

2,7-Dimethyl-4-triisobutylsilyloxyoct-7-en-5-yne

Inchi: InChI=1S/C22H42OSi/c1-17(2)11-12-22(13-18(3)4)23-24(14-19(5)6,15-20(7)8)16-21(9)1
InchiKey: KRBCJAWQCUEWLR-UHFFFAOYSA-N
Formula: C22H42OSi
SMILES: C=C(C)C#CC(CC(C)C)O[Si](CC(C)C)(CC(C)C)CC(C)C
Mol. weight [g/mol]: 350.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.96		Crippen Method
logp	6.911		Crippen Method
rinpol	1762.00		NIST Webbook
rinpol	1762.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299465&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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