2H-1-Benzopyran-2-one, 5,7-dimethoxy-

Other names:	Coumarin, 5,7-dimethoxy-
	Citraptene
	Citropten
	Citroptene
	Limetin
	Limettin
	5,7-Dimethoxycoumarin
	5,7-Dimethoxy-2H-chromen-2-one
	5,7-Dimethoxy-2H-1-benzo-pyran-2-one
	5,7-Dimethyloxy-2H-1-benzopyran-2-one
	NSC 102793
	5,7-dimethoxy-2-benzopyrone
Inchi:	InChI=1S/C11H10O4/c1-13-7-5-9(14-2)8-3-4-11(12)15-10(8)6-7/h3-6H,1-2H3
InchiKey:	NXJCRELRQHZBQA-UHFFFAOYSA-N
Formula:	C11H10O4
SMILES:	COc1cc(OC)c2ccc(=O)oc2c1
Mol. weight [g/mol]:	206.19
CAS:	487-06-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.67		Crippen Method
logp	1.810		Crippen Method
mcvol	146.110	ml/mol	McGowan Method
rinpol	1916.00		NIST Webbook
rinpol	1992.80		NIST Webbook
rinpol	1916.00		NIST Webbook
rinpol	1992.80		NIST Webbook
rinpol	1916.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C487069&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