3,5-Di-tert-butyl-4-hydroxybenzoic acid, tert-butyldimethylsilyl ester

Other names: 3,5-Di-tert-butyl-4-hydroxybenzoic acid, tbdms derivative
Inchi: InChI=1S/C21H36O3Si/c1-19(2,3)15-12-14(13-16(17(15)22)20(4,5)6)18(23)24-25(10,11)
InchiKey: KBKIFSSJQAIYIG-UHFFFAOYSA-N
Formula: C21H36O3Si
SMILES: CC(C)(C)c1cc(C(=O)O[Si](C)(C)C(C)(C)C)cc(C(C)(C)C)c1O
Mol. weight [g/mol]: 364.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.03		Crippen Method
logp	6.149		Crippen Method
rinpol	2167.40		NIST Webbook
rinpol	2167.40		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U352485&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