1-phenyl,3-methylsilatrane

Inchi: InChI=1S/C13H19NSi/c1-12-11-15(9-7-14(12)8-10-15)13-5-3-2-4-6-13/h2-6,12H,7-11H2,
InchiKey: BOLMDUBAAVELJD-UHFFFAOYSA-N
Formula: C13H19NSi
SMILES: CC1C[Si]2(c3ccccc3)CCN1CC2
Mol. weight [g/mol]: 217.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.29		Crippen Method
logp	2.060		Crippen Method
rinpol	2075.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R307738&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