

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/ci9903071>

Crippen Method: https://www.cheméo.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

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