

# «alpha»-Bisabolol, trimethylsilyl ether

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | «ALPHA»-bisabolol, tms derivative   |
| <b>Inchi:</b>               | InChI=1S/C18H34OSi/c1-15(2)9-8-14-18(4,19-20(5,6)7)17-12-10-16(3)11-13-17/h9-10,1 |
| <b>InchiKey:</b>            | XKSLVSPUDWKMNV-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C18H34OSi   |
| <b>SMILES:</b>              | CC(C)=CCCC(C)(O[Si](C)(C)C)C1CC=C(C)CC1   |
| <b>Mol. weight [g/mol]:</b> | 294.55  |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -3.97   |      | Crippen Method |
| logp          | 6.089   |      | Crippen Method |
| rinsol        | 1743.40 |      | NIST Webbook   |
| rinsol        | 1743.40 |      | 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=U334013&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U334013&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/62-993-1/alpha-Bisabolol-trimethylsilyl-ether.pdf>

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