

# Tetracosanoic acid, trimethylsilyl ester

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Tetracosanoic acid, TMS<br>Lignoceric acid, tms derivative                       |
| <b>Inchi:</b>               | InChI=1S/C27H56O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25 |
| <b>InchiKey:</b>            | MFKGSZQXHZDMAM-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C27H56O2Si   |
| <b>SMILES:</b>              | CCCCCCCCCCCCCCCCCCCCCCCC(=O)O[Si](C)(C)C   |
| <b>Mol. weight [g/mol]:</b> | 440.82   |
| <b>CAS:</b>                 | 74367-37-6   |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -8.04   |      | Crippen Method |
| logp          | 9.967   |      | Crippen Method |
| rinpol        | 2829.00 |      | NIST Webbook   |
| rinpol        | 2826.80 |      | NIST Webbook   |
| rinpol        | 2835.00 |      | NIST Webbook   |
| rinpol        | 2837.00 |      | NIST Webbook   |
| rinpol        | 2850.00 |      | NIST Webbook   |
| rinpol        | 2839.00 |      | NIST Webbook   |
| rinpol        | 2835.00 |      | NIST Webbook   |
| rinpol        | 2838.00 |      | NIST Webbook   |
| rinpol        | 2848.00 |      | 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=C74367376&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C74367376&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

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

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