

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

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:	<chem>COc1ccc(-c2oc3cc(OC)c(OC)c(O)c3c(=O)c2OC)cc1OC</chem>
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/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=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

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