

# 2,8,9-Trioxa-5-aza-1-silabicyclo[3.3.3]undecane,

Other names:

## 1-methyl-

1-Methylsilatrane

Methylsilatrane

Methylsilatran

1-Methyl-2,8,9-trioxa-5-aza-1-silabicyclo(3.3.3)undecane

**Inchi:** InChI=1S/C7H15NO3Si/c1-12-9-5-2-8(3-6-10-12)4-7-11-12/h2-7H2,1H3

**InchiKey:** DZLQWMNVOBAZGC-UHFFFAOYSA-N

**Formula:** C7H15NO3Si

**SMILES:** C[Si]12OCCN(CCO1)CCO2

**Mol. weight [g/mol]:** 189.28

**CAS:** 2288-13-3

## Physical Properties

Property code	Value	Unit	Source
ie	8.70	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
ie	8.50 ± 0.10	eV	NIST Webbook
ie	8.49	eV	NIST Webbook
log10ws	2.41		Crippen Method
logp	-0.066		Crippen Method
rinpol	1387.00		NIST Webbook
ripol	2258.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2288133&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

**ie:** Ionization energy

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**rinpol:** Non-polar retention indices  
**ripol:** Polar retention indices

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