cis-1,2-Indanediol, DTBS

Inchi: InChI=1S/C17H26O2Si/c1-16(2,3)20(17(4,5)6)18-14-11-12-9-7-8-10-13(12)15(14)19-20/
InchiKey: CZQZZACQVQCFKC-CABCVRRESA-N
Formula: C17H26O2Si
SMILES: CC(C)(C)[Si]1(C(C)(C)C)OC2Cc3ccccc3C2O1
Mol. weight [g/mol]: 290.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	4.742		Crippen Method
rinpol	1760.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R115341&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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