Benzoic acid, 2-hydroxy-3-(2,3-dioxypropyl), methyl ester, DTBS #1

Inchi: InChI=1S/C19H30O5Si/c1-18(2,3)25(19(4,5)6)23-12-14(24-25)11-13-9-8-10-15(16(13)20

InchiKey: JFTRHZPZIPLBMY-UHFFFAOYSA-N

Formula: C19H30O5Si

SMILES: COC(=O)c1cccc(CC2CO[Si](C(C)(C)C)(C(C)(C)C)O2)c1O

Mol. weight [g/mol]: 366.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	4.179		Crippen Method
rinpol	2295.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R41146&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