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

Other names: Phenylsilatrane
1-Phenylsilatrane
1-Fenylosilatranu
Fenylsilatran
Silatrane, phenyl-
1-phenyl-2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undecane

Inchi: InChI=1S/C12H17NO3Si/c1-2-4-12(5-3-1)17-14-9-6-13(7-10-15-17)8-11-16-17/h1-5H,6-1

InchiKey: IJOIPPSHQCEBDH-UHFFFAOYSA-N

Formula: C12H17NO3Si

SMILES: c1ccc([Si]23OCCN(CCO2)CCO3)cc1

Mol. weight [g/mol]: 251.35

CAS: 2097-19-0

Physical Properties

Property code	Value	Unit	Source
ie	8.20	eV	NIST Webbook
ie	8.80 ± 0.10	eV	NIST Webbook
log10ws	-2.76		Crippen Method
logp	0.212		Crippen Method
rinpol	2242.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2097190&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