1-(4-Chlorophenyl)-4,4-dimethyl-3-(1,2,4-triazol-1-yl trimethylsilyl ether

Other names: 1-(4-Chlorophenyl)-4,4-dimethyl-3-(1H-1,2,4-triazol-1-ylmethyl)-3-pentanol, TMS ether

Inchi: InChI=1S/C19H30ClN3OSi/c1-18(2,3)19(24-25(4,5)6,13-23-15-21-14-22-23)12-11-16-7-9 TMS ether

InchiKey: NPTSCAQIVNWXHW-UHFFFAOYSA-N

Formula: C19H30ClN3OSi

SMILES: CC(C)(C)C(CCc1ccc(Cl)cc1)(Cn1cncn1)O[Si](C)(C)C

Mol. weight [g/mol]: 380.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	5.201		Crippen Method
rinpol	2487.00		NIST Webbook
rinpol	2487.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373457&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