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

Inchi:	InChI=1S/C22H24O9/c1-24-12-9-8-11(10-13(12)25-2)16-19(27-4)15(23)14-17(26-3)20(2
InchiKey:	SSXJHQZOHUYEGD-UHFFFAOYSA-N
Formula:	C22H24O9
SMILES:	COc1ccc(-c2oc3c(OC)c(OC)c(OC)c(OC)c3c(=O)c2OC)cc1OC
Mol. weight [g/mol]:	432.42
CAS:	1178-24-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.87		Crippen Method
logp	3.520		Crippen Method
mcvol	306.690	ml/mol	McGowan Method
rinpol	3342.40		NIST Webbook
rinpol	3375.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1178241&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices

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