

3-(2,5-Dimethoxyphenyl)propionic acid, TBDMS

Inchi:	InChI=1S/C17H28O4Si/c1-17(2,3)22(6,7)21-16(18)11-8-13-12-14(19-4)9-10-15(13)20-5/
InchiKey:	GERRSFDZHZHCTL-UHFFFAOYSA-N
Formula:	C17H28O4Si
SMILES:	COc1ccc(OC)c(CCC(=O)O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]:	324.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.36		Crippen Method
logp	4.185		Crippen Method
rinpol	2057.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R563309&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/47-170-1/3-2-5-Dimethoxyphenyl-propionic-acid-TBDMS.pdf>

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