

# Benzoic acid, 3-heptafluorobutyrylthio-, tert.-butyldimethylsilyl ester

**Inchi:** InChI=1S/C17H19F7O3SSi/c1-14(2,3)29(4,5)27-12(25)10-7-6-8-11(9-10)28-13(26)15(18)  
**InchiKey:** ODZNXTMEELFNDS-UHFFFAOYSA-N  
**Formula:** C17H19F7O3SSi  
**SMILES:** CC(C)(C)[Si](C)(C)OC(=O)c1cccc(SC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1  
**Mol. weight [g/mol]:** 464.47

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	6.300		Crippen Method
rinpol	1775.00		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=U375166&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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