N-(3-Bromo-4-hydroxy-phenyl)-4-nitro-benzenesu N,O-di(tert.-butydimethylsilyl)-

Inchi: InChI=1S/C24H37BrN2O5SSi2/c1-23(2,3)34(7,8)27(33(30,31)20-14-11-18(12-15-20)26(2

InchiKey: BZEYTWSTAFSKJO-UHFFFAOYSA-N

Formula: C24H37BrN2O5SSi2

SMILES: CC(C)(C)[Si](C)(C)Oc1ccc(N([Si](C)(C)C(C)(C)C)S(=O)(=O)c2ccc([N+](=O)[O-])cc2)cc1B

Mol. weight [g/mol]: 601.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.10		Crippen Method
logp	7.942		Crippen Method
rinpol	3336.00		NIST Webbook
rinpol	3336.00		NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374409&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices