

# Phytanic acid, TBDMS

**Inchi:** InChI=1S/C26H52O2Si/c1-21(2)14-11-15-22(3)16-12-17-23(4)18-13-19-24(5)20-25(27)2  
**InchiKey:** OYBWOZDHGGAVPJ-CNCACEPUSA-N  
**Formula:** C26H52O2Si  
**SMILES:** CC(=CC(=O)O[Si](C)(C)C(C)(C)C)CCCC(C)CCCC(C)CCCC(C)C  
**Mol. weight [g/mol]:** 424.78

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.75		Crippen Method
logp	8.920		Crippen Method
rinpol	2437.00		NIST Webbook

## Sources

**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)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R564837&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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