3,3-Dimethyl-1-(4-phenylphenoxy)-1-(1,2,4-triazol-trimethylsilyl ether

Inchi: InChI=1S/C23H31N3O2Si/c1-23(2,3)21(28-29(4,5)6)22(26-17-24-16-25-26)27-20-14-12-

InchiKey: DADILEVWHMREEQ-UHFFFAOYSA-N

Formula: C23H31N3O2Si

SMILES: CC(C)(C)C(O[Si](C)(C)C)C(Oc1ccc(-c2ccccc2)cc1)n1cncn1

Mol. weight [g/mol]: 409.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.61		Crippen Method
logp	5.789		Crippen Method
rinpol	2724.00		NIST Webbook
rinpol	2724.00		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=U372989&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices