1-Propyloxy-silatrane

Inchi: InChI=1S/C9H19NO4Si/c1-2-6-11-15-12-7-3-10(4-8-13-15)5-9-14-15/h2-9H2,1H3
InchiKey: MJXMRNLFYVDGQC-UHFFFAOYSA-N
Formula: C9H19NO4Si
SMILES: CCCO[Si]12OCCN(CCO1)CCO2
Mol. weight [g/mol]: 233.34

Physical Properties

Property code	Value	Unit	Source
log10ws	1.90		Crippen Method
logp	0.228		Crippen Method
rinpol	1689.00		NIST Webbook
ripol	2858.00		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=R145961&Units=SI

Legend

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