Benzeneacetic acid, «alpha»,4-bis[(tert-butyldimethylsilyl)oxy]-3-meth
tert-butyldimethylsilyl ester

Other names:	DL-4-Hydroxy-3-methoxymandelic acid, bis(tert-butyldimethylsilyl) ether,
	tert-butyldimethylsilyl ester
	tert-Butyl(dimethyl)silyl
	pyrrol[tert-butyl(dimethyl)silyl]oxymorpho(4-pyrrol[tert-butyl(dimethyl)silyl]oxymorpho-3-m
	Vanillylmandelic acid, triTBDMS
	Vanillylmandelic acid, TBDMS
	Vanillylmandelic acid, 3tbdms derivative
Inchi:	InChI=1S/C27H52O5Si3/c1-25(2,3)33(11,12)30-21-18-17-20(19-22(21)29-10)23(31-34(1
InchiKey:	CGCMIBHFTPWWNW-UHFFFAOYSA-N
Formula:	C27H52O5Si3
SMILES:	COc1cc(C(O[Si](C)(C)C(C)(C)C)C(=O)O[Si](C)(C)C(C)(C)C)ccc1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	540.96
CAS:	78324-20-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Crippen Method
logp	8.691		Crippen Method
rinpol	2511.00		NIST Webbook
rinpol	2481.40		NIST Webbook
rinpol	2519.00		NIST Webbook
rinpol	2481.40		NIST Webbook
rinpol	2519.00		NIST Webbook
rinpol	2511.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78324206&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices