

3-Aminobenzoic acid, N-acetyl-, tert.-butyldimethylsilyl ester

Inchi:	InChI=1S/C15H23NO3Si/c1-11(17)16-13-9-7-8-12(10-13)14(18)19-20(5,6)15(2,3)4/h7-10
InchiKey:	RSYMRTAFDNATCA-UHFFFAOYSA-N
Formula:	C15H23NO3Si
SMILES:	CC(=O)Nc1cccc(C(=O)O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]:	293.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.06		Crippen Method
logp	3.807		Crippen Method
rinpol	2199.00		NIST Webbook
rinpol	2199.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375086&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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<https://www.chemeo.com/cid/117-783-3/3-Aminobenzoic-acid-N-acetyl-tert-butyldimethylsilyl-ester.pdf>

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