

# Benzaldehyde, 2-hydroxy, 3-nitro-5-tert.-octyl, oxime, TMS

<b>Inchi:</b>	InChI=1S/C17H30N2O4Si2/c1-17(2,3)14-10-13(12-18-23-25(7,8)9)16(22-24(4,5)6)15(11
<b>InchiKey:</b>	BYXZOFDQJNYVAG-UHFFFAOYSA-N
<b>Formula:</b>	C17H30N2O4Si2
<b>SMILES:</b>	CC(C)(C)c1cc(C=NO[Si](C)(C)C)c(O[Si](C)(C)C)c([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	382.60

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.48		Crippen Method
logp	5.291		Crippen Method
rinpol	2241.00		NIST Webbook

## Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R58262&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R58262&amp;Units=SI</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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