

# Isotalactone, TMS

**Inchi:** InChI=1S/C21H28O5Si2/c1-13-9-14-10-15-11-16(23-2)12-17(25-27(3,4)5)18(15)20(26-2)  
**InchiKey:** FNFKEZVUVTWIAE-UHFFFAOYSA-N  
**Formula:** C21H28O5Si2  
**SMILES:** C=C1Cc2cc3cc(OC)cc(O[Si](C)(C)C)c3c(O[Si](C)(C)C)c2C(=O)O1  
**Mol. weight [g/mol]:** 416.62

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	5.502		Crippen Method
rinpol	2599.00		NIST Webbook
rinpol	2599.00		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=R158259&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/31-787-4/Isotalactone-TMS.pdf>

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