sec-Butyl tert-butyldimethylsilyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, sec-butyl tert-butyldimethylsilyl ester
Inchi: InChI=1S/C18H28O4Si/c1-8-13(2)21-16(19)14-11-9-10-12-15(14)17(20)22-23(6,7)18(3,4
InchiKey: WIKZZVBXCNNYNS-UHFFFAOYSA-N
Formula: C18H28O4Si
SMILES: CCC(C)OC(=O)c1ccccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 336.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.47		Crippen Method
logp	4.804		Crippen Method
rinpol	1999.00		NIST Webbook
rinpol	1999.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373657&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