

Benzoic acid, 2-heptafluorobutyryloxy-, trimethylsilyl ester

Inchi: InChI=1S/C14H13F7O4Si/c1-26(2,3)25-10(22)8-6-4-5-7-9(8)24-11(23)12(15,16)13(17,18)
InchiKey: FYJONWYIRGBNEX-UHFFFAOYSA-N
Formula: C14H13F7O4Si
SMILES: C[Si](C)(C)OC(=O)c1ccccc1OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 406.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.04		Crippen Method
logp	4.417		Crippen Method
rinpol	1383.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375211&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

Latest version available from:

<https://www.chemeo.com/cid/124-354-1/Benzoic-acid-2-heptafluorobutyryloxy-trimethylsilyl-ester.pdf>

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