

4-[2-(4-Allyl-2,6-dimethoxy-phenoxy)-1-hydroxy-propyl]-2,6-dimethoxy-phenol

TES

InchiKey:

InChI=1S/C34H56O6Si2/c1-13-20-26-21-28(35-9)32(29(22-26)36-10)25(8)33(39-41(14-2

Formula:

C34H56O6Si2

SMILES:

C=CCc1cc(OC)c(C(C)C(O[Si](CC)(CC)CC)c2cc(OC)c(O[Si](CC)(CC)CC)c(OC)c2)c(OC)

Mol. weight [g/mol]:

616.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.20		Crippen Method
logp	9.700		Crippen Method
rinpol	3360.00		NIST Webbook
rinpol	3360.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R294310&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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