tert-Butyldimethylsilyl 3-oxobutan-2-yl phthalate

Other names: 1,2-Benzenedicarboxylic acid, 3-oxobutan-2-yl, tert-Butyldimethylsilyl ester
Inchi: InChI=1S/C18H26O5Si/c1-12(19)13(2)22-16(20)14-10-8-9-11-15(14)17(21)23-24(6,7)18
InchiKey: OOVUXUDJQGASPA-UHFFFAOYSA-N
Formula: C18H26O5Si
SMILES: CC(=O)C(C)OC(=O)c1ccccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 350.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	3.983		Crippen Method
rinpol	2127.00		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=U373506&Units=SI

Legend

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