

# 1-Pentylsilatrane

|                      |                                                                                |
|----------------------|--------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C11H23NO3Si/c1-2-3-4-11-16-13-8-5-12(6-9-14-16)7-10-15-16/h2-11H2,1H3 |
| InchiKey:            | WIERTAILZLPRGK-UHFFFAOYSA-N                                                    |
| Formula:             | C11H23NO3Si                                                                    |
| SMILES:              | CCCCC[Si]12OCCN(CCO1)CCO2                                                      |
| Mol. weight [g/mol]: | 245.39                                                                         |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | 0.74    |      | Crippen Method |
| logp          | 1.494   |      | Crippen Method |
| rinpol        | 1721.00 |      | NIST Webbook   |
| ripol         | 2532.00 |      | NIST Webbook   |
| ripol         | 2532.00 |      | NIST Webbook   |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R145887&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R145887&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| Crippen Method: | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                         |

## Legend

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

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