(E)-6-(3,4-Dimethoxystyryl)-4-methoxy-2H-pyran-2

Inchi:	InChI=1S/C16H16O5/c1-18-13-9-12(21-16(17)10-13)6-4-11-5-7-14(19-2)15(8-11)20-3/h4
InchiKey:	GBJRDULCMRSYSL-GQCTYLIASA-N
Formula:	C16H16O5
SMILES:	COc1cc(C=Cc2ccc(OC)c(OC)c2)oc(=O)c1
Mol. weight [g/mol]:	288.30
CAS:	56070-89-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.59		Crippen Method
logp	2.836		Crippen Method
mcvol	213.830	ml/mol	McGowan Method
rinpol	2880.80		NIST Webbook
rinpol	2880.80		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56070894&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

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