2-Methyl-4-triisobutylsilyloxyoct-5-yne

Inchi: InChI=1S/C21H42OSi/c1-10-11-12-21(13-17(2)3)22-23(14-18(4)5,15-19(6)7)16-20(8)9/h
InchiKey: GTMZNKKNWLSATM-UHFFFAOYSA-N
Formula: C21H42OSi
SMILES: CCC#CC(CC(C)C)O[Si](CC(C)C)(CC(C)C)CC(C)C
Mol. weight [g/mol]: 338.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.69		Crippen Method
logp	6.745		Crippen Method
rinpol	1718.00		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=U299464&Units=SI

Legend

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