

# Citronellic acid, tert-butyldimethylsilyl ester

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Citronellic acid, tbdms derivative  |
| <b>Inchi:</b>               | InChI=1S/C16H32O2Si/c1-13(2)10-9-11-14(3)12-15(17)18-19(7,8)16(4,5)6/h10,14H,9,11 |
| <b>InchiKey:</b>            | PAYDULIHYPMYID-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C16H32O2Si  |
| <b>SMILES:</b>              | CC(C)=CCCC(C)CC(=O)O[Si](C)(C)C(C)(C)C  |
| <b>Mol. weight [g/mol]:</b> | 284.51  |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -3.05   |      | Crippen Method |
| logp          | 5.307   |      | Crippen Method |
| rinsol        | 1607.30 |      | NIST Webbook   |
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## 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=U333630&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333630&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>rinsol:</b>  | Non-polar retention indices         |

Latest version available from:

<https://www.chemeo.com/cid/117-880-5/Citronellic-acid-tert-butyldimethylsilyl-ester.pdf>

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