

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

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

InchiKey: BYBDEQLGVDSXML-UHFFFAOYSA-N

Formula: C₁₄H₁₃F₆NO₄Si

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

Mol. weight [g/mol]: 401.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Crippen Method
logp	3.662		Crippen Method
rinpol	1454.00		NIST Webbook
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Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375129&Units=SI>

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

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.chemeo.com/cid/117-052-4/4-Aminobenzoic-acid-N-N-bis-trifluoroacetyl-trimethylsilyl-ester.pdf>

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