

# 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/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

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

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