

2-(4-Allyl-2,6-dimethoxy-phenoxy)-1-(3,4-dimethoxy-phenyl)-propan-1-ol, TMS

Inchi: InChI=1S/C25H36O6Si/c1-10-11-18-14-22(28-5)25(23(15-18)29-6)30-17(2)24(31-32(7,8))
InchiKey: PGPFNHBPJKCGHV-UHFFFAOYSA-N
Formula: C25H36O6Si
SMILES: C=CCc1cc(OC)c(OC(C)C(O[Si](C)(C)C)c2ccc(OC)c(OC)c2)c(OC)c1
Mol. weight [g/mol]: 460.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.56		Crippen Method
logp	5.810		Crippen Method
rinpol	2655.00		NIST Webbook
rinpol	2655.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R294261&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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