

# 3-Deoxytetronic acid, TMS

**Inchi:** InChI=1S/C7H14O2Si/c1-10(2,3)9-7-5-4-6-8-7/h5H,4,6H2,1-3H3  
**InchiKey:** ROCZJWMPGISRQB-UHFFFAOYSA-N  
**Formula:** C7H14O2Si  
**SMILES:** C[Si](C)(C)OC1=CCCO1  
**Mol. weight [g/mol]:** 158.27

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.28		Crippen Method
logp	2.100		Crippen Method
rinpol	1460.00		NIST Webbook

## Sources

**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)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R594175&Units=SI>

## Legend

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

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<https://www.chemeo.com/cid/98-638-6/3-Deoxytetronic-acid-TMS.pdf>

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