4H-1-Benzopyran-4-one, 5,7-dimethoxy-2-phenyl-

Other names: Flavone, 5,7-dimethoxy-
Chrysin - dimethyl ether
Dimethylchrysin
5,7-Dimethoxyflavone, TMS

Inchi: InChI=1S/C17H14O4/c1-19-12-8-15(20-2)17-13(18)10-14(21-16(17)9-12)11-6-4-3-5-7-11

InchiKey: JRFZSUMZAUHNSL-UHFFFAOYSA-N

Formula: C17H14O4

SMILES: COc1cc(OC)c2c(=O)cc(-c3ccccc3)oc2c1

Mol. weight [g/mol]: 282.29

CAS: 21392-57-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.27		Crippen Method
logp	3.477		Crippen Method
mcvol	206.890	ml/mol	McGowan Method
rinpol	2588.00		NIST Webbook
rinpol	2588.00		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=C21392574&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