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/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices