

# «alpha»-Cellobiose TMS

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Other names:         | «alpha»-D(+)-Cellobiose, TMS                                                     |
| Inchi:               | InChI=1S/C36H86O11Si8/c1-48(2,3)37-25-27-29(31(43-51(10,11)12)34(46-54(19,20)21) |
| InchiKey:            | QJZFYVYJIGWEKIR-UNVZJPJOSA-N                                                     |
| Formula:             | C36H86O11Si8                                                                     |
| SMILES:              | C[Si](C)(C)OCC1OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1OC1OC(CO[Si](C)   |
| Mol. weight [g/mol]: | 919.75                                                                           |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | 8.84    |      | Crippen Method |
| logp          | 9.476   |      | Crippen Method |
| rinpol        | 2758.00 |      | NIST Webbook   |

## Sources

|                 |                                                                                                                                         |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                               |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                       |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R24510&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R24510&amp;Units=SI</a> |

## Legend

|          |                                     |
|----------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l  |
| logp:    | Octanol/Water partition coefficient |
| rinpol:  | Non-polar retention indices         |

Latest version available from:

<https://www.chemeo.com/cid/57-099-0/alpha-Cellobiose-TMS.pdf>

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