3,5,6,7-Tetramethoxy-2-(4-methoxyphenyl)-4h-chr

Inchi:	InChI=1S/C20H20O7/c1-22-12-8-6-11(7-9-12)17-20(26-5)16(21)15-13(27-17)10-14(23-2
InchiKey:	OWNRDLYPIYHOQK-UHFFFAOYSA-N
Formula:	C20H20O7
SMILES:	COc1ccc(-c2oc3cc(OC)c(OC)c(OC)c3c(=O)c2OC)cc1
Mol. weight [g/mol]:	372.37
CAS:	4472-73-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.63		Crippen Method
logp	3.503		Crippen Method
mcvol	266.770	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=C4472735&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

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