

# 2-Oxobutanoic acid, 4-methylthio, oxime, bis-TMS

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 2-Keto-4-methiol-butyric acid, oxime, TMS   |
| <b>Inchi:</b>               | InChI=1S/C11H25NO3SSi2/c1-16-9-8-10(12-15-18(5,6)7)11(13)14-17(2,3)4/h8-9H2,1-7H1 |
| <b>InchiKey:</b>            | QHUCALKSWWWQAO-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C11H25NO3SSi2   |
| <b>SMILES:</b>              | CSCCC(=NO[Si](C)(C)C)C(=O)O[Si](C)(C)C  |
| <b>Mol. weight [g/mol]:</b> | 307.56  |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | 1.48    |      | Crippen Method |
| logp          | 3.325   |      | Crippen Method |
| rinpol        | 1514.00 |      | NIST Webbook   |
| rinpol        | 1512.00 |      | NIST Webbook   |
| rinpol        | 1514.00 |      | NIST Webbook   |
| rinpol        | 1512.00 |      | NIST Webbook   |
| rinpol        | 1514.00 |      | 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=R112773&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R112773&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         |

Latest version available from:

<https://www.chemeo.com/cid/58-556-1/2-Oxobutanoic-acid-4-methylthio-oxime-bis-TMS.pdf>

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