

5,7,8-trimethoxycoumarin

Inchi:	InChI=1S/C12H12O5/c1-14-8-6-9(15-2)12(16-3)11-7(8)4-5-10(13)17-11/h4-6H,1-3H3
InchiKey:	MSFXSDYNQKVMJTJ-UHFFFAOYSA-N
Formula:	C12H12O5
SMILES:	COc1cc(OC)c2ccc(=O)oc2c1OC
Mol. weight [g/mol]:	236.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.79		Crippen Method
logp	1.819		Crippen Method
mcvol	166.070	ml/mol	McGowan Method
rinsol	2107.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R422283&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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<https://www.chemeo.com/cid/85-617-3/5-7-8-trimethoxycoumarin.pdf>

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