1-isobutyloxy-silatrane

Inchi: InChI=1S/C10H21NO4Si/c1-10(2)9-15-16-12-6-3-11(4-7-13-16)5-8-14-16/h10H,3-9H2,1-
InchiKey: GAFJIOMMGWYIMT-UHFFFAOYSA-N
Formula: C10H21NO4Si
SMILES: CC(C)CO[Si]12OCCN(CCO1)CCO2
Mol. weight [g/mol]: 247.36

Physical Properties

Property code	Value	Unit	Source
log10ws	1.73		Crippen Method
logp	0.474		Crippen Method
rinpol	1724.00		NIST Webbook
rinpol	1724.00		NIST Webbook
ripol	2849.00		NIST Webbook
ripol	2849.00		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=R145703&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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