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

Other names: 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/ci990307l

Crippen Method: 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