tert-Butyldimethylsilyl octan-2-yl phthalate

Other names: 1,2-Benzenedicarboxylic acid, octan-2-yl tert-butyldimethylsilyl ester
Inchi: InChI=1S/C22H36O4Si/c1-8-9-10-11-14-17(2)25-20(23)18-15-12-13-16-19(18)21(24)26-
InchiKey: MKWZNYAQTHTJDZ-UHFFFAOYSA-N
Formula: C22H36O4Si
SMILES: CCCCCCC(C)OC(=O)c1ccccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 392.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Crippen Method
logp	6.364		Crippen Method
rinpol	2353.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373620&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices