

2-(4-Allyl-2,6-dimethoxy-phenoxy)-1-(3,4,5-trimethoxyphenyl)propan-1-ol-TES

TES

InchiKey:

InChI=1S/C29H44O7Si/c1-11-15-21-16-23(30-6)29(24(17-21)31-7)35-20(5)27(36-37(12-13)14)28

AKSDDYGGFYIBDD-UHFFFAOYSA-N

Formula:

C₂₉H₄₄O₇Si

SMILES:

C=CCc1cc(OC)c(OC(C)C(O[Si](CC)(CC)CC)c2cc(OC)c(OC)c(OC)c2)c(OC)c1

Mol. weight [g/mol]:

532.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.94		Crippen Method
logp	6.989		Crippen Method
rinpol	3020.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R294221&Units=SI>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

rinpol:

Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/79-989-8/2-4-Allyl-2-6-dimethoxy-phenoxy-1-3-4-5-trimethoxy-phenyl-propan-1-ol-TES>.

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