

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

Inchi: InChI=1S/C15H20F3NO3Si/c1-14(2,3)23(4,5)22-12(20)10-7-6-8-11(9-10)19-13(21)15(16)
InchiKey: RASMRNGTRUITRD-UHFFFAOYSA-N
Formula: C15H20F3NO3Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cccc(NC(=O)C(F)(F)F)c1
Mol. weight [g/mol]: 347.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Crippen Method
logp	4.349		Crippen Method
rinsol	1852.00		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=U375083&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
rinsol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/117-779-8/3-Aminobenzoic-acid-N-trifluoroacetyl-tert-butyldimethylsilyl-ester.pdf>

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