# Benzoic acid, 2-acetylthio-, trimethylsilyl ester

**Inchi:** InChI=1S/C12H16O3SSi/c1-9(13)16-11-8-6-5-7-10(11)12(14)15-17(2,3)4/h5-8H,1-4H3
**InchiKey:** ROIBKRHXZKIPFN-UHFFFAOYSA-N
**Formula:** C12H16O3SSi
**SMILES:** CC(=O)Sc1ccccc1C(=O)O[Si](C)(C)C
**Mol. weight [g/mol]:** 268.40

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -1.54 | | Crippen Method |
| logp | 3.317 | | Crippen Method |
| rinpol | 1728.00 | | NIST Webbook |
| rinpol | 1728.00 | | NIST Webbook |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U375203&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

## Legend

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