

5-[2-(4-Allyl-2,6-dimethoxy-phenoxy)-1-hydroxy-propyl]-2-methoxy-phenol-TES

TES

InchiKey:

InChI=1S/C33H54O5Si2/c1-12-19-26-22-30(35-10)32(31(23-26)36-11)25(8)33(38-40(16

Formula:

C33H54O5Si2

SMILES:

C=CCc1cc(OC)c(C(C)C(O[Si](CC)(CC)CC)c2ccc(OC)c(O[Si](CC)(CC)CC)c2)c(OC)c1

Mol. weight [g/mol]:

586.95

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.08		Crippen Method
logp	9.691		Crippen Method
rinpol	3310.00		NIST Webbook
rinpol	3310.00		NIST Webbook

Sources

Crippen Method:

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

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R294434&Units=SI>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

rinpol:

Non-polar retention indices

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