2-Methoxy-5-nitrophenol, tert-butyldimethylsilyl ether

Other names: 2-Methoxy-5-nitrophenol, tbdms derivative
Inchi: InChI=1S/C13H21NO4Si/c1-13(2,3)19(5,6)18-12-9-10(14(15)16)7-8-11(12)17-4/h7-9H,1-
InchiKey: ZZKQYNAFDWPSPY-UHFFFAOYSA-N
Formula: C13H21NO4Si
SMILES: COc1ccc([N+](=O)[O-])cc1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 283.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	3.987		Crippen Method
rinpol	1946.40		NIST Webbook
rinpol	1946.40		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U352891&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