1-(p-methylphenyl)-silatrane

Other names: 2,8,9-Trioxa-5-aza-1-silabicyclo(3.3.3)undecane, 1-(p-tolyl)-
Inchi: InChI=1S/C13H19NO3Si/c1-12-2-4-13(5-3-12)18-15-9-6-14(7-10-16-18)8-11-17-18/h2-5
InchiKey: PRBBCDUTXWBPNJ-UHFFFAOYSA-N
Formula: C13H19NO3Si
SMILES: Cc1ccc([Si]23OCCN(CCO2)CCO3)cc1
Mol. weight [g/mol]: 265.38
CAS: 37905-22-9

Physical Properties

Property code	Value	Unit	Source
ie	8.00	eV	NIST Webbook
ie	8.50 ± 0.10	eV	NIST Webbook
log10ws	-3.24		Crippen Method
logp	0.520		Crippen Method
rinpol	2197.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37905229&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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