

1-Hexene, 2,4,6-[diphenyl-trimethylsilyl] (isomer # 1)

Inchi: InChI=1S/C21H28Si/c1-18(19-11-7-5-8-12-19)17-21(15-16-22(2,3)4)20-13-9-6-10-14-20
InchiKey: DVYDDCIOXQYFCS-UHFFFAOYSA-N
Formula: C₂₁H₂₈Si
SMILES: C=C(CC(CC[Si](C)(C)C)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 308.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	6.602		Crippen Method
rinpol	2056.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R97406&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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