

# B-Tagatofuranose, TMS

**Inchi:** InChI=1S/C21H52O6Si5/c1-28(2,3)22-16-18-19(25-30(7,8)9)20(26-31(10,11)12)21(24-18)23  
**InchiKey:** PLNWQGWZBNJIQM-DOIPELPJSA-N  
**Formula:** C<sub>21</sub>H<sub>52</sub>O<sub>6</sub>Si<sub>5</sub>  
**SMILES:** C[Si](C)(C)OCC1OC(CO[Si](C)(C)C)(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C  
**Mol. weight [g/mol]:** 541.06

## Physical Properties

Property code	Value	Unit	Source
log10ws	5.77		Crippen Method
logp	6.076		Crippen Method
ripol	1753.00		NIST Webbook
ripol	1753.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R46007&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**ripol:** Polar retention indices

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<https://www.chemeo.com/cid/70-927-5/B-Tagatofuranose-TMS.pdf>

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