1-(p-methylphenoxy)-silatrane

Inchi: InChI=1S/C13H19NO4Si/c1-12-2-4-13(5-3-12)18-19-15-9-6-14(7-10-16-19)8-11-17-19/h2
InchiKey: JSMJJRXGICSIMK-UHFFFAOYSA-N
Formula: C13H19NO4Si
SMILES: Cc1ccc(O[Si]23OCCN(CCO2)CCO3)cc1
Mol. weight [g/mol]: 281.38

Physical Properties

Property code	Value	Unit	Source
log10ws	0.42		Crippen Method
logp	1.188		Crippen Method
rinpol	2384.00		NIST Webbook
rinpol	2384.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R145941&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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