

# Decanoic acid, trimethylsilyl ester

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Decanoic acid, tms derivative   |
| <b>Inchi:</b>               | InChI=1S/C13H28O2Si/c1-5-6-7-8-9-10-11-12-13(14)15-16(2,3)4/h5-12H2,1-4H3 |
| <b>InchiKey:</b>            | FGTNBYWFNITQJR-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C13H28O2Si  |
| <b>SMILES:</b>              | CCCCCCCCC(=O)O[Si](C)(C)C   |
| <b>Mol. weight [g/mol]:</b> | 244.45  |
| <b>CAS:</b>                 | 55494-15-0  |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -2.18   |      | Crippen Method |
| logp          | 4.505   |      | Crippen Method |
| rinpol        | 1455.00 |      | NIST Webbook   |
| rinpol        | 1450.00 |      | NIST Webbook   |
| rinpol        | 1453.00 |      | NIST Webbook   |
| rinpol        | 1450.00 |      | NIST Webbook   |
| rinpol        | 1450.00 |      | NIST Webbook   |
| rinpol        | 1453.00 |      | NIST Webbook   |
| rinpol        | 1449.90 |      | NIST Webbook   |
| rinpol        | 1446.00 |      | NIST Webbook   |
| rinpol        | 1451.00 |      | NIST Webbook   |
| rinpol        | 1453.00 |      | NIST Webbook   |
| rinpol        | 1450.00 |      | NIST Webbook   |
| rinpol        | 1460.00 |      | NIST Webbook   |
| rinpol        | 1462.00 |      | NIST Webbook   |
| rinpol        | 1446.00 |      | NIST Webbook   |
| rinpol        | 1453.00 |      | NIST Webbook   |
| rinpol        | 1460.00 |      | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C55494150&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55494150&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                     |

# Legend

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

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