1-isoropyloxy-silatrane

Inchi:	InChI=1S/C9H19NO4Si/c1-9(2)14-15-11-6-3-10(4-7-12-15)5-8-13-15/h9H,3-8H2,1-2H3
InchiKey:	MMGCYKXCCAJHDV-UHFFFAOYSA-N
Formula:	C9H19NO4Si
SMILES:	CC(C)O[Si]12OCCN(CCO1)CCO2
Mol. weight [g/mol]:	233.34

Physical Properties

Property code	Value	Unit	Source
log10ws	1.79		Crippen Method
logp	0.226		Crippen Method
rinpol	1599.00		NIST Webbook
rinpol	1599.00		NIST Webbook
ripol	2672.00		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=R145738&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

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