trans-Diethylstilbestrol, bis(tert-butyldimethylsilyl) ether

Other names: [4-((1E)-1-Ethyl-2-(4-[(tert-butyldimethylsilyl)oxy]phenyl)-1-butenyl)phenoxy](tert-butyldim
Inchi: InChI=1S/C30H48O2Si2/c1-13-27(23-15-19-25(20-16-23)31-33(9,10)29(3,4)5)28(14-2)24
InchiKey: NRFANCKTHNLRHQ-BYYHNAKLSA-N
Formula: C30H48O2Si2
SMILES: CCC(=C(CC)c1ccc(O[Si](C)(C)C(C)(C)C)cc1)c1ccc(O[Si](C)(C)C(C)(C)C)cc1
Mol. weight [g/mol]: 496.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.28		Crippen Method
logp	10.185		Crippen Method
rinpol	2927.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373395&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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