1-Phenoxysilatrane

Inchi: InChI=1S/C12H17NO4Si/c1-2-4-12(5-3-1)17-18-14-9-6-13(7-10-15-18)8-11-16-18/h1-5H
InchiKey: VXZOISSTUSCPNB-UHFFFAOYSA-N
Formula: C12H17NO4Si
SMILES: c1ccc(O[Si]23OCCN(CCO2)CCO3)cc1
Mol. weight [g/mol]: 267.35
CAS: 3463-22-7

Physical Properties

Property code	Value	Unit	Source
log10ws	0.90		Crippen Method
logp	0.880		Crippen Method
rinpol	2288.00		NIST Webbook
rinpol	2288.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3463227&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