3-(4-Hydroxyphenyl)propionic acid, tert-butyldimethylsilyl ether, tert-butyldimethylsilyl ester

Other names: 3-(4-Hydroxyphenyl)propionic acid, TBDMS
Phloretic acid, 2tbdms derivative

Inchi: InChI=1S/C21H38O3Si2/c1-20(2,3)25(7,8)23-18-14-11-17(12-15-18)13-16-19(22)24-26(9

InchiKey: IGVDMGCCKOIHCG-UHFFFAOYSA-N

Formula: C21H38O3Si2

SMILES: CC(C)(C)[Si](C)(C)OC(=O)CCc1ccc(O[Si](C)(C)C(C)(C)C)cc1

Mol. weight [g/mol]: 394.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.38		Crippen Method
logp	6.552		Crippen Method
rinpol	2236.90		NIST Webbook
rinpol	2246.00		NIST Webbook
rinpol	2246.00		NIST Webbook
rinpol	2236.90		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U352426&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices