Benzoic acid, 2-hydroxy-3-methoxycarbonyl, DTBS

Inchi: InChI=1S/C17H24O5Si/c1-16(2,3)23(17(4,5)6)21-13-11(14(18)20-7)9-8-10-12(13)15(19)22-23(16,17)OC2=O

InchiKey: QNRVGUQFEJCZGN-UHFFFAOYSA-N

Formula: C17H24O5Si

SMILES: COC(=O)c1cccc2c1O[Si](C(C)(C)C)(C(C)(C)C)OC2=O

Mol. weight [g/mol]: 336.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	4.065		Crippen Method
rinpol	2000.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R41182&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