1-(m-chlorophenyl), 4,4,7,10-tetramethylsilatrane, b

Inchi: InChI=1S/C16H24ClNO3Si/c1-12-9-18-10-13(2)21-22(20-12,19-11-16(18,3)4)15-7-5-6-14

InchiKey: YEWYNBNHVJSFRD-UHFFFAOYSA-N

Formula: C16H24ClNO3Si

SMILES: CC1CN2CC(C)O[Si](c3cccc(Cl)c3)(OCC2(C)C)O1

Mol. weight [g/mol]: 341.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.46		Crippen Method
logp	2.420		Crippen Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		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=R145758&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices