

# 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(16,17)2  
**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/ci9903071>  
**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=U375172&Units=SI>

## Legend

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

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