

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)11-6-4-3-5-7-1

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
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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=C21392574&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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