1-(Phenylethyl)-silatrane

Inchi: InChI=1S/C14H21NO3Si/c1-2-4-14(5-3-1)6-13-19-16-10-7-15(8-11-17-19)9-12-18-19/h1-
InchiKey: BDTNXGFFEHWUHY-UHFFFAOYSA-N
Formula: C14H21NO3Si
SMILES: c1ccc(CC[Si]23OCCN(CCO2)CCO3)cc1
Mol. weight [g/mol]: 279.41

Physical Properties

Property code	Value	Unit	Source
log10ws	0.38		Crippen Method
logp	1.547		Crippen Method
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook
ripol	3335.00		NIST Webbook
ripol	3335.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R145936&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.