

1-chloromethyl, 4,4,7,10-tetramethylsilatrane, a

Inchi: InChI=1S/C11H22ClNO3Si/c1-9-5-13-6-10(2)16-17(8-12,15-9)14-7-11(13,3)4/h9-10H,5-8
InchiKey: COMDYUPDFIYCJZ-UHFFFAOYSA-N
Formula: C11H22ClNO3Si
SMILES: CC1CN2CC(C)O[Si](CCl)(OCC2(C)C)O1
Mol. weight [g/mol]: 279.84

Physical Properties

Property code	Value	Unit	Source
log10ws	0.16		Crippen Method
logp	1.638		Crippen Method
rinpol	1869.00		NIST Webbook
rinpol	1869.00		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=R145565&Units=SI>

Legend

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

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