1,2-Propanediol, 3-(3,4-methylenedioxyphenyl), DTBS

Inchi: InChI=1S/C17H26O5Si/c1-16(2,3)23(17(4,5)6)20-10-15(22-23)21-12-7-8-13-14(9-12)19-

InchiKey: BHWRFRGTLUYCSP-UHFFFAOYSA-N

Formula: C17H26O5Si

SMILES: CC(C)(C)[Si]1(C(C)(C)C)OCC(Oc2ccc3c(c2)OCO3)O1

Mol. weight [g/mol]: 338.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	4.209		Crippen Method
rinpol	2105.00		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=R41057&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices