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

Inchi: InChI=1S/C14H21NO3Si/c1-12-10-15-8-9-16-19(17-12,18-13(2)11-15)14-6-4-3-5-7-14/h3
InchiKey: HOBATWHQQHWNCD-UHFFFAOYSA-N
Formula: C14H21NO3Si
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/ci990307l
Crippen Method: https://www.chemeo.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