Benzoic acid, 4-methoxy-, tert.-butyldimethylsilyl ester

Inchi: InChI=1S/C14H22O3Si/c1-14(2,3)18(5,6)17-13(15)11-7-9-12(16-4)10-8-11/h7-10H,1-6H3

InchiKey: CSDAFUDOYGPYMF-UHFFFAOYSA-N

Formula: C14H22O3Si

SMILES: COc1ccc(C(=O)O[Si](C)(C)C(C)(C)C)cc1

Mol. weight [g/mol]: 266.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.98		Crippen Method
logp	3.857		Crippen Method
rinpol	1777.00		NIST Webbook
rinpol	1777.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374508&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices