

(3,4-Dihydroxyphenyl)acetic acid, tert-butyldimethylsilyl ester

Other names: tert-Butyl(dimethyl)silyl (3,4-dihydroxyphenyl)acetate

3,4-Dihydroxyphenylacetic acid, tbdms derivative

Inchi: InChI=1S/C14H22O4Si/c1-14(2,3)19(4,5)18-13(17)9-10-6-7-11(15)12(16)8-10/h6-8,15-1

InchiKey: IDCIAIKDEYHTQE-UHFFFAOYSA-N

Formula: C14H22O4Si

SMILES: CC(C)(C)[Si](C)(C)OC(=O)Cc1ccc(O)c(O)c1

Mol. weight [g/mol]: 282.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.80		Crippen Method
logp	3.189		Crippen Method
rinpol	2065.80		NIST Webbook
rinpol	2065.80		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=U332726&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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