21-15(18)13(7
InchiKey:	XWIYFDMXXLINPU-WNWIJWBNSA-N
Formula:	C17H12O7
SMILES:	COc1cc2c(c3oc(=O)c4c(c13)CCOC4=O)C1C=COC1O2
Mol. weight [g/mol]:	328.27
CAS:	1165-39-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.21		Crippen Method
logp	1.860		Crippen Method
mcvol	207.080	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=C1165395&Units=SI

Legend

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

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