4-Bromophenoxyacetic acid, tert-butyldimethylsilyl ester

Other names: tert-Butyl(dimethyl)silyl (4-bromophenoxy)acetate
4-Bromophenoxyacetic acid, tbdms derivative
Inchi: InChI=1S/C14H21BrO3Si/c1-14(2,3)19(4,5)18-13(16)10-17-12-8-6-11(15)7-9-12/h6-9H,1
InchiKey: SAKKGSWHVUYUEC-UHFFFAOYSA-N
Formula: C14H21BrO3Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)COc1ccc(Br)cc1
Mol. weight [g/mol]: 345.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.60		Crippen Method
logp	4.376		Crippen Method
rinpol	1952.80		NIST Webbook
rinpol	1952.80		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=U333182&Units=SI

Legend

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