4-Aminobenzoic acid, N-heptafluorobutyryl-, tert.-butyldimethylsilyl ester

Inchi: InChI=1S/C17H20F7NO3Si/c1-14(2,3)29(4,5)28-12(26)10-6-8-11(9-7-10)25-13(27)15(18

InchiKey: VBNAKOBBVKCNNL-UHFFFAOYSA-N

Formula: C17H20F7NO3Si

SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccc(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1

Mol. weight [g/mol]: 447.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Crippen Method
logp	5.620		Crippen Method
rinpol	1907.00		NIST Webbook
rinpol	1907.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375089&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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https://www.chemeo.com/cid/62-524-1/4-Aminobenzoic-acid-N-heptafluorobutyryl-tert-butyldimethylsilyl-ester.pdf

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