Benzenepropanoic acid, «alpha»,4-bis[(tert-butyldimethylsilyl)oxy]-, tert-butyldimethylsilyl ester

Other names: 4-Hydroxyphenyllactic acid, TBDMS
4-Hydroxyphenyllactate, TBDMS
p-Hydroxyphenyllactic acid, DMTBS
4-Hydroxyphenyllactic acid, triTBDMS
4-Hydroxyphenyllactic acid, 3tbdms derivative

Inchi: InChI=1S/C27H52O4Si3/c1-25(2,3)32(10,11)29-22-18-16-21(17-19-22)20-23(30-33(12,1

InchiKey: PUXQURXXIQTAIM-UHFFFAOYSA-N

Formula: C27H52O4Si3

SMILES: CC(C)(C)[Si](C)(C)OC(=O)C(Cc1ccc(O[Si](C)(C)C(C)(C)C)cc1)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 524.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.14		Crippen Method
logp	8.552		Crippen Method
rinpol	2600.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2596.00		NIST Webbook
rinpol	2602.00		NIST Webbook
rinpol	2596.00		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=U221802&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices