

3-Aminobenzoic acid, N,N-bis(trifluoroacetyl)-, trimethylsilyl ester

Inchi: InChI=1S/C14H13F6NO4Si/c1-26(2,3)25-10(22)8-5-4-6-9(7-8)21(11(23)13(15,16)17)12(24)14

InchiKey: YQTBKTWWSEVLO-UHFFFAOYSA-N

Formula: C₁₄H₁₃F₆NO₄Si

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

Mol. weight [g/mol]: 401.33

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -2.22 | | Crippen Method |
| logp | 3.662 | | Crippen Method |
| rinpol | 1410.00 | | NIST Webbook |
| rinpol | 1410.00 | | NIST Webbook |

Sources

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

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375109&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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