Propanoic acid, 3-hydroxy-2-phenyl, DTBS

Inchi: InChI=1S/C17H26O3Si/c1-16(2,3)21(17(4,5)6)19-12-14(15(18)20-21)13-10-8-7-9-11-13/h
InchiKey: MHRXQMCRVMHBTF-UHFFFAOYSA-N
Formula: C17H26O3Si
SMILES: CC(C)(C)[Si]1(C(C)(C)C)OCC(c2ccccc2)C(=O)O1
Mol. weight [g/mol]: 306.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Crippen Method
logp	4.386		Crippen Method
rinpol	2000.00		NIST Webbook
rinpol	2000.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R41338&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