Tocopherol-«delta»-tms-derivative (high mass adjustment=100%)

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]: 474.83
CAS: 52704-11-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.28		Crippen Method
logp	9.732		Crippen Method
rinpol	2900.00		NIST Webbook
rinpol	2913.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52704117&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