

# 2,8,9-Trioxa-5-aza-1-silabicyclo[3.3.3]undecane, 3,7-dimethyl-1-phenyl-

InChI: C1=CC=C(C=C1)OC2C(C)OC(O2)Si3C4CC5CC6CC(C4)CC5N6  
InChIKey: HOBATWHQQHWNCD-UHFFFAOYSA-N

**Formula:** C<sub>14</sub>H<sub>21</sub>NO<sub>3</sub>Si  
**SMILES:** CC1CN2CCO[Si](c3ccccc3)(O1)OC(C)C2  
**Mol. weight [g/mol]:** 279.41  
**CAS:** 2097-20-3

## Physical Properties

Property code	Value	Unit	Source
ie	8.00	eV	NIST Webbook
ie	8.70 ± 0.10	eV	NIST Webbook
log10ws	-3.82		Crippen Method
logp	0.989		Crippen Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2097203&Units=SI&Mask=3FFF>

## Legend

**ie:** Ionization energy  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient

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