2-(4-Allyl-2,6-dimethoxy-phenoxy)-1 -benzo[1,3]dioxol-5-yl-propan-1-ol, TES

Inchi: InChI=1S/C27H38O7Si/c1-8-12-20-15-24(28-6)26(25(16-20)29-7)32-19(5)27(34-35(9-2,1

InchiKey: SPKUYYPPLYHQLT-UHFFFAOYSA-N

Formula: C27H38O7Si

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

Mol. weight [g/mol]: 502.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.67		Crippen Method
logp	6.355		Crippen Method
rinpol	2940.00		NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R294281&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices