Benzoic acid, 2-hydroxy-3-methyl-4-methoxy, DTBS

Inchi: InChI=1S/C17H26O4Si/c1-11-13(19-8)10-9-12-14(11)20-22(16(2,3)4,17(5,6)7)21-15(12)

InchiKey: BZUHHCGKFPAUOT-UHFFFAOYSA-N

Formula: C17H26O4Si

SMILES: COc1ccc2c(c1C)O[Si](C(C)(C)C)(C(C)(C)C)OC2=O

Mol. weight [g/mol]: 322.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.47		Crippen Method
logp	4.595		Crippen Method
rinpol	2045.00		NIST Webbook
rinpol	2045.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R41203&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