2H-1-Benzopyran-2-one, 6,7-dimethoxy-4-methyl-

Other names: Coumarin, 6,7-dimethoxy-4-methyl-
4-Methyl-6,7-dimethoxycoumarin
6,7-Dimethoxy-4-methylcoumarin

Inchi: InChI=1S/C12H12O4/c1-7-4-12(13)16-9-6-11(15-3)10(14-2)5-8(7)9/h4-6H,1-3H3

InchiKey: GBYDSYPGGDKWGZ-UHFFFAOYSA-N

Formula: C12H12O4

SMILES: COc1cc2oc(=O)cc(C)c2cc1OC

Mol. weight [g/mol]: 220.22

CAS: 4281-40-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.15		Crippen Method
logp	2.119		Crippen Method
mcvol	160.200	ml/mol	McGowan Method
rinpol	2166.00		NIST Webbook
rinpol	2166.00		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=C4281407&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