«beta»-(4-Methoxyphenyl)propionic acid, TBDMS

Inchi: InChI=1S/C16H26O3Si/c1-12(13-8-10-14(18-5)11-9-13)15(17)19-20(6,7)16(2,3)4/h8-12H

InchiKey: SNMHIIDDYKJDLI-UHFFFAOYSA-N

Formula: C16H26O3Si

SMILES: COc1ccc(C(C)C(=O)O[Si](C)(C)C(C)(C)C)cc1

Mol. weight [g/mol]: 294.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	4.347		Crippen Method
rinpol	1900.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R562742&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices