4H-1-Benzopyran-4-one, 5-hydroxy-6,7-dimethoxy-2-(4-methoxyphenyl)-

Other names: 5-Hydroxy-6,7-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one
Salvigenin

Inchi: InChI=1S/C18H16O6/c1-21-11-6-4-10(5-7-11)13-8-12(19)16-14(24-13)9-15(22-2)18(23-3

InchiKey: QCDYOIZVELGOLZ-UHFFFAOYSA-N

Formula: C18H16O6

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

Mol. weight [g/mol]: 328.32

CAS: 19103-54-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.94		Crippen Method
logp	3.191		Crippen Method
mcvol	232.720	ml/mol	McGowan Method
rinpol	3232.60		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=C19103549&Units=SI

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

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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