4H-1-Benzopyran-4-one, 5-hydroxy-2-(4-hydroxyphenyl)-3,7-dimethoxy-

Other names: Flavone, 4',5-dihydroxy-3,7-dimethoxy-
Jaranol
Kaempferol 3,7-dimethyl ether
Kumatakenin
3,7-Di-O-methyl kaempferol
4',5-Dihydroxy-3,7-dimethoxyflavone
Kaempferol, 3,7-dimethyl
5-Hydroxy-2-(4-hydroxyphenyl)-3,7-dimethoxy-4H-chromen-4-one

Inchi: InChI=1S/C17H14O6/c1-21-11-7-12(19)14-13(8-11)23-16(17(22-2)15(14)20)9-3-5-10(18

InchiKey: BJBUTJQYZDYRMJ-UHFFFAOYSA-N

Formula: C17H14O6

SMILES: COc1cc(O)c2c(=O)c(OC)c(-c3ccc(O)cc3)oc2c1

Mol. weight [g/mol]: 314.29

CAS: 3301-49-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.37		Crippen Method
logp	2.888		Crippen Method
mcvol	218.630	ml/mol	McGowan Method
rinpol	3067.20		NIST Webbook
rinpol	3067.20		NIST Webbook

Sources

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=C3301493&Units=SI

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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices