3-Nitrobenzoic acid, tert-butyldimethylsilyl ester

Other names: Benzoic acid, 3-nitro-, tert-butyldimethylsilyl ester
3-Nitrobenzoic acid BDMS
Inchi: InChI=1S/C13H19NO4Si/c1-13(2,3)19(4,5)18-12(15)10-7-6-8-11(9-10)14(16)17/h6-9H,1-
InchiKey: GJZBAVMSSINKTD-UHFFFAOYSA-N
Formula: C13H19NO4Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 281.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	3.757		Crippen Method
rinpol	1860.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373105&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