# Timolol, PFB-TMS

**Inchi:** InChI=1S/C20H31F7N4O4SSi/c1-17(2,3)31(16(32)18(21,22)19(23,24)20(25,26)27)11-13
**InchiKey:** JLNCXADSXSCRFZ-UHFFFAOYSA-N
**Formula:** C20H31F7N4O4SSi
**SMILES:** CC(C)(C)N(CC(COc1nsnc1N1CCOCC1)O[Si](C)(C)C)C(=O)C(F)(F)C(F)(F)C(F)(F)F
**Mol. weight [g/mol]:** 584.62

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -3.05 | | Crippen Method |
| logp | 4.434 | | Crippen Method |
| rinpol | 2853.00 | | NIST Webbook |
| rinpol | 2853.00 | | NIST Webbook |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R175061&Units=SI

## Legend

**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**rinpol:** Non-polar retention indices