Benzoic acid, 2,3-dihydroxy, methyl ester, DTBS

Inchi: InChI=1S/C16H24O4Si/c1-15(2,3)21(16(4,5)6)19-12-10-8-9-11(13(12)20-21)14(17)18-7/

InchiKey: DVSCEVIMVUSJJT-UHFFFAOYSA-N

Formula: C16H24O4Si

SMILES: COC(=O)c1cccc2c1O[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	1910.00		NIST Webbook
rinpol	1910.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R41100&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