3',4',5,6,7,8-Hexamethoxyflavone

Other names:	2-(3,4-dimethoxyphenyl)-5,6,7,8-tetramethoxy-4H-1-benzopyran-4-one
	2-(3,4-dimethoxyphenyl)-5,6,7,8-tetramethoxy-4H-chromen-4-one
	4H-1-Benzopyran-4-one, 2-(3,4-dimethoxyphenyl)-5,6,7,8-tetramethoxy-
	Flavone, 5,6,7,8,3',4'-hexamethoxy
	Nobiletin
Inchi:	InChI=1S/C21H22O8/c1-23-13-8-7-11(9-15(13)24-2)14-10-12(22)16-17(25-3)19(26-4)21
InchiKey:	MRIAQLRQZPPODS-UHFFFAOYSA-N
Formula:	C21H22O8
SMILES:	COc1ccc(-c2cc(=O)c3c(OC)c(OC)c(OC)c(OC)c3o2)cc1OC
Mol. weight [g/mol]:	402.39
CAS:	478-01-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.75		Crippen Method
logp	3.512		Crippen Method
mcvol	286.730	ml/mol	McGowan Method
rinpol	3380.90		NIST Webbook
rinpol	3392.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C478013&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measuring and validation for isothermal solubility data of solid 2-(3,4-Dimethoxyphenyl)-5,6,7,8-tetramethoxychromen-4-one (nobiletin) in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.jct.2015.08.018

Legend

log10ws:	Log10 of Water solubility in mol/l

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