3-Hydroxymandelic acid, O,O-bis(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester

Other names: tert-Butyl(dimethyl)silyl
pyrrol[tert-butyl(dimethyl)silyl]oxymorpho(3-pyrrol[tert-butyl(dimethyl)silyl]oxymorphophen
3-Hydroxymandelic acid, 3tbdms derivative

Inchi: InChI=1S/C26H50O4Si3/c1-24(2,3)31(10,11)28-21-18-16-17-20(19-21)22(29-32(12,13)2

InchiKey: IUYHMCKPQSHYDV-UHFFFAOYSA-N

Formula: C26H50O4Si3

SMILES: CC(C)(C)[Si](C)(C)OC(=O)C(O[Si](C)(C)C(C)(C)C)c1cccc(O[Si](C)(C)C(C)(C)C)c1

Mol. weight [g/mol]: 510.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	8.682		Crippen Method
rinpol	2343.50		NIST Webbook
rinpol	2343.50		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U332761&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

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