

# Tagatose, acyclic, TMS

**Other names:** Tagatose, TMS  
**Inchi:** InChI=1S/C21H52O6Si5/c1-28(2,3)23-16-18(22)20(26-31(10,11)12)21(27-32(13,14)15)1  
**InchiKey:** LDUCAYFXHYLHLP-NJYVYQBISA-N  
**Formula:** C<sub>21</sub>H<sub>52</sub>O<sub>6</sub>Si<sub>5</sub>  
**SMILES:** C[Si](C)(C)OCC(=O)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C  
**Mol. weight [g/mol]:** 541.06

## Physical Properties

Property code	Value	Unit	Source
log10ws	6.08		Crippen Method
logp	5.919		Crippen Method
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1853.00		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=R46043&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  
**rinpol:** Non-polar retention indices  
**ripol:** Polar retention indices

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<https://www.chemeo.com/cid/66-743-4/Tagatose-acyclic-TMS.pdf>

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