

4-Aminobenzoic acid, N,N-bis(trifluoroacetyl)-, tert.-butyldimethylsilyl ester

Other names:

4-Aminobenzoic acid, N-trifluoroacetyl-, tert.-butyldimethylsilyl ester

Inchi:

InChI=1S/C17H19F6NO4Si/c1-15(2,3)29(4,5)28-12(25)10-6-8-11(9-7-10)24(13(26)16(18

InchiKey:

AAVOIDNYWCERPX-UHFFFAOYSA-N

Formula:

C17H19F6NO4Si

SMILES:

CC(C)(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]:

443.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	4.833		Crippen Method
rinpol	1905.00		NIST Webbook
rinpol	1905.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U375096&Units=SI>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

rinpol:

Non-polar retention indices

Latest version available from:

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