

3-Aminobenzoic acid, N-pentafluoropropionyl-, tert.-butyldimethylsilyl ester

InChI: InChI=1S/C16H12O5F5NO3Si/c1-11(2,3)26(4,5)25-12(23)10-7-6-8-11(9-10)22-13(24)15(17)
InChIKey: SFCJKHGDMCHBKS-UHFFFAOYSA-N

Formula: C16H20F5NO3Si

SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cccc(NC(=O)C(F)(F)C(F)(F)F)c1

Mol. weight [g/mol]: 397.41

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.46 | | Crippen Method |
| logp | 4.985 | | Crippen Method |
| rinpol | 1821.00 | | NIST Webbook |
| rinpol | 1821.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375081&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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