

# Benzenebutanoic acid, «alpha»,4-dihydroxy-3-methoxy, tris-TMS

**Inchi:** InChI=1S/C20H38O5Si3/c1-22-19-15-16(11-13-17(19)23-26(2,3)4)12-14-18(24-27(5,6)7)  
**InchiKey:** HJRCFCJKFFOCLL-UHFFFAOYSA-N  
**Formula:** C20H38O5Si3  
**SMILES:** COc1cc(CCC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)ccc1O[Si](C)(C)C  
**Mol. weight [g/mol]:** 442.77

## Physical Properties

Property code	Value	Unit	Source
log10ws	1.09		Crippen Method
logp	5.440		Crippen Method
rinpol	2147.00		NIST Webbook
rinpol	2147.00		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=R100171&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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