

# 3,5-Dinitrobenzyl alcohol, benzyldimethylsilyl ether

<b>Inchi:</b>	InChI=1S/C16H18N2O5Si/c1-24(2,12-13-6-4-3-5-7-13)23-11-14-8-15(17(19)20)10-16(9-
<b>InchiKey:</b>	HBTOAUWRLJLJSL-UHFFFAOYSA-N
<b>Formula:</b>	C16H18N2O5Si
<b>SMILES:</b>	C[Si](C)(Cc1cccc1)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	346.41

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	4.007		Crippen Method
rinpol	2556.00		NIST Webbook
rinpol	2556.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U376142&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376142&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>rinpol:</b>	Non-polar retention indices

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