# 3-O-methyl dopamine, PFB-TMS

**Inchi:** InChI=1S/C19H20F5NO3Si/c1-27-12-9-10(5-6-11(12)28-29(2,3)4)7-8-25-19(26)13-14(20
**InchiKey:** LMCZYNQIPQCNAP-UHFFFAOYSA-N
**Formula:** C19H20F5NO3Si
**SMILES:** COc1cc(CCNC(=O)c2c(F)c(F)c(F)c(F)c2F)ccc1O[Si](C)(C)C
**Mol. weight [g/mol]:** 433.44

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -4.64 | | Crippen Method |
| logp | 4.577 | | Crippen Method |
| rinpol | 2126.00 | | NIST Webbook |
| rinpol | 2126.00 | | 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=R305752&Units=SI

## Legend

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