

# GA28 methyl ester TMS ether

|                             |                                                                                  |
|-----------------------------|----------------------------------------------------------------------------------|
| <b>Other names:</b>         | GA28, methyl ester TMS<br>GA28, MeTMS                                            |
| <b>Inchi:</b>               | InChI=1S/C29H48O8Si2/c1-18-16-27-17-28(18,37-39(9,10)11)14-12-19(27)29(25(32)35- |
| <b>InchiKey:</b>            | FFCBOCPBFUTUOW-FENPKODMSA-N                                                      |
| <b>Formula:</b>             | C29H48O8Si2                                                                      |
| <b>SMILES:</b>              | C=C1CC23CC1(O[Si](C)(C)C)CCC2C1(C(=O)OC)CCC(O[Si](C)(C)C)C(C)(C(=O)OC)C1         |
| <b>Mol. weight [g/mol]:</b> | 580.86                                                                           |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -1.03   |      | Crippen Method |
| logp          | 5.095   |      | Crippen Method |
| rinpol        | 2723.00 |      | NIST Webbook   |
| rinpol        | 2710.00 |      | NIST Webbook   |
| rinpol        | 2710.00 |      | NIST Webbook   |
| rinpol        | 2720.00 |      | NIST Webbook   |
| rinpol        | 2724.00 |      | NIST Webbook   |
| rinpol        | 2733.00 |      | 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=R79387&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R79387&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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