

# Benzoic acid, 3-trifluoroacetylthio-, trimethylsilyl ester

**Inchi:** InChI=1S/C12H13F3O3SSi/c1-20(2,3)18-10(16)8-5-4-6-9(7-8)19-11(17)12(13,14)15/h4-7  
**InchiKey:** XHLBNQMTZDRIFX-UHFFFAOYSA-N  
**Formula:** C12H13F3O3SSi  
**SMILES:** C[Si](C)(C)OC(=O)c1cccc(SC(=O)C(F)(F)F)c1  
**Mol. weight [g/mol]:** 322.38

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -2.20   |      | Crippen Method |
| logp          | 3.859   |      | Crippen Method |
| rinpol        | 1528.00 |      | NIST Webbook   |
| rinpol        | 1528.00 |      | NIST Webbook   |

## Sources

**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=U375174&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

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

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