4H-1-Benzopyran-4-one, 2-(3,4-dimethoxyphenyl)-5-hydroxy-3,6,7-trimetho

Other names: Flavone, 5-hydroxy-3,3',4',6,7-pentamethoxy-
Artemetin
Artemisetin
Erianthin
5-Hydroxy-3,6,7,3',4'-pentamethoxyflavone

Inchi: InChI=1S/C20H20O8/c1-23-11-7-6-10(8-12(11)24-2)18-20(27-5)17(22)15-13(28-18)9-14

InchiKey: RIGYMJVFEJNCKD-UHFFFAOYSA-N

Formula: C20H20O8

SMILES: COc1ccc(-c2oc3cc(OC)c(OC)c(O)c3c(=O)c2OC)cc1OC

Mol. weight [g/mol]: 388.37

CAS: 479-90-3

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	3381.20		NIST Webbook
rinpol	3381.20		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C479903&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