

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/ci990307I>

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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