# Benzoic acid, 3-pentafluoropropionylthio-, trimethylsilyl ester

**Inchi:** InChI=1S/C13H13F5O3SSi/c1-23(2,3)21-10(19)8-5-4-6-9(7-8)22-11(20)12(14,15)13(16,1

**InchiKey:** VTSNDDFHHPTDHK-UHFFFAOYSA-N

**Formula:** C13H13F5O3SSi

**SMILES:** C[Si](C)(C)OC(=O)c1cccc(SC(=O)C(F)(F)C(F)(F)F)c1

**Mol. weight [g/mol]:** 372.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -2.93 | | Crippen Method |
| logp | 4.495 | | Crippen Method |
| rinpol | 1527.00 | | NIST Webbook |
| rinpol | 1527.00 | | 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=U375172&Units=SI

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices