

1-isopropyl,3,7,10-trimethylsilatrane, e

Inchi:	InChI=1S/C12H25NO3Si/c1-9(2)17-14-10(3)6-13(7-11(4)15-17)8-12(5)16-17/h9-12H,6-8
InchiKey:	MFNQPKFQWOSBLY-UHFFFAOYSA-N
Formula:	C12H25NO3Si
SMILES:	CC1CN2CC(C)O[Si](C(C)C)(O1)OC(C)C2
Mol. weight [g/mol]:	259.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.02		Crippen Method
logp	1.880		Crippen Method
rinpol	1441.00		NIST Webbook
rinpol	1441.00		NIST Webbook
ripol	1962.00		NIST Webbook
ripol	1962.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R145723&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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