

Benzoic acid, 3,4-dimethoxy-, trimethylsilyl ester

Other names:	Trimethylsilyl 3,4-dimethoxybenzoate Veratric acid, tms derivative
Inchi:	InChI=1S/C12H18O4Si/c1-14-10-7-6-9(8-11(10)15-2)12(13)16-17(3,4)5/h6-8H,1-5H3
InchiKey:	JZIXRRXJQVBHJP-UHFFFAOYSA-N
Formula:	C12H18O4Si
SMILES:	COc1ccc(C(=O)O[Si](C)(C)C)cc1OC
Mol. weight [g/mol]:	254.35
CAS:	2078-16-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.84		Crippen Method
logp	2.696		Crippen Method
rinpol	1684.00		NIST Webbook
rinpol	1680.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2078162&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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<https://www.chemeo.com/cid/10-838-0/Benzoic-acid-3-4-dimethoxy-trimethylsilyl-ester.pdf>

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