1,2-Cyclododecanediol, DTBS

Inchi: InChI=1S/C20H40O2Si/c1-19(2,3)23(20(4,5)6)21-17-15-13-11-9-7-8-10-12-14-16-18(17)22-23/h17-18H,7-16H2,1-6H3/t17-,18-/m1/s1
InchiKey: RLPUWUWWCZGDJU-UHFFFAOYSA-N
Formula: C20H40O2Si
SMILES: CC(C)(C)[Si]1(C(C)(C)C)OC2CCCCCCCCCCC2O1
Mol. weight [g/mol]: 340.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.02		Crippen Method
logp	6.727		Crippen Method
rinpol	2140.00		NIST Webbook
rinpol	2140.00		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=R115212&Units=SI

Legend

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