4H-1-Benzopyran-4-one, 5-hydroxy-2-(4-hydroxyphenyl)-6,7-dimethoxy-

Other names: Flavone, 4',5-dihydroxy-6,7-dimethoxy-
Cirsimaritin
Scrophulein
6-Methoxygenkwanin
6,7-Dimethoxyscutellarein

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

InchiKey: ZIIAJIWLQUVGHB-UHFFFAOYSA-N

Formula: C17H14O6

SMILES: COc1cc2oc(-c3ccc(O)cc3)cc(=O)c2c(O)c1OC

Mol. weight [g/mol]: 314.29

CAS: 6601-62-3

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	3287.00		NIST Webbook
rinpol	3287.00		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=C6601623&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