

# Gluconic acid lactone, TMS # 1

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Glucono-1,5-lactone, TMS # 1<br>GLUCONIC ACID LACTONE 4TMS-1                       |
| <b>Inchi:</b>               | InChI=1S/C18H42O6Si4/c1-25(2,3)20-13-14-15(22-26(4,5)6)16(23-27(7,8)9)17(18(19)21) |
| <b>InchiKey:</b>            | VNGTZLYNGGLPIZ-NXOAAHMSSA-N  |
| <b>Formula:</b>             | C18H42O6Si4  |
| <b>SMILES:</b>              | C[Si](C)(C)OCC1OC(=O)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C                  |
| <b>Mol. weight [g/mol]:</b> | 466.86   |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | 4.89    |      | Crippen Method |
| logp          | 4.424   |      | Crippen Method |
| rinsol        | 1913.00 |      | NIST Webbook   |
| rinsol        | 1915.00 |      | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <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>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R400872&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R400872&amp;Units=SI</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         |

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