

# 2-propyl-3-hydroxy-pentanoic acid, TMS

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Other names:         | 2-Propyl-3-hydroxypentanoic acid, diTMS<br>2-propyl-3-hydroxy-pentanoic acid, TMS |
| Inchi:               | InChI=1S/C14H32O3Si2/c1-9-11-12(14(15)17-19(6,7)8)13(10-2)16-18(3,4)5/h12-13H,9-1 |
| InchiKey:            | ZQFAKXFWMDHIJN-UHFFFAOYSA-N                                                       |
| Formula:             | C14H32O3Si2                                                                       |
| SMILES:              | CCCC(C(=O)O[Si](C)(C)C)C(CC)O[Si](C)(C)C                                          |
| Mol. weight [g/mol]: | 304.58                                                                            |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| logp          | 4.411   |      | Crippen Method |
| rinpol        | 1393.00 |      | NIST Webbook   |
| rinpol        | 1392.00 |      | NIST Webbook   |
| rinpol        | 1394.00 |      | NIST Webbook   |
| rinpol        | 1392.00 |      | NIST Webbook   |
| rinpol        | 1402.00 |      | NIST Webbook   |
| rinpol        | 1393.00 |      | NIST Webbook   |

## Sources

|                           |                                                                                                                                         |
|---------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method:           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                       |
| Cheméo Relay (1.0):       |                                                                                                                                         |
| Cheméo Relay (1.0, beta): |                                                                                                                                         |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U72014&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U72014&amp;Units=SI</a> |
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                               |

## Legend

|         |                                     |
|---------|-------------------------------------|
| logp:   | Octanol/Water partition coefficient |
| rinpol: | Non-polar retention indices         |

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