

# «beta»-Neolactose, TMS

**Inchi:** InChI=1S/C36H86O11Si8/c1-48(2,3)37-25-27-30(43-51(10,11)12)32(45-53(16,17)18)34(44-52)  
**InchiKey:** BKRCJVHGUNBEML-DKRGELLUSA-N  
**Formula:** C<sub>36</sub>H<sub>86</sub>O<sub>11</sub>Si<sub>8</sub>  
**SMILES:** C[Si](C)(C)OCC1OC(O[Si](C)(C)C)C(OC2OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)  
**Mol. weight [g/mol]:** 919.75

## Physical Properties

Property code	Value	Unit	Source
log10ws	8.84		Crippen Method
logp	9.476		Crippen Method
rinpol	2650.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R68049&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:** Log<sub>10</sub> of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**rinpol:** Non-polar retention indices

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