3-(2-Methoxyphenyl)propionic acid, TBDMS

Inchi: InChI=1S/C16H26O3Si/c1-16(2,3)20(5,6)19-15(17)12-11-13-9-7-8-10-14(13)18-4/h7-10H
InchiKey: LYDDBKKICYSAMV-UHFFFAOYSA-N
Formula: C16H26O3Si
SMILES: COc1ccccc1CCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 294.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	4.176		Crippen Method
rinpol	1849.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R563314&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