1-(o-chlorophenyl)-silatrane

Inchi: InChI=1S/C12H16ClNO3Si/c13-11-3-1-2-4-12(11)18-15-8-5-14(6-9-16-18)7-10-17-18/h1-
InchiKey: XKLVDAGNHGKDPR-UHFFFAOYSA-N
Formula: C12H16ClNO3Si
SMILES: Clc1ccccc1[Si]12OCCN(CCO1)CCO2
Mol. weight [g/mol]: 285.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	0.865		Crippen Method
rinpol	2267.00		NIST Webbook
rinpol	2267.00		NIST Webbook

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=R145812&Units=SI

Legend

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