Sterigmatocystin

Other names:	7H-Furo[3',2':4,5]furo[2,3-c]xanthen-7-one, 3a,12c-dihydro-8-hydroxy-6-methoxy-, (3aR-cis)- 7H-Furo[3',2':4,5]furo[2,3-c]xanthen-7-one, 3a,12c-dihydro-8-hydroxy-6-methoxy- NSC 204985 3a,12c-Dihydro-8-hydroxy-6-methoxy-7H-furo(3',2':4,5)furo(2,3-c)xanthen-7-one 8-Hydroxy-6-methoxy-3a,12c-dihydro-7H-furo[3',2':4,5]furo[2,3-c]xanthen-7-one (3aR-cis)3a,12c-dihydro-8-hydroxy-6-methoxy-7H-furo[3',2':4,5]furo[2,3-c]xanthen-7-one
Inchi:	InChI=1S/C18H12O6/c1-21-11-7-12-13(8-5-6-22-18(8)24-12)17-15(11)16(20)14-9(19)3-2
InchiKey:	UTSVPXMQSFGQTM-UHFFFAOYSA-N
Formula:	C18H12O6
SMILES:	COc1cc2c(c3oc4cccc(O)c4c(=O)c13)C1C=COC1O2
Mol. weight [g/mol]:	324.28
CAS:	10048-13-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.04		Crippen Method
logp	3.006		Crippen Method
mcvol	211.000	ml/mol	McGowan Method
rinpol	2999.00		NIST Webbook
rinpol	2999.00		NIST Webbook

Sources

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=C10048132&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices