Pectolinaringenin

Other names:	4H-1-Benzopyran-4-one, 5,7-dihydroxy-6-methoxy-2-(4-methoxyphenyl)- Flavone, 5,7-dihydroxy-4',6-dimethoxy- Pectolinarigenin 5,7-Dihydroxy-4',6-dimethoxyflavone 5,7-Dihydroxy-6,4'-dimethoxyflavone 5,7-dihydroxy-6-methoxy-2-(4-methoxyphenyl)-4-benzopyrone Pectolinargenin
Inchi:	InChI=1S/C17H14O6/c1-21-10-5-3-9(4-6-10)13-7-11(18)15-14(23-13)8-12(19)17(22-2)16
InchiKey:	GPQLHGCIAUEJQK-UHFFFAOYSA-N
Formula:	C17H14O6
SMILES:	COc1ccc(-c2cc(=O)c3c(O)c(OC)c(O)cc3o2)cc1
Mol. weight [g/mol]:	314.29
CAS:	520-12-7

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	3038.90		NIST Webbook
rinpol	3038.90		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C520127&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