

tert-Butyldimethylsilyl 4-nitrobenzoate

Other names:	4-Nitrobenzoic acid, tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C13H19NO4Si/c1-13(2,3)19(4,5)18-12(15)10-6-8-11(9-7-10)14(16)17/h6-9H,1
InchiKey:	TVYJISKNYVTYMG-UHFFFAOYSA-N
Formula:	C13H19NO4Si
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	281.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	3.757		Crippen Method
rinpol	1866.00		NIST Webbook
rinpol	1866.00		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=U373050&Units=SI

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/34-943-7/tert-Butyldimethylsilyl-4-nitrobenzoate.pdf>

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