Benzoic acid, 3-amino-, tert-butyldimethylsilyl ester

Inchi: InChI=1S/C13H21NO2Si/c1-13(2,3)17(4,5)16-12(15)10-7-6-8-11(14)9-10/h6-9H,14H2,1-

InchiKey: LEMFTLBDBKRTJX-UHFFFAOYSA-N

Formula: C13H21NO2Si

SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cccc(N)c1

Mol. weight [g/mol]: 251.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	3.431		Crippen Method
rinpol	1844.00		NIST Webbook
rinpol	1844.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374524&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