Benzoic acid, 4-methoxy-3-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:	Trimethylsilyl isovanillate, trimethylsilyl ether
	3-Hydroxy-4-methoxybenzoic acid, trimethylsilyl ether, trimethylsilyl ester
	Isovanillic acid, trimethylsilyl ether, trimethylsilyl ester
	Bis(trimethylsilyl)isovanillate
	Isovanillic acid, 2tms derivative
Inchi:	InChI=1S/C14H24O4Si2/c1-16-12-9-8-11(14(15)18-20(5,6)7)10-13(12)17-19(2,3)4/h8-10
InchiKey:	DSTNHSZUWMFBDU-UHFFFAOYSA-N
Formula:	C14H24O4Si2
SMILES:	COc1ccc(C(=O)O[Si](C)(C)C)cc1O[Si](C)(C)C
Mol. weight [g/mol]:	312.51
CAS:	68595-68-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.27		Crippen Method
logp	3.901		Crippen Method
rinpol	1761.00		NIST Webbook
rinpol	1760.70		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1760.70		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68595686&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