

4-Aminobenzoic acid, N-trifluoroacetyl-, trimethylsilyl ester

Inchi: InChI=1S/C12H14F3NO3Si/c1-20(2,3)19-10(17)8-4-6-9(7-5-8)16-11(18)12(13,14)15/h4-7
InchiKey: QUKQQUVXDFDGEM-UHFFFAOYSA-N
Formula: C12H14F3NO3Si
SMILES: C[Si](C)(C)OC(=O)c1ccc(NC(=O)C(F)(F)F)cc1
Mol. weight [g/mol]: 305.33

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -1.47 | | Crippen Method |
| logp | 3.179 | | Crippen Method |
| rinpol | 1662.00 | | NIST Webbook |
| rinpol | 1662.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375128&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

Latest version available from:

<https://www.cheméo.com/cid/117-051-5/4-Aminobenzoic-acid-N-trifluoroacetyl-trimethylsilyl-ester.pdf>

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