5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-chromen-4

Other names:	4',5,7-trihydroxyflavone
	apigenin
Inchi:	InChI=1S/C15H10O5/c16-9-3-1-8(2-4-9)13-7-12(19)15-11(18)5-10(17)6-14(15)20-13/h1-
InchiKey:	KZNIFHPLKGYRTM-UHFFFAOYSA-N
Formula:	C15H10O5
SMILES:	O=c1cc(-c2ccc(O)cc2)oc2cc(O)cc(O)c12
Mol. weight [g/mol]:	270.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.14		Cheméo Relay (1.0)
logp	2.577		Crippen Method
mcvol	184.580	ml/mol	McGowan Method
tf	565.46	K	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Measurement and correlation of solubilities of apigenin and apigenin 7-O-rutinoside in seven solvents at different temperatures:	https://www.doi.org/10.1016/j.jct.2010.09.013
Solubilities of Apigenin in Ethanol + Water at Different Temperatures:	https://www.doi.org/10.1021/je1001208

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point