

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

TPS

InchiKey:

InChI=1S/C39H66O6Si2/c1-11-18-32-27-34(30-40)39(37(28-32)42-10)43-31(8)38(45-47)

Formula:

C39H66O6Si2

SMILES:

C=CCc1cc(CO)c(OC(C)C(O[Si](CCC)(CCC)CCC)c2ccc(O[Si](CCC)(CCC)CCC)c(OC)c2

Mol. weight [g/mol]:

687.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.50		Crippen Method
logp	11.180		Crippen Method
rinpol	3540.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R306186&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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