

Benzoic acid, 4-heptafluorobutyrylthio-, tert.-butyldimethylsilyl ester

Inchi: InChI=1S/C17H19F7O3SSi/c1-14(2,3)29(4,5)27-12(25)10-6-8-11(9-7-10)28-13(26)15(18)
InchiKey: IJFWVOTYOSSYGA-UHFFFAOYSA-N
Formula: C17H19F7O3SSi
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccc(SC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1
Mol. weight [g/mol]: 464.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	6.300		Crippen Method
rinsol	1828.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375181&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/114-813-2/Benzoic-acid-4-heptafluorobutyrylthio-tert-butyldimethylsilyl-ester.pdf>

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