4-Aminobenzoic acid, N-(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester

Other names: Benzoic acid, 4-amino, TBDMS

Inchi: InChI=1S/C19H35NO2Si2/c1-18(2,3)23(7,8)20-16-13-11-15(12-14-16)17(21)22-24(9,10)19(4,5)6/h11-14,20H,1-10H3

InchiKey: MWRAWVXPRARZSM-UHFFFAOYSA-N

Formula: C19H35NO2Si2

SMILES: CC(C)(C)[Si](C)(C)Nc1ccc(C(=O)O[Si](C)(C)C(C)(C)C)cc1

Mol. weight [g/mol]: 365.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.01		Crippen Method
logp	6.266		Crippen Method
rinpol	1850.00		NIST Webbook
rinpol	1850.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U364387&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