Trimethylsilyl 3,5-dimethoxy-4-(trimethylsilyloxy)benzoate

Other names: Benzoic acid, 3,5-dimethoxy-4-[(trimethylsilyl)oxy]-, trimethylsilyl ester
Syringic acid d--tms
Syringic acid-di-TMS
Syringic acid, TMS
Syringic acid, 2tms derivative

Inchi: InChI=1S/C15H26O5Si2/c1-17-12-9-11(15(16)20-22(6,7)8)10-13(18-2)14(12)19-21(3,4)5

InchiKey: KWOFGVXBWXVAJU-UHFFFAOYSA-N

Formula: C15H26O5Si2

SMILES: COc1cc(C(=O)O[Si](C)(C)C)cc(OC)c1O[Si](C)(C)C

Mol. weight [g/mol]: 342.53

CAS: 10517-29-0

Physical Properties

Property code	Value	Unit	Source
log10ws	0.15		Crippen Method
logp	3.909		Crippen Method
rinpol	1884.00		NIST Webbook
rinpol	1888.00		NIST Webbook
rinpol	1884.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10517290&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