

# D-mannose, TMS diethyldithioacetal derivative

**Inchi:** InChI=1S/C25H62O5S2Si5/c1-18-31-25(32-19-2)24(30-37(15,16)17)23(29-36(12,13)14)  
**InchiKey:** CNMNOZHMKGENSD-LWSSLDFYSA-N  
**Formula:** C25H62O5S2Si5  
**SMILES:** CCSC(SCC)C(O[Si](C)(C)C)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]:** 647.31

## Physical Properties

Property code	Value	Unit	Source
log10ws	3.20		Crippen Method
logp	8.551		Crippen Method
rinpol	2359.00		NIST Webbook
rinpol	2359.00		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=R502804&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/13-297-8/D-mannose-TMS-diethyldithioacetal-derivative.pdf>

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