

Aflatoxin B2

Other names:

Cyclopenta[c]furo[3',2':4,5]furo[2,3-h][1]benzopyran-1,11-dione,
2,3,6a,8,9,9a-hexahydro-4-methoxy-, (6aR-cis)-
Cyclopenta[c]furo[3',2':4,5]furo[2,3-h][1]benzopyran-1,11-dione,
2,3,6a«alpha»,8,9,9a«alpha»-hexahydro-4-methoxy-
Dihydroaflatoxin B1

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2,3,6a«alpha»,8,9,9a«alpha»-hexahydro-4-methoxycyclopenta[c]furo[2',3':4,5]furo[2,3-h]

Inchi:

InChI=1S/C17H14O6/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:

WWSYXEZEXMQWHT-WNWIJWBNSA-N

Formula:

C17H14O6

SMILES:

COc1cc2c(c3oc(=O)c4c(c13)CCC4=O)C1CCOC1O2

Mol. weight [g/mol]:

314.29

CAS:

7220-81-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.28		Crippen Method
logp	2.153		Crippen Method
mcvol	205.510	ml/mol	McGowan Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C7220817&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/90-202-7/Aflatoxin-B2.pdf>

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