Tocopherol-.delta.-TMS-Derivative (High Mass Adjustment=50%)

Other names: Tocopherol-«delta»-tms-derivative (high mass adjustment=0%)
Tocopherol-«delta»-tms-derivative (high mass adjustment=50%)
.delta.-Tocopherol, O-trimethylsilyl-

Inchi: InChI=1S/C30H54O2Si/c1-23(2)13-10-14-24(3)15-11-16-25(4)17-12-19-30(6)20-18-27-2

InchiKey: OCAXNUPKBRKNKO-UHFFFAOYSA-N

Formula: C30H54O2Si

SMILES: Cc1cc(O[Si](C)(C)C)cc2c1OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2

Mol. weight [g/mol]: 474.85

Physical Properties

Property code	Value	Unit	Source
logp	9.732		Crippen Method
rinpol	2913.00		NIST Webbook
rinpol	2900.00		NIST Webbook
rinpol	2900.00		NIST Webbook
rinpol	2913.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52704117&Units=SI

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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