

3-Nitrophenol, tert-butyldimethylsilyl ether

Other names:	tert-Butyl(dimethyl)(3-nitrophenoxy)silane 3-nitrophenol, TBDMS 3-Nitrophenol, tbdms derivative
Inchi:	InChI=1S/C12H19NO3Si/c1-12(2,3)17(4,5)16-11-8-6-7-10(9-11)13(14)15/h6-9H,1-5H3
InchiKey:	MCSGRWOMRNBFLF-UHFFFAOYSA-N
Formula:	C12H19NO3Si
SMILES:	CC(C)(C)[Si](C)(C)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	253.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	3.979		Crippen Method
rinpol	1689.40		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333428&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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