3,4-Dihydroxybenzoic acid, bis(tert-butyldimethylsilyl) ether, tert-butyldimethylsilyl ester

Other names: Protocatechoic acid, 3tbdms derivative
Inchi: InChI=1S/C25H48O4Si3/c1-23(2,3)30(10,11)27-20-17-16-19(22(26)29-32(14,15)25(7,8)9
InchiKey: JCJACHCJNGAAAR-UHFFFAOYSA-N
Formula: C25H48O4Si3
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccc(O[Si](C)(C)C(C)(C)C)c(O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]: 496.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	8.617		Crippen Method
rinpol	2538.00		NIST Webbook
rinpol	2511.00		NIST Webbook
rinpol	2529.00		NIST Webbook
rinpol	2510.10		NIST Webbook
rinpol	2510.10		NIST Webbook
rinpol	2529.00		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=U352467&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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