Benzoic acid, 4-chloro-, tert-butyldimethylsilyl ester

Other names: 4-Chlorobenzoic acid, tbdms derivative
Inchi: InChI=1S/C13H19ClO2Si/c1-13(2,3)17(4,5)16-12(15)10-6-8-11(14)9-7-10/h6-9H,1-5H3
InchiKey: BLGLFFJMLCSQGT-UHFFFAOYSA-N
Formula: C13H19ClO2Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 270.83
CAS: 105040-96-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	4.502		Crippen Method
rinpol	1663.50		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=C105040968&Units=SI

Legend

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