

# A-Tagatopyranose, TMS

**Inchi:** InChI=1S/C22H54O5Si5/c1-28(2,3)23-18-22(27-32(13,14)15)17-16-19(24-29(4,5)6)20(21)22  
**InchiKey:** VMYYSEVTKSVMQL-ZGJBTBESSA-N  
**Formula:** C22H54O5Si5  
**SMILES:** C[Si](C)(C)OCC1(O[Si](C)(C)C)CCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C  
**Mol. weight [g/mol]:** 539.09

## Physical Properties

Property code	Value	Unit	Source
log10ws	4.94		Crippen Method
logp	6.882		Crippen Method
ripol	1776.00		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=R45952&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  
**ripol:** Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/72-490-8/A-Tagatopyranose-TMS.pdf>

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