4H-1-Benzopyran-4-one, 5-hydroxy-7-methoxy-2-(4-methoxyphenyl)-

Other names: Flavone, 5-hydroxy-4',7-dimethoxy-
Apigenin 4',7-dimethyl ether
Apigenin 7,4'-dimethyl ether
Genkwanin 4'-methyl ether
4',7-Dimethylapigenin
5-Hydroxy-4',7-dimethoxyflavone
5-Hydroxy-7,4'-dimethoxyflavone
4',7-Dimethoxy-5-hydroxy flavone
5-Hydroxy-7-methoxy-2-(4-methoxyphenyl)-4H-chromen-4-one
Apigenin, 7,4'-dimethyl
NSC 94547
5-hydroxy-7-methoxy-2-(4-methoxyphenyl)-4-benzopyrone

Inchi: InChI=1S/C17H14O5/c1-20-11-5-3-10(4-6-11)15-9-14(19)17-13(18)7-12(21-2)8-16(17)22

InchiKey: LZERJKGWTQYMBB-UHFFFAOYSA-N

Formula: C17H14O5

SMILES: COc1ccc(-c2cc(=O)c3c(O)cc(OC)cc3o2)cc1

Mol. weight [g/mol]: 298.29

CAS: 5128-44-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.82		Crippen Method
logp	3.183		Crippen Method
mcvol	212.760	ml/mol	McGowan Method
rinpol	2964.00		NIST Webbook
rinpol	2964.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5128449&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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