

# (S)-2-Butyl glucuronide, TMS

**Inchi:** InChI=1S/C22H50O7Si4/c1-15-16(2)24-22-20(28-32(9,10)11)18(27-31(6,7)8)17(26-30(3,4)21)5  
**InchiKey:** BYQDUSVVYSRQEK-UUFSNNOVSA-N  
**Formula:** C<sub>22</sub>H<sub>50</sub>O<sub>7</sub>Si<sub>4</sub>  
**SMILES:** CCC(C)OC1OC(C(=O)O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C  
**Mol. weight [g/mol]:** 538.97

## Physical Properties

Property code	Value	Unit	Source
log10ws	3.40		Crippen Method
logp	5.565		Crippen Method
rinpol	2099.00		NIST Webbook
rinpol	2099.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R554751&Units=SI>  
**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)

## 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/124-814-0/S-2-Butyl-glucuronide-TMS.pdf>

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