

# Benzoic acid, 2-heptafluorobutyrylthio-, trimethylsilyl ester

**Inchi:** InChI=1S/C14H13F7O3SSi/c1-26(2,3)24-10(22)8-6-4-5-7-9(8)25-11(23)12(15,16)13(17,18)14  
**InchiKey:** DWAYYTIDJIHYJH-UHFFFAOYSA-N  
**Formula:** C14H13F7O3SSi  
**SMILES:** C[Si](C)(C)OC(=O)c1ccccc1SC(=O)C(F)(F)C(F)(F)C(F)(F)F  
**Mol. weight [g/mol]:** 422.39

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Crippen Method
logp	5.130		Crippen Method
rinpol	1535.00		NIST Webbook
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## 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=U375200&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

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

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