6,7-Dimethoxy-2-phenethyl-4H-chromen-4-one

Other names:	6,7-Dimethoxy-2-phenethylchromone
	4H-1-Benzopyran-4-one, 6,7-dimethoxy-2-(2-phenylethyl)-
Inchi:	InChI=1S/C19H18O4/c1-21-18-11-15-16(20)10-14(23-17(15)12-19(18)22-2)9-8-13-6-4-3
InchiKey:	MVQOWXHYPYRBOE-UHFFFAOYSA-N
Formula:	C19H18O4
SMILES:	COc1cc2oc(CCc3ccccc3)cc(=O)c2cc1OC
Mol. weight [g/mol]:	310.34
CAS:	84294-87-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.09		Crippen Method
logp	3.595		Crippen Method
mcvol	235.070	ml/mol	McGowan Method
rinpol	2891.40		NIST Webbook
rinpol	2891.40		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84294871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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