

Benzoic acid, 4-amino-, tert-butyldimethylsilyl ester

Other names:	tert-Butyl(dimethyl)silyl 4-aminobenzoate
Inchi:	InChI=1S/C13H21NO2Si/c1-13(2,3)17(4,5)16-12(15)10-6-8-11(14)9-7-10/h6-9H,14H2,1-
InchiKey:	VUPIPMFSIIDWGU-UHFFFAOYSA-N
Formula:	C13H21NO2Si
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)c1ccc(N)cc1
Mol. weight [g/mol]:	251.40
CAS:	155056-93-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	3.431		Crippen Method
rinpol	1919.00		NIST Webbook
rinpol	1908.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C155056932&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/52-822-1/Benzoic-acid-4-amino-tert-butyldimethylsilyl-ester.pdf>

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