

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

Inchi: InChI=1S/C17H19F7O4Si/c1-14(2,3)29(4,5)28-12(25)10-6-8-11(9-7-10)27-13(26)15(18,19)20
InchiKey: QJZXZFSNZCAWAD-UHFFFAOYSA-N
Formula: C17H19F7O4Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1
Mol. weight [g/mol]: 448.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.30		Crippen Method
logp	5.587		Crippen Method
rinpol	1643.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375041&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/45-682-5/Benzoic-acid-4-heptafluorobutyryloxy-tert-butyldimethylsilyl-ester.pdf>

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