Benzoic acid, 2-hydroxy-4,6-dimethyl, DTBS

Inchi: InChI=1S/C17H26O3Si/c1-11-9-12(2)14-13(10-11)19-21(16(3,4)5,17(6,7)8)20-15(14)18/h
InchiKey: DQOUYPLOHNAWOJ-UHFFFAOYSA-N
Formula: C17H26O3Si
SMILES: Cc1cc(C)c2c(c1)O[Si](C(C)(C)C)(C(C)(C)C)OC2=O
Mol. weight [g/mol]: 306.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	4.895		Crippen Method
rinpol	1890.00		NIST Webbook
rinpol	1890.00		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=R41221&Units=SI

Legend

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