3-Aminobenzoic acid, N-acetyl-, trimethylsilyl ester

Inchi: InChI=1S/C12H17NO3Si/c1-9(14)13-11-7-5-6-10(8-11)12(15)16-17(2,3)4/h5-8H,1-4H3,(H

InchiKey: OKBYTWHKBWAONE-UHFFFAOYSA-N

Formula: C12H17NO3Si

SMILES: CC(=O)Nc1cccc(C(=O)O[Si](C)(C)C)c1

Mol. weight [g/mol]: 251.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.80		Crippen Method
logp	2.637		Crippen Method
rinpol	1958.00		NIST Webbook
rinpol	1958.00		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=U375111&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices