

# 1-(p-methylphenyl)-silatrane

<b>Other names:</b>	2,8,9-Trioxa-5-aza-1-silabicyclo(3.3.3)undecane, 1-(p-tolyl)-
<b>Inchi:</b>	InChI=1S/C13H19NO3Si/c1-12-2-4-13(5-3-12)18-15-9-6-14(7-10-16-18)8-11-17-18/h2-5
<b>InchiKey:</b>	PRBBCDUTXWBPNJ-UHFFFAOYSA-N
<b>Formula:</b>	C13H19NO3Si
<b>SMILES:</b>	<chem>Cc1ccc([Si]23OCCN(CCO2)CCO3)cc1</chem>
<b>Mol. weight [g/mol]:</b>	265.38
<b>CAS:</b>	37905-22-9

## Physical Properties

Property code	Value	Unit	Source
ie	8.00	eV	NIST Webbook
ie	8.50 ± 0.10	eV	NIST Webbook
log10ws	-3.24		Crippen Method
logp	0.520		Crippen Method
rinpol	2197.00		NIST Webbook

## 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=C37905229&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C37905229&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>ie:</b>	Ionization energy
<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/33-800-6/1-p-methylphenyl-silatrane.pdf>

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