

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

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 | 2106.00 | | NIST Webbook |
| rinpol | 2106.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R97410&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/72-545-7/1-Hexene-2-4-6-diphenyl-trimethylsilyl-isomer-2.pdf>

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