

tert-Butyldimethylsilyl 4-((tert-butyldimethylsilyl)oxy)-3,5-dimethoxybenzoate

Other names: 530-57-4, BDMS
Syringic acid, TBDMS

Inchi: InChI=1S/C21H38O5Si2/c1-20(2,3)27(9,10)25-18-16(23-7)13-15(14-17(18)24-8)19(22)2

InchiKey: IMVHVWFNMTWNB-TUHFFFAOYSA-N

Formula: C₂₁H₃₈O₅Si₂

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

Mol. weight [g/mol]: 426.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.36		Crippen Method
logp	6.250		Crippen Method
rinpol	2392.00		NIST Webbook
rinpol	2393.00		NIST Webbook
rinpol	2354.00		NIST Webbook
rinpol	2392.00		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=U385875&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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