2-(4-Allyl-2,6-dimethoxy-phenoxy)-1-benzo[1,3]dio
TMS

InChI: InChI=1S/C24H32O7Si/c1-8-9-17-12-21(25-3)23(22(13-17)26-4)29-16(2)24(31-32(5,6)7)

InchiKey: QTAQACPASHCDRX-UHFFFAOYSA-N

Formula: C24H32O7Si

SMILES: C=CCc1cc(OC)c(OC(C)C(Oc2ccc3c(c2)OCO3)O[Si](C)(C)C)c(OC)c1

Mol. weight [g/mol]: 460.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.42		Crippen Method
logp	5.185		Crippen Method
rinpol	2630.00		NIST Webbook
rinpol	2630.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R294296&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices