7H-Furo[3,2-g][1]benzopyran-7-one, 4,9-dimethoxy-

Other names: Isopimpinellin
5,8-Dimethoxypsoralen
5,8-Dimethoxypsoralene
5,8-Dimethoxy-6,7-furanocoumarin

Inchi: InChI=1S/C13H10O5/c1-15-10-7-3-4-9(14)18-12(7)13(16-2)11-8(10)5-6-17-11/h3-6H,1-2

InchiKey: DFMAXQKDIGCMTL-UHFFFAOYSA-N

Formula: C13H10O5

SMILES: COc1c2ccoc2c(OC)c2oc(=O)ccc12

Mol. weight [g/mol]: 246.22

CAS: 482-27-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.21		Crippen Method
logp	2.556		Crippen Method
mcvol	165.000	ml/mol	McGowan Method
rinpol	2250.00		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2240.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C482279&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