

1-Diphenylethenylsilyloxytridec-2-yne

Inchi: InChI=1S/C27H36OSi/c1-3-5-6-7-8-9-10-11-12-13-20-25-28-29(4-2,26-21-16-14-17-22-23-24)/Si1
InchiKey: CKCPRLVUIPYTMX-UHFFFAOYSA-N
Formula: C27H36OSi
SMILES: C=C[Si](OCC#CCCCCCCCCCC)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 404.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.16		Crippen Method
logp	6.022		Crippen Method
rinpol	3015.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299566&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.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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<https://www.chemeo.com/cid/30-383-3/1-Diphenylethenylsilyloxytridec-2-yne.pdf>

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