

Benzoic acid, 3-heptafluorobutyrylthio-, trimethylsilyl ester

Inchi: InChI=1S/C14H13F7O3SSi/c1-26(2,3)24-10(22)8-5-4-6-9(7-8)25-11(23)12(15,16)13(17,18)14
InchiKey: BFCMSCGSIFAJTK-UHFFFAOYSA-N
Formula: C14H13F7O3SSi
SMILES: C[Si](C)(C)OC(=O)c1cccc(SC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 422.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Crippen Method
logp	5.130		Crippen Method
rinpol	1561.00		NIST Webbook
rinpol	1561.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375170&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/28-194-6/Benzoic-acid-3-heptafluorobutyrylthio-trimethylsilyl-ester.pdf>

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