

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:	<chem>COc1cc2oc(=O)cc(C)c2cc1OC</chem>
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
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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