

2-(3,4-Dimethoxyphenyl)-5-hydroxy-6,7,8-trimethoxy-4H-chromen-4-one

Inchi: InChI=1S/C20H20O8/c1-23-12-7-6-10(8-14(12)24-2)13-9-11(21)15-16(22)18(25-3)20(27)
InchiKey: DOFJNFPSMUCECH-UHFFFAOYSA-N
Formula: C20H20O8
SMILES: COc1ccc(-c2cc(=O)c3c(O)c(OC)c(OC)c(OC)c3o2)cc1OC
Mol. weight [g/mol]: 388.37
CAS: 2174-59-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.18		Crippen Method
logp	3.209		Crippen Method
mcvol	272.640	ml/mol	McGowan Method
rinpol	3355.00		NIST Webbook
rinpol	3355.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C2174596&Units=SI>

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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