Benzoic acid, 3,4-dihydroxy, methyl ester, DTBS

Inchi: InChI=1S/C16H24O4Si/c1-15(2,3)21(16(4,5)6)19-12-9-8-11(14(17)18-7)10-13(12)20-21/
InchiKey: URKUFCXHMWIYOY-UHFFFAOYSA-N
Formula: C16H24O4Si
SMILES: COC(=O)c1ccc2c(c1)O[Si](C(C)(C)C)(C(C)(C)C)O2
Mol. weight [g/mol]: 308.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	4.287		Crippen Method
rinpol	1795.00		NIST Webbook
rinpol	1795.00		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=R41285&Units=SI

Legend

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