

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

TPS

InchiKey:

InChI=1S/C40H68O7Si2/c1-12-19-32-26-34(30-41)39(35(27-32)42-9)45-31(8)38(46-48(2

Formula:

C40H68O7Si2

SMILES:

C=CCc1cc(CO)c(OC(C)C(O[Si](CCC)(CCC)CCC)c2cc(OC)c(O[Si](CCC)(CCC)CCC)c(O

Mol. weight [g/mol]:

717.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.62		Crippen Method
logp	11.188		Crippen Method
rinpol	3595.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R306166&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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