

# 3-Nitrobenzoic acid, trimethylsilyl ester

<b>Other names:</b>	Benzoic acid, 3-nitro-, trimethylsilyl ester Benzoic acid, m-nitro-, trimethylsilyl ester m-Nitrobenzoic acid, trimethylsilyl ester
<b>Inchi:</b>	InChI=1S/C10H13NO4Si/c1-16(2,3)15-10(12)8-5-4-6-9(7-8)11(13)14/h4-7H,1-3H3
<b>InchiKey:</b>	PDIIQWNPRAHHQZ-UHFFFAOYSA-N
<b>Formula:</b>	C10H13NO4Si
<b>SMILES:</b>	C[Si](C)(C)OC(=O)c1cccc([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	239.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.25		Crippen Method
logp	2.587		Crippen Method
rinpol	1619.00		NIST Webbook
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## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U373086&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U373086&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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<https://www.chemeo.com/cid/42-687-3/3-Nitrobenzoic-acid-trimethylsilyl-ester.pdf>

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