

tert-Butyldimethylsilyl 3,4-dimethoxybenzoate

Other names:	Benzoic acid, 3,4-dimethoxy-, t-butyldimethylsilyl ester
Inchi:	InChI=1S/C15H24O4Si/c1-15(2,3)20(6,7)19-14(16)11-8-9-12(17-4)13(10-11)18-5/h8-10H
InchiKey:	OTFQZYPHSOASKT-UHFFFAOYSA-N
Formula:	C15H24O4Si
SMILES:	COc1ccc(C(=O)O[Si](C)(C)C(C)(C)C)cc1OC
Mol. weight [g/mol]:	296.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.10		Crippen Method
logp	3.866		Crippen Method
rinpol	1990.00		NIST Webbook
rinpol	1958.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1958.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373070&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/83-625-6/tert-Butyldimethylsilyl-3-4-dimethoxybenzoate.pdf>

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