

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: VBNAKOBVVKCNL-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/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/62-524-1/4-Aminobenzoic-acid-N-heptafluorobutyryl-tert-butyldimethylsilyl-ester.pdf>

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