Benzoic acid, 2-hydroxy-5-methyl-3-(1,1-dimethylethyl), DTBS

InChI: InChI=1S/C20H32O3Si/c1-13-11-14-16(15(12-13)18(2,3)4)22-24(19(5,6)7,20(8,9)10)23-17(14)21/h11-12H,1-10H3

InchiKey: RNNQAKPTUWSRGS-UHFFFAOYSA-N

Formula: C20H32O3Si

SMILES: Cc1cc2c(c(C(C)(C)C)c1)O[Si](C(C)(C)C)(C(C)(C)C)OC2=O

Mol. weight [g/mol]: 348.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.66		Crippen Method
logp	5.884		Crippen Method
rinpol	2110.00		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=R41249&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices