

# Benzoic acid, 3-heptafluorobutyryloxy-, trimethylsilyl ester

**Inchi:** InChI=1S/C14H13F7O4Si/c1-26(2,3)25-10(22)8-5-4-6-9(7-8)24-11(23)12(15,16)13(17,18)  
**InchiKey:** KBWXVIOHTOGUNJ-UHFFFAOYSA-N  
**Formula:** C<sub>14</sub>H<sub>13</sub>F<sub>7</sub>O<sub>4</sub>Si  
**SMILES:** C[Si](C)(C)OC(=O)c1cccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1  
**Mol. weight [g/mol]:** 406.32

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.04		Crippen Method
logp	4.417		Crippen Method
rinpol	1395.00		NIST Webbook
rinpol	1395.00		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=U375031&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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