1,3-dimethylsilatrane

Inchi: InChI=1S/C8H17NO3Si/c1-8-7-9-3-5-10-13(2,12-8)11-6-4-9/h8H,3-7H2,1-2H3
InchiKey: SJSYJCKBYWTBQM-UHFFFAOYSA-N
Formula: C8H17NO3Si
SMILES: CC1CN2CCO[Si](C)(OCC2)O1
Mol. weight [g/mol]: 203.31

Physical Properties

Property code	Value	Unit	Source
log10ws	1.88		Crippen Method
logp	0.323		Crippen Method
rinpol	1380.00		NIST Webbook
rinpol	1380.00		NIST Webbook
ripol	2163.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R145456&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
ripol: Polar retention indices