

# 4-nitrophenol, TBDMS

<b>Other names:</b>	4-Nitrophenol, tert-butyldimethylsilyl ether 1-Dimethyl(tert-butyl)silyloxy-4-nitrobenzene
<b>Inchi:</b>	InChI=1S/C12H19NO3Si/c1-12(2,3)17(4,5)16-11-8-6-10(7-9-11)13(14)15/h6-9H,1-5H3
<b>InchiKey:</b>	AQPYYGDGBSMJJI-UHFFFAOYSA-N
<b>Formula:</b>	C12H19NO3Si
<b>SMILES:</b>	CC(C)(C)[Si](C)(C)Oc1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	253.37

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	3.979		Crippen Method
rinpola	1784.40		NIST Webbook
rinpola	1732.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U307925&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307925&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>rinpola:</b>	Non-polar retention indices

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<https://www.chemeo.com/cid/18-287-4/4-nitrophenol-TBDMS.pdf>

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