Benzoic acid, 2-acetyloxy-, tert.-butyldimethylsilyl ester

Inchi: InChI=1S/C15H22O4Si/c1-11(16)18-13-10-8-7-9-12(13)14(17)19-20(5,6)15(2,3)4/h7-10H

InchiKey: PTUZUDDOZGCNTE-UHFFFAOYSA-N

Formula: C15H22O4Si

SMILES: CC(=O)Oc1ccccc1C(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 294.42

CAS: 129512-44-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	3.774		Crippen Method
rinpol	1752.00		NIST Webbook
rinpol	1790.80		NIST Webbook
rinpol	1752.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C129512443&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