tert-Butyldimethylsilyl 8-chlorooctyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, 8-chlorooctyl tert-butyldimethylsilyl ester
Inchi: InChI=1S/C22H35ClO4Si/c1-22(2,3)28(4,5)27-21(25)19-15-11-10-14-18(19)20(24)26-17-
InchiKey: VPMKCWDDCUSVRG-UHFFFAOYSA-N
Formula: C22H35ClO4Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccccc1C(=O)OCCCCCCCCCCl
Mol. weight [g/mol]: 427.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.18		Crippen Method
logp	6.585		Crippen Method
rinpol	2751.00		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=U373651&Units=SI

Legend

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