«alpha»-Tocopherol, TMS

Inchi: InChI=1S/C32H58O2Si/c1-23(2)15-12-16-24(3)17-13-18-25(4)19-14-21-32(8)22-20-29-2
InchiKey: MJWXSUWKOCZGBM-CAHKVJEUSA-N
Formula: C32H58O2Si
SMILES: Cc1c(C)c2c(c(C)c1O[Si](C)(C)C)CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2
Mol. weight [g/mol]: 502.89

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.23		Crippen Method
logp	10.348		Crippen Method
rinpol	3143.00		NIST Webbook
rinpol	3149.00		NIST Webbook
rinpol	3143.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R573287&Units=SI

Legend

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