

# B-Tagatopyranose, TMS

**Other names:** «beta»-D(-)-Tagatose, pyranose, TMS  
**Inchi:** InChI=1S/C21H52O6Si5/c1-28(2,3)23-17-21(27-32(13,14)15)20(26-31(10,11)12)19(25-3  
**InchiKey:** PJXWXHJDJODISP-HAMDTZRPSA-N  
**Formula:** C<sub>21</sub>H<sub>52</sub>O<sub>6</sub>Si<sub>5</sub>  
**SMILES:** C[Si](C)(C)OCC1(O[Si](C)(C)C)OCC(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
rinpola	1879.00		NIST Webbook
rinpola	1924.00		NIST Webbook
rinpola	1924.00		NIST Webbook
ripola	1698.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R46011&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**rinpola:** Non-polar retention indices  
**ripola:** Polar retention indices

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<https://www.chemeo.com/cid/21-213-1/B-Tagatopyranose-TMS.pdf>

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