

# 3-Methylcrotonylglycine, di-TMS

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Glycine, N-(3-methyl-2-butenoyl), bis-TMS<br>3-Methylcrotonyl glycine, TMS      |
| <b>Inchi:</b>               | InChI=1S/C13H27NO3Si2/c1-11(2)9-12(16-18(3,4)5)14-10-13(15)17-19(6,7)8/h9H,10H2 |
| <b>InchiKey:</b>            | QFGAKQFBTMQVCA-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C13H27NO3Si2  |
| <b>SMILES:</b>              | CC(C)=CC(=NCC(=O)O[Si](C)(C)C)O[Si](C)(C)C                                      |
| <b>Mol. weight [g/mol]:</b> | 301.53  |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | 1.17    |      | Crippen Method |
| logp          | 3.581   |      | Crippen Method |
| rinpol        | 1560.00 |      | NIST Webbook   |
| rinpol        | 1578.00 |      | NIST Webbook   |
| rinpol        | 1572.00 |      | NIST Webbook   |
| rinpol        | 1584.00 |      | NIST Webbook   |
| rinpol        | 1563.00 |      | NIST Webbook   |
| rinpol        | 1588.00 |      | NIST Webbook   |
| rinpol        | 1588.00 |      | 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=R51624&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R51624&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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