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

Other names:	1-Ethylsilatrane
	Ethylsilatrane
	1-ethyl-2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undecane
Inchi:	InChI=1S/C8H17NO3Si/c1-2-13-10-6-3-9(4-7-11-13)5-8-12-13/h2-8H2,1H3
InchiKey:	BJMVMCLSNWRFSD-UHFFFAOYSA-N
Formula:	C8H17NO3Si
SMILES:	CC[Si]12OCCN(CCO1)CCO2
Mol. weight [g/mol]:	203.31
CAS:	2097-16-7

Physical Properties

Property code	Value	Unit	Source
log10ws	1.99		Crippen Method
logp	0.324		Crippen Method
rinpol	1462.00		NIST Webbook
rinpol	1462.00		NIST Webbook
ripol	2294.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2097167&Units=SI

Legend

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