

# D(-)-Tagatose, aldol, TMS

**Inchi:** InChI=1S/C21H52O6Si5/c1-28(2,3)23-17-19(25-30(7,8)9)21(27-32(13,14)15)20(26-31(10,11)12)22-16-18-4-5-6-3  
**InchiKey:** PPTMWEDTYQRQBC-VKEMMKHGSA-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[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(C=O)O[Si](C)(C)C  
**Mol. weight [g/mol]:** 541.06

## Physical Properties

Property code	Value	Unit	Source
log10ws	5.97		Crippen Method
logp	5.917		Crippen Method
rinpol	1934.00		NIST Webbook
rinpol	1934.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R441299&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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  
**rinpol:** Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/63-905-7/D-Tagatose-aldol-TMS.pdf>

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